



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2023 – 05:49 AM EDT

PDB ID : 1Z7Q  
Title : Crystal structure of the 20s proteasome from yeast in complex with the proteasome activator PA26 from Trypanosome brucei at 3.2 angstroms resolution  
Authors : Forster, A.; Whitby, F.G.; Hill, C.P.  
Deposited on : 2005-03-26  
Resolution : 3.22 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](mailto: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>.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

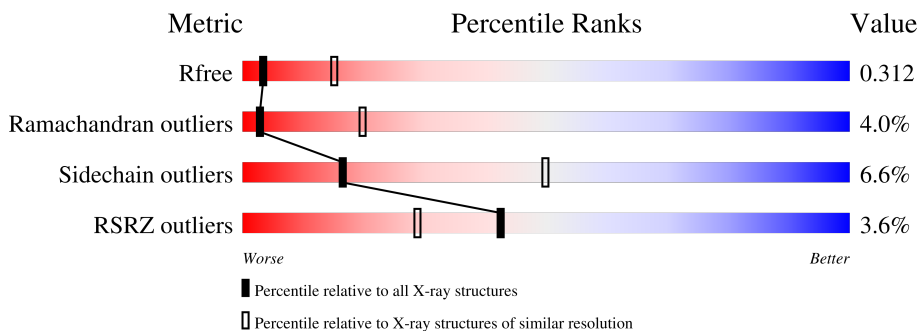
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.22 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	1335 (3.24-3.20)
Ramachandran outliers	138981	1437 (3.24-3.20)
Sidechain outliers	138945	1436 (3.24-3.20)
RSRZ outliers	127900	1291 (3.24-3.20)

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  $\geq 3$ , 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	A	252	 4% 83% 12% . .
1	O	252	 4% 83% 12% . .
2	B	250	 3% 86% 13% .
2	P	250	 4% 86% 12% .
3	C	258	 2% 81% 12% . 6%
3	Q	258	 4% 81% 12% . 6%

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Mol	Chain	Length	Quality of chain
4	D	254	 2% 85% 10% 5%
4	R	254	 3% 85% 10% 5%
5	E	260	 6% 85% 10% 6%
5	S	260	 5% 84% 10% 6%
6	F	234	 % 90% 9% .
6	T	234	 % 89% 10% .
7	G	288	 % 73% 10% . 16%
7	U	288	 5% 74% 10% . 16%
8	H	196	 3% 85% 14% .
8	V	196	 3% 84% 16% .
9	I	222	 2% 88% 11% .
9	W	222	 2% 88% 11% .
10	J	205	 % 92% 7% .
10	X	205	 % 93% 6% .
11	K	198	 3% 88% 12% .
11	Y	198	 2% 89% 11% .
12	L	212	 % 94% 6% .
12	Z	212	 % 93% 6% .
13	M	222	 % 89% 11% .
13	a	222	 % 89% 11% .
14	N	233	 % 88% 12% .
14	b	233	 3% 88% 12% .
15	c	231	 3% 94% 5% .
15	d	231	 3% 93% 6% .
15	e	231	 5% 91% 7% .

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Mol	Chain	Length	Quality of chain
15	f	231	 % 89% 6% ..
15	g	231	 3% 90% 7% ..
15	h	231	 5% 92% 8%
15	i	231	 7% 91% 7% .
15	j	231	 5% 94% 5% .
15	k	231	 10% 92% 6% .
15	l	231	 6% 91% 7% .
15	m	231	 6% 90% 6% ..
15	n	231	 8% 90% 7% ..
15	o	231	 7% 92% 8%
15	p	231	 3% 90% 6% ..

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 74222 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 Proteasome component C7-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	243	Total 1921	C 1221	N 322	O 370	S 8	0	0	0
1	O	243	Total 1921	C 1221	N 322	O 370	S 8	0	0	0

- Molecule 2 is a protein called Proteasome component Y7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	249	Total 1907	C 1214	N 314	O 376	S 3	0	0	0
2	P	249	Total 1907	C 1214	N 314	O 376	S 3	0	0	0

- Molecule 3 is a protein called Proteasome component Y13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	243	Total 1900	C 1199	N 320	O 378	S 3	0	0	0
3	Q	243	Total 1900	C 1199	N 320	O 378	S 3	0	0	0

- Molecule 4 is a protein called Proteasome component PRE6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	241	Total 1890	C 1181	N 331	O 374	S 4	0	0	0
4	R	241	Total 1890	C 1181	N 331	O 374	S 4	0	0	0

- Molecule 5 is a protein called Proteasome component PUP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	245	Total	C	N	O	S	0	0	0
			1888	1179	317	385	7			
5	S	245	Total	C	N	O	S	0	0	0
			1888	1179	317	385	7			

- Molecule 6 is a protein called Proteasome component PRE5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	234	Total	C	N	O	S	0	0	0
			1803	1134	313	351	5			
6	T	234	Total	C	N	O	S	0	0	0
			1803	1134	313	351	5			

- Molecule 7 is a protein called Proteasome component C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	243	Total	C	N	O	S	0	0	0
			1892	1203	329	356	4			
7	U	243	Total	C	N	O	S	0	0	0
			1892	1203	329	356	4			

- Molecule 8 is a protein called Proteasome component PRE3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
8	V	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

- Molecule 9 is a protein called Proteasome component PUP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			
9	W	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			

- Molecule 10 is a protein called Proteasome component PUP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	X	204	1581	1010	258	305	8	0	0	0

- Molecule 11 is a protein called Proteasome component C11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	198	1585	1005	269	305	6	0	0	0
11	Y	198	1585	1005	269	305	6	0	0	0

- Molecule 12 is a protein called Proteasome component PRE2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	212	1646	1045	282	312	7	0	0	0
12	Z	212	1646	1045	282	312	7	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	33	ARG	LYS	conflict	UNP P30656
Z	33	ARG	LYS	conflict	UNP P30656

- Molecule 13 is a protein called Potential proteasome component C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	M	222	1757	1115	303	335	4	0	0	0
13	a	222	1757	1115	303	335	4	0	0	0

- Molecule 14 is a protein called Proteasome component PRE4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	N	233	1824	1154	312	351	7	0	0	0
14	b	233	1824	1154	312	351	7	0	0	0

- Molecule 15 is a protein called proteasome activator protein PA26.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	c	230	1760	1101	310	343	6	219	0	0
15	d	230	1760	1101	310	343	6	219	0	0
15	e	230	1760	1101	310	343	6	219	0	0
15	f	230	1760	1101	310	343	6	219	0	0
15	g	230	1760	1101	310	343	6	219	0	0
15	h	230	1760	1101	310	343	6	219	0	0
15	i	230	1760	1101	310	343	6	249	0	0
15	j	230	1760	1101	310	343	6	219	0	0
15	k	230	1760	1101	310	343	6	219	0	0
15	l	230	1760	1101	310	343	6	219	0	0
15	m	230	1760	1101	310	343	6	219	0	0
15	n	230	1760	1101	310	343	6	219	0	0
15	o	230	1760	1101	310	343	6	219	0	0
15	p	230	1760	1101	310	343	6	249	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	1049	VAL	THR	conflict	UNP Q9U8G2
c	?	-	SER	deletion	UNP Q9U8G2
c	1171	GLY	-	insertion	UNP Q9U8G2
d	1049	VAL	THR	conflict	UNP Q9U8G2
d	?	-	SER	deletion	UNP Q9U8G2
d	1171	GLY	-	insertion	UNP Q9U8G2
e	1049	VAL	THR	conflict	UNP Q9U8G2
e	?	-	SER	deletion	UNP Q9U8G2
e	1171	GLY	-	insertion	UNP Q9U8G2
f	1049	VAL	THR	conflict	UNP Q9U8G2
f	?	-	SER	deletion	UNP Q9U8G2
f	1171	GLY	-	insertion	UNP Q9U8G2

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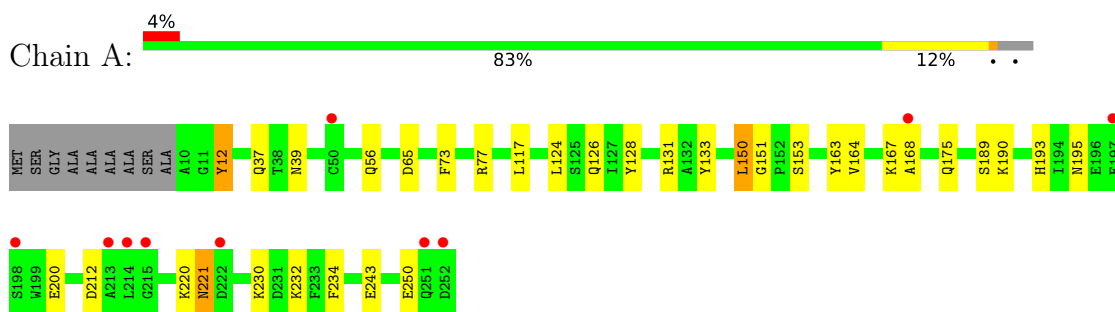
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Chain	Residue	Modelled	Actual	Comment	Reference
g	1049	VAL	THR	conflict	UNP Q9U8G2
g	?	-	SER	deletion	UNP Q9U8G2
g	1171	GLY	-	insertion	UNP Q9U8G2
h	1049	VAL	THR	conflict	UNP Q9U8G2
h	?	-	SER	deletion	UNP Q9U8G2
h	1171	GLY	-	insertion	UNP Q9U8G2
i	1049	VAL	THR	conflict	UNP Q9U8G2
i	?	-	SER	deletion	UNP Q9U8G2
i	1171	GLY	-	insertion	UNP Q9U8G2
j	1049	VAL	THR	conflict	UNP Q9U8G2
j	?	-	SER	deletion	UNP Q9U8G2
j	1171	GLY	-	insertion	UNP Q9U8G2
k	1049	VAL	THR	conflict	UNP Q9U8G2
k	?	-	SER	deletion	UNP Q9U8G2
k	1171	GLY	-	insertion	UNP Q9U8G2
l	1049	VAL	THR	conflict	UNP Q9U8G2
l	?	-	SER	deletion	UNP Q9U8G2
l	1171	GLY	-	insertion	UNP Q9U8G2
m	1049	VAL	THR	conflict	UNP Q9U8G2
m	?	-	SER	deletion	UNP Q9U8G2
m	1171	GLY	-	insertion	UNP Q9U8G2
n	1049	VAL	THR	conflict	UNP Q9U8G2
n	?	-	SER	deletion	UNP Q9U8G2
n	1171	GLY	-	insertion	UNP Q9U8G2
o	1049	VAL	THR	conflict	UNP Q9U8G2
o	?	-	SER	deletion	UNP Q9U8G2
o	1171	GLY	-	insertion	UNP Q9U8G2
p	1049	VAL	THR	conflict	UNP Q9U8G2
p	?	-	SER	deletion	UNP Q9U8G2
p	1171	GLY	-	insertion	UNP Q9U8G2

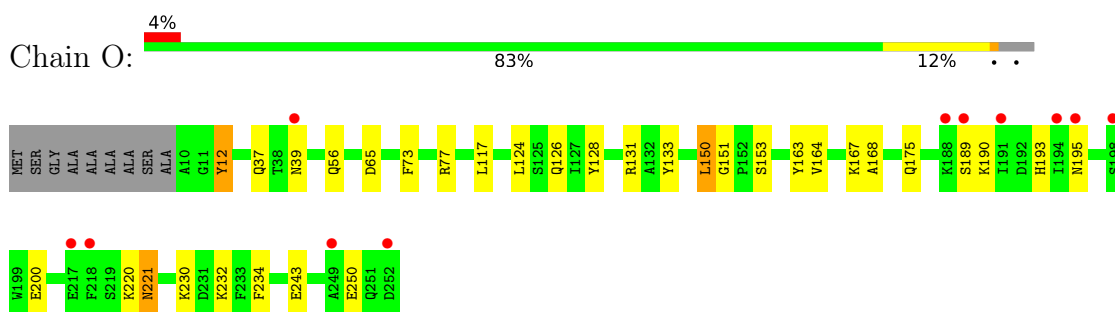
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

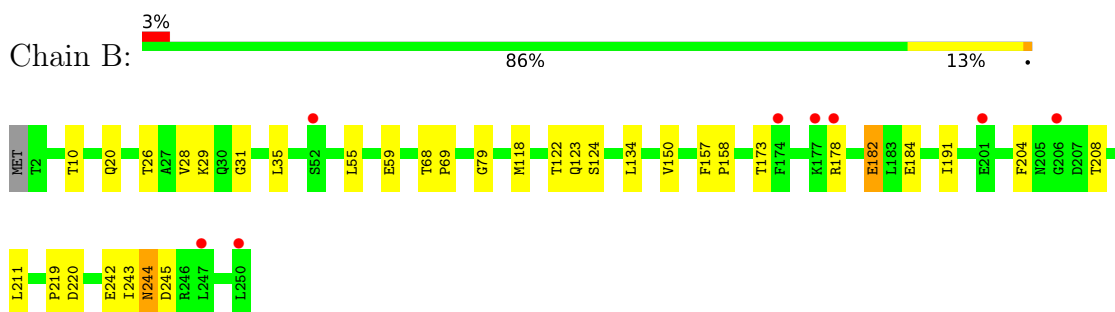
- Molecule 1: Proteasome component C7-alpha



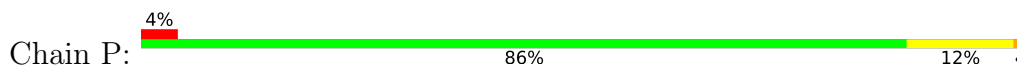
- Molecule 1: Proteasome component C7-alpha

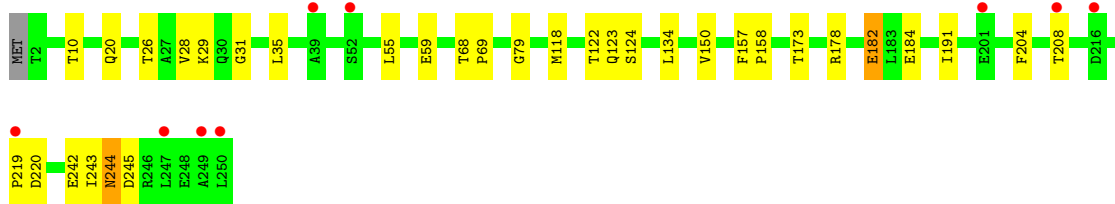


- Molecule 2: Proteasome component Y7

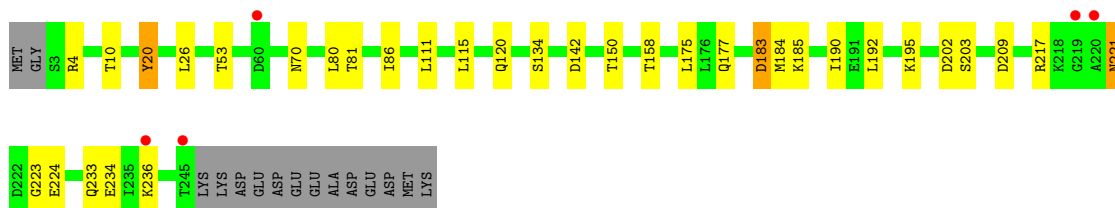
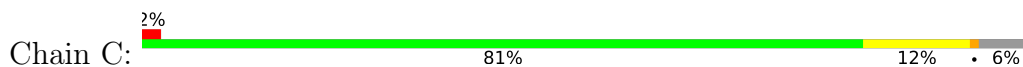


- Molecule 2: Proteasome component Y7

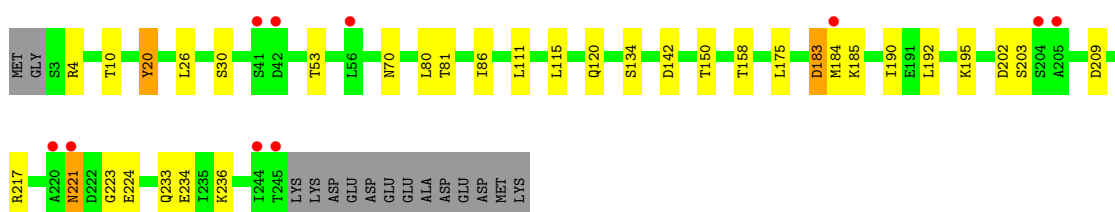
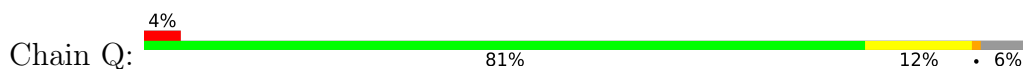




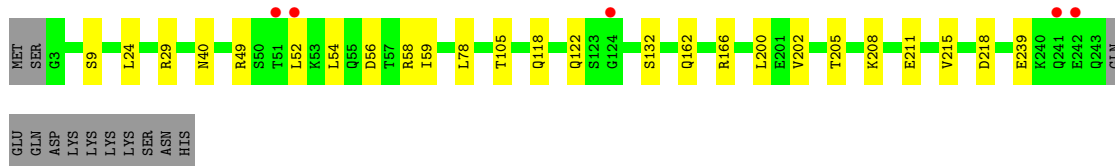
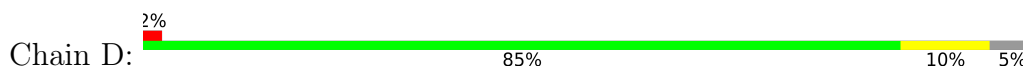
- Molecule 3: Proteasome component Y13



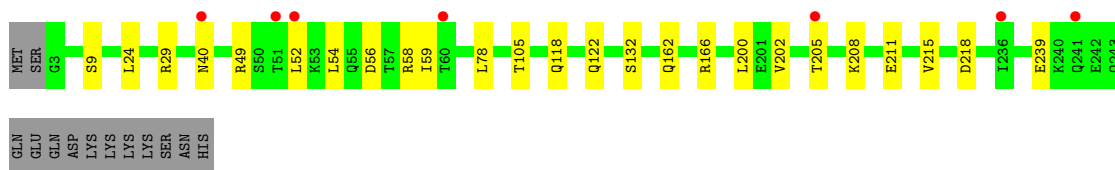
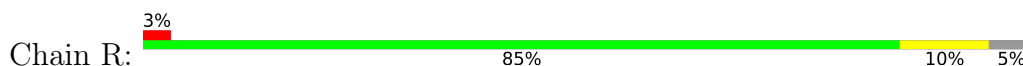
- Molecule 3: Proteasome component Y13



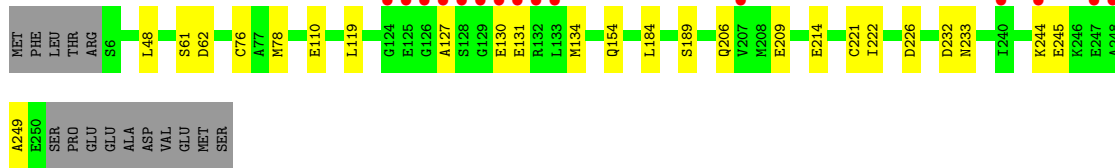
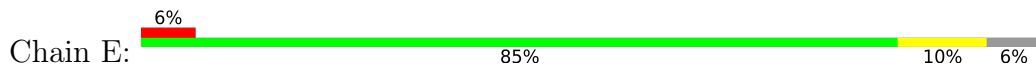
- Molecule 4: Proteasome component PRE6



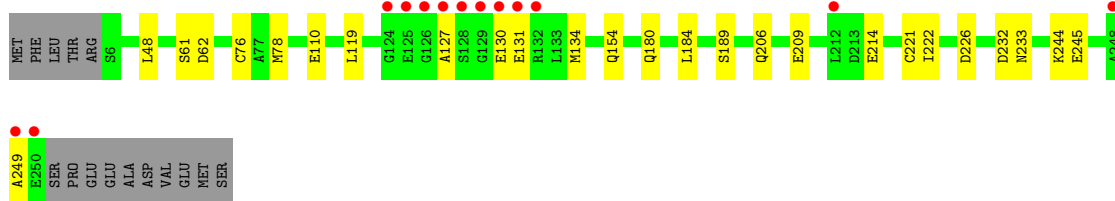
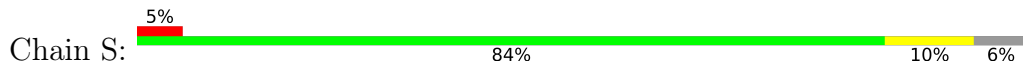
- Molecule 4: Proteasome component PRE6



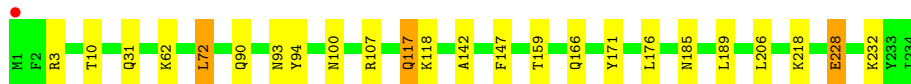
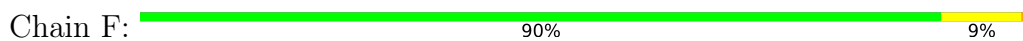
- Molecule 5: Proteasome component PUP2



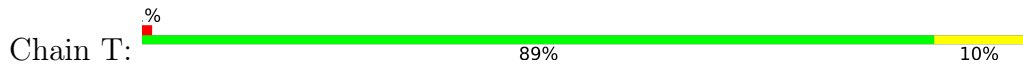
- Molecule 5: Proteasome component PUP2



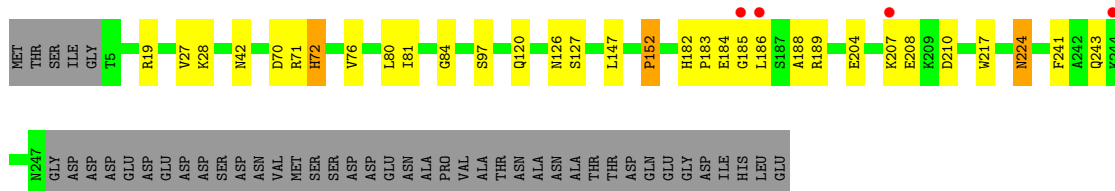
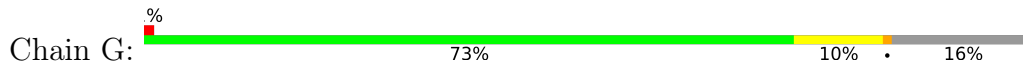
- Molecule 6: Proteasome component PRE5



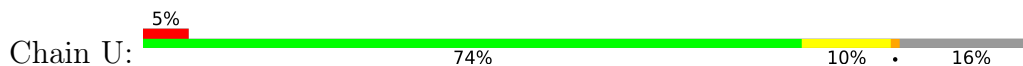
- Molecule 6: Proteasome component PRE5

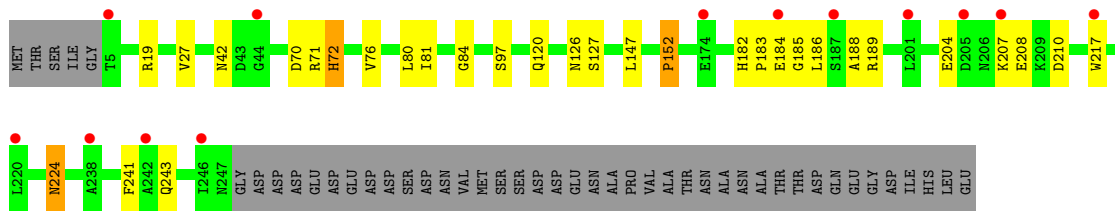


- Molecule 7: Proteasome component C1

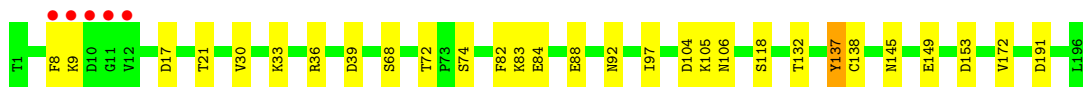
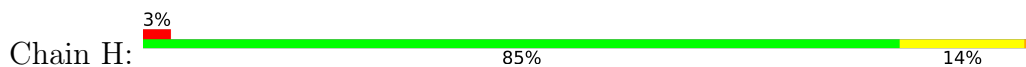


- Molecule 7: Proteasome component C1

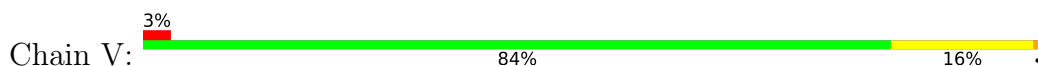




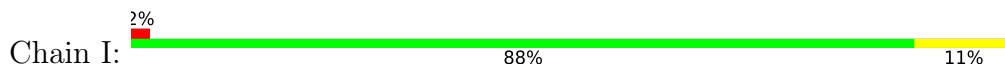
• Molecule 8: Proteasome component PRE3



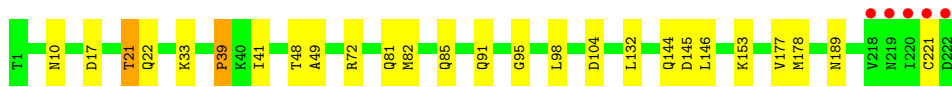
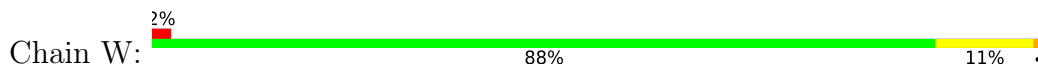
• Molecule 8: Proteasome component PRE3



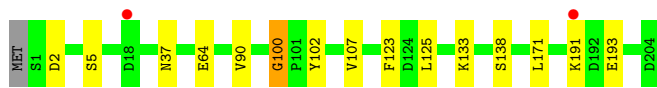
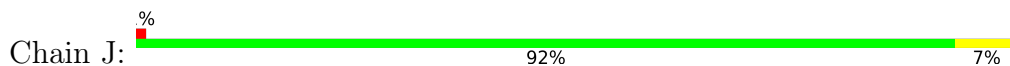
• Molecule 9: Proteasome component PUP1



• Molecule 9: Proteasome component PUP1



• Molecule 10: Proteasome component PUP3




• Molecule 10: Proteasome component PUP3

Chain X:  93% 6%

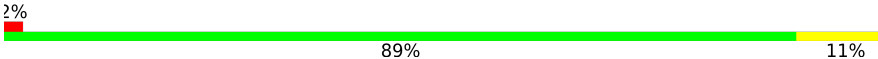


- Molecule 11: Proteasome component C11

Chain K:  3% 88% 12%



- Molecule 11: Proteasome component C11

Chain Y:  2% 89% 11%



- Molecule 12: Proteasome component PRE2

Chain L:  94% 6%



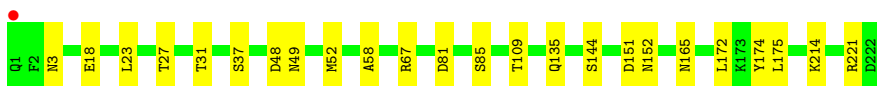
- Molecule 12: Proteasome component PRE2

Chain Z:  93% 6%




- Molecule 13: Potential proteasome component C5

Chain M:  89% 11%

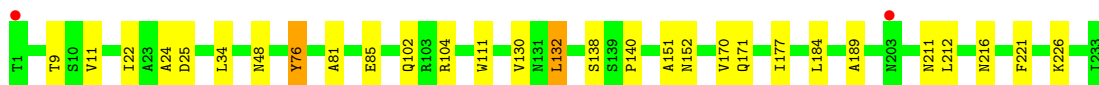
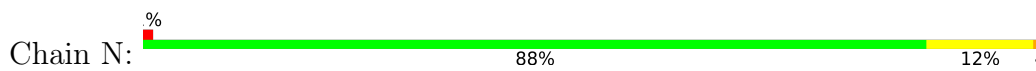


- Molecule 13: Potential proteasome component C5

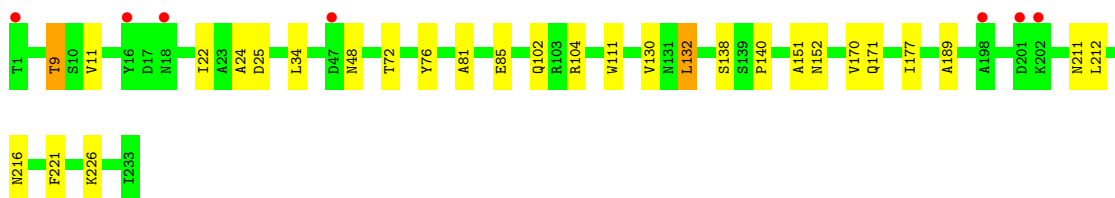
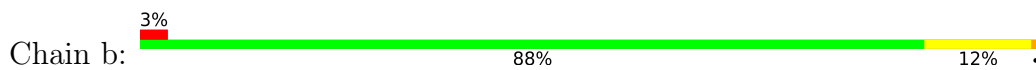
Chain a:  89% 11%



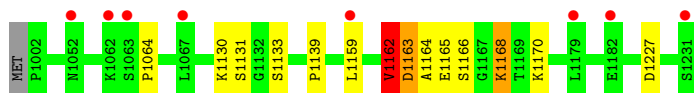
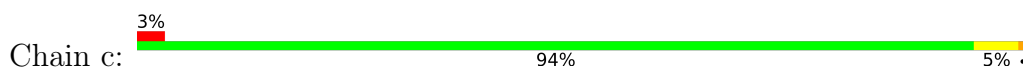
- Molecule 14: Proteasome component PRE4



- Molecule 14: Proteasome component PRE4



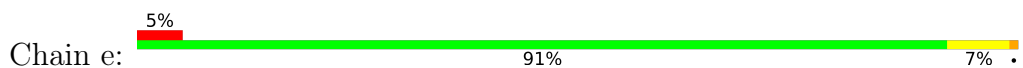
- Molecule 15: proteasome activator protein PA26



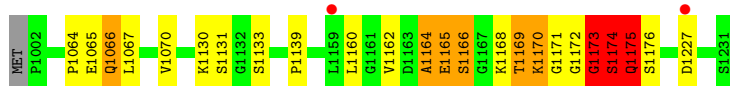
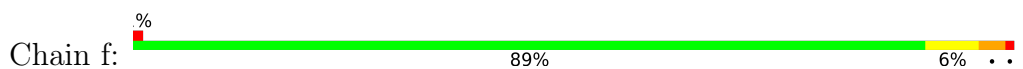
- Molecule 15: proteasome activator protein PA26



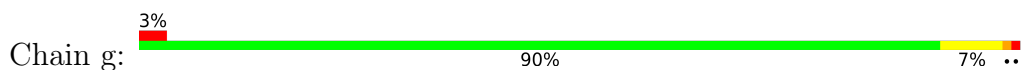
- Molecule 15: proteasome activator protein PA26



- Molecule 15: proteasome activator protein PA26

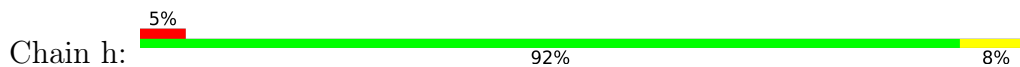


- Molecule 15: proteasome activator protein PA26

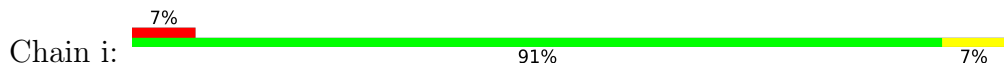




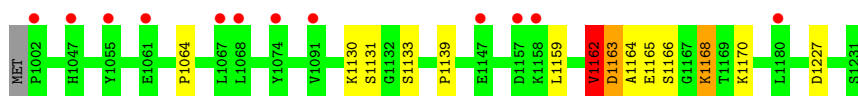
- Molecule 15: proteasome activator protein PA26



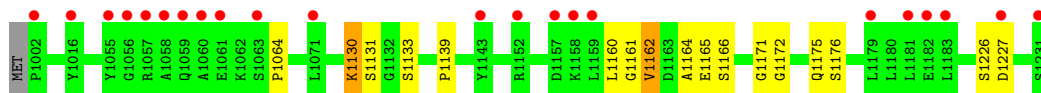
- Molecule 15: proteasome activator protein PA26



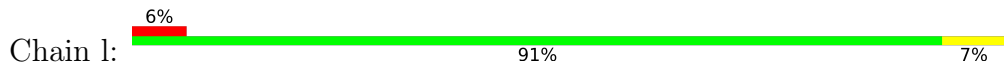
- Molecule 15: proteasome activator protein PA26



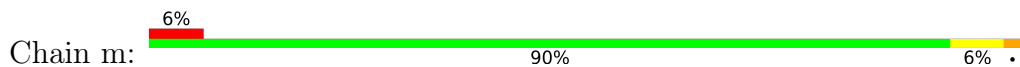
- Molecule 15: proteasome activator protein PA26



- Molecule 15: proteasome activator protein PA26

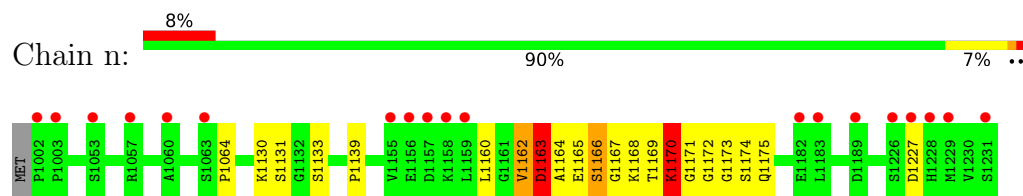


- Molecule 15: proteasome activator protein PA26

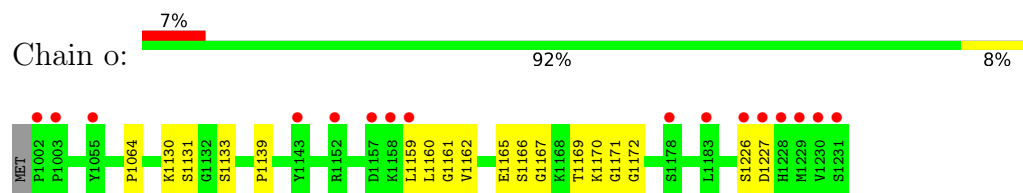




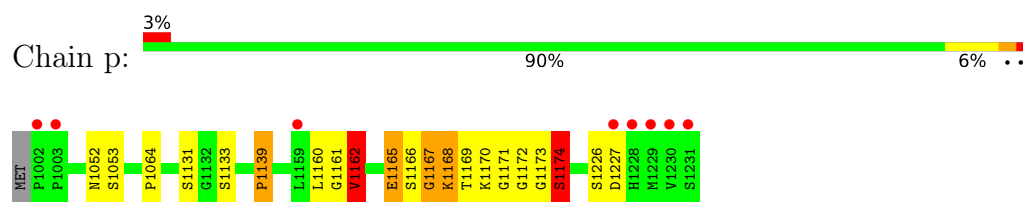
- Molecule 15: proteasome activator protein PA26



- Molecule 15: proteasome activator protein PA26



- Molecule 15: proteasome activator protein PA26



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	192.96Å 232.13Å 296.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.80 – 3.22 39.84 – 3.22	Depositor EDS
% Data completeness (in resolution range)	89.1 (39.80-3.22) 88.2 (39.84-3.22)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 3.25Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.263 , 0.308 0.275 , 0.312	Depositor DCC
$R_{free}$ test set	1264 reflections (0.67%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.3	Xtrriage
Anisotropy	0.529	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 53.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	74222	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	A	0.50	0/1959	0.70	1/2652 (0.0%)
1	O	0.49	0/1959	0.70	1/2652 (0.0%)
2	B	0.47	0/1944	0.73	0/2632
2	P	0.46	0/1944	0.72	0/2632
3	C	0.47	0/1930	0.69	0/2613
3	Q	0.47	0/1930	0.69	0/2613
4	D	0.47	0/1919	0.69	0/2598
4	R	0.45	0/1919	0.69	0/2598
5	E	0.49	0/1914	0.70	0/2579
5	S	0.47	0/1914	0.70	0/2579
6	F	0.48	0/1831	0.71	1/2473 (0.0%)
6	T	0.48	0/1831	0.70	0/2473
7	G	0.47	0/1932	0.68	0/2609
7	U	0.46	0/1932	0.67	0/2609
8	H	0.51	0/1541	0.74	0/2087
8	V	0.48	0/1541	0.73	0/2087
9	I	0.49	0/1716	0.71	0/2326
9	W	0.48	0/1716	0.70	0/2326
10	J	0.49	0/1611	0.76	2/2174 (0.1%)
10	X	0.50	0/1611	0.75	1/2174 (0.0%)
11	K	0.56	0/1613	0.74	0/2173
11	Y	0.53	0/1613	0.73	0/2173
12	L	0.54	0/1683	0.74	1/2277 (0.0%)
12	Z	0.54	0/1683	0.74	1/2277 (0.0%)
13	M	0.49	0/1795	0.73	0/2420
13	a	0.50	0/1795	0.73	0/2420
14	N	0.49	0/1855	0.75	0/2514
14	b	0.49	0/1855	0.75	0/2514
15	c	0.57	2/1786 (0.1%)	0.77	6/2415 (0.2%)
15	d	0.70	9/1786 (0.5%)	0.88	15/2415 (0.6%)
15	e	0.82	11/1786 (0.6%)	1.01	22/2415 (0.9%)
15	f	0.74	5/1786 (0.3%)	1.19	18/2415 (0.7%)
15	g	0.91	9/1786 (0.5%)	1.17	20/2415 (0.8%)
15	h	0.77	7/1786 (0.4%)	0.94	20/2415 (0.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
15	i	1.22	17/1786 (1.0%)	1.43	28/2415 (1.2%)
15	j	0.56	2/1786 (0.1%)	0.77	6/2415 (0.2%)
15	k	0.69	9/1786 (0.5%)	0.88	16/2415 (0.7%)
15	l	0.81	11/1786 (0.6%)	1.01	21/2415 (0.9%)
15	m	0.73	5/1786 (0.3%)	1.18	18/2415 (0.7%)
15	n	0.91	9/1786 (0.5%)	1.17	20/2415 (0.8%)
15	o	0.76	7/1786 (0.4%)	0.94	20/2415 (0.8%)
15	p	1.23	17/1786 (1.0%)	1.43	28/2415 (1.2%)
All	All	0.63	120/75490 (0.2%)	0.85	266/102064 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	O	0	1
3	C	0	1
3	Q	0	1
14	N	0	1
15	e	0	1
15	f	0	4
15	g	0	1
15	i	0	4
15	l	0	1
15	m	0	4
15	n	0	1
15	p	0	4
All	All	0	25

All (120) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	i	1172	GLY	C-N	32.26	1.91	1.33
15	p	1172	GLY	C-N	32.26	1.91	1.33
15	g	1163	ASP	C-O	14.32	1.50	1.23
15	n	1163	ASP	C-O	14.30	1.50	1.23
15	i	1173	GLY	N-CA	13.87	1.66	1.46
15	p	1173	GLY	N-CA	13.85	1.66	1.46
15	g	1168	LYS	N-CA	13.72	1.73	1.46
15	n	1168	LYS	N-CA	13.70	1.73	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	n	1168	LYS	CA-C	13.62	1.88	1.52
15	g	1168	LYS	CA-C	13.60	1.88	1.52
15	n	1169	THR	N-CA	13.05	1.72	1.46
15	g	1169	THR	N-CA	13.04	1.72	1.46
15	o	1170	LYS	C-N	-12.80	1.10	1.33
15	h	1170	LYS	C-N	-12.80	1.10	1.33
15	e	1175	GLN	C-O	-12.72	0.99	1.23
15	l	1175	GLN	C-O	-12.70	0.99	1.23
15	p	1172	GLY	C-O	11.93	1.42	1.23
15	i	1172	GLY	C-O	11.86	1.42	1.23
15	m	1066	GLN	CA-CB	11.06	1.78	1.53
15	f	1066	GLN	CA-CB	11.06	1.78	1.53
15	p	1162	VAL	C-N	10.99	1.59	1.34
15	i	1162	VAL	C-N	10.88	1.59	1.34
15	p	1167	GLY	CA-C	10.31	1.68	1.51
15	n	1168	LYS	C-N	9.53	1.55	1.34
15	g	1168	LYS	C-N	9.51	1.55	1.34
15	n	1167	GLY	CA-C	8.93	1.66	1.51
15	g	1167	GLY	CA-C	8.85	1.66	1.51
15	k	1165	GLU	N-CA	8.67	1.63	1.46
15	i	1167	GLY	CA-C	8.55	1.65	1.51
15	d	1165	GLU	N-CA	8.54	1.63	1.46
15	e	1167	GLY	CA-C	8.52	1.65	1.51
15	l	1167	GLY	CA-C	8.52	1.65	1.51
15	l	1175	GLN	C-N	-8.42	1.14	1.34
15	e	1175	GLN	C-N	-8.41	1.14	1.34
15	f	1175	GLN	C-O	-8.33	1.07	1.23
15	m	1175	GLN	C-O	-8.26	1.07	1.23
15	i	1173	GLY	CA-C	-8.25	1.38	1.51
15	p	1173	GLY	CA-C	-8.25	1.38	1.51
15	f	1175	GLN	C-N	-8.08	1.15	1.34
15	p	1170	LYS	N-CA	8.08	1.62	1.46
15	i	1170	LYS	N-CA	8.02	1.62	1.46
15	e	1170	LYS	N-CA	8.01	1.62	1.46
15	l	1170	LYS	N-CA	8.01	1.62	1.46
15	m	1175	GLN	C-N	-8.01	1.15	1.34
15	p	1172	GLY	N-CA	-8.00	1.34	1.46
15	i	1172	GLY	N-CA	-7.99	1.34	1.46
15	i	1169	THR	N-CA	7.72	1.61	1.46
15	e	1169	THR	N-CA	7.67	1.61	1.46
15	p	1169	THR	N-CA	7.66	1.61	1.46
15	l	1169	THR	N-CA	7.65	1.61	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	i	1173	GLY	C-N	-7.54	1.16	1.34
15	p	1173	GLY	C-N	-7.48	1.16	1.34
15	h	1161	GLY	N-CA	-7.29	1.35	1.46
15	o	1161	GLY	N-CA	-7.20	1.35	1.46
15	o	1170	LYS	N-CA	7.18	1.60	1.46
15	i	1172	GLY	CA-C	-7.16	1.40	1.51
15	h	1170	LYS	N-CA	7.12	1.60	1.46
15	p	1172	GLY	CA-C	-7.10	1.40	1.51
15	e	1172	GLY	N-CA	-7.06	1.35	1.46
15	d	1165	GLU	CA-C	7.03	1.71	1.52
15	k	1165	GLU	CA-C	6.99	1.71	1.52
15	l	1172	GLY	N-CA	-6.99	1.35	1.46
15	o	1169	THR	N-CA	6.84	1.60	1.46
15	h	1169	THR	N-CA	6.82	1.59	1.46
15	h	1169	THR	CA-C	6.82	1.70	1.52
15	o	1169	THR	CA-C	6.78	1.70	1.52
15	k	1166	SER	N-CA	6.59	1.59	1.46
15	d	1171	GLY	N-CA	6.58	1.55	1.46
15	d	1171	GLY	CA-C	6.55	1.62	1.51
15	k	1171	GLY	CA-C	6.53	1.62	1.51
15	d	1166	SER	N-CA	6.53	1.59	1.46
15	e	1170	LYS	CA-C	6.52	1.70	1.52
15	l	1170	LYS	CA-C	6.51	1.69	1.52
15	p	1170	LYS	CA-C	6.51	1.69	1.52
15	g	1167	GLY	C-N	6.51	1.49	1.34
15	n	1167	GLY	C-N	6.49	1.49	1.34
15	k	1171	GLY	N-CA	6.47	1.55	1.46
15	i	1170	LYS	CA-C	6.47	1.69	1.52
15	e	1169	THR	CA-C	6.26	1.69	1.52
15	l	1169	THR	CA-C	6.26	1.69	1.52
15	i	1169	THR	CA-C	6.23	1.69	1.52
15	p	1169	THR	CA-C	6.23	1.69	1.52
15	g	1174	SER	CA-CB	-5.95	1.44	1.52
15	d	1164	ALA	C-N	5.94	1.47	1.34
15	n	1174	SER	CA-CB	-5.91	1.44	1.52
15	k	1164	ALA	C-N	5.91	1.47	1.34
15	p	1170	LYS	C-N	5.89	1.43	1.33
15	e	1170	LYS	C-N	5.88	1.43	1.33
15	i	1170	LYS	C-N	5.88	1.43	1.33
15	l	1170	LYS	C-N	5.84	1.43	1.33
15	p	1161	GLY	N-CA	-5.83	1.37	1.46
15	h	1167	GLY	CA-C	5.81	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	i	1161	GLY	N-CA	-5.78	1.37	1.46
15	o	1167	GLY	CA-C	5.74	1.61	1.51
15	m	1173	GLY	C-O	-5.70	1.14	1.23
15	k	1161	GLY	N-CA	5.68	1.54	1.46
15	f	1173	GLY	C-O	-5.67	1.14	1.23
15	d	1161	GLY	N-CA	5.67	1.54	1.46
15	j	1162	VAL	CA-C	5.61	1.67	1.52
15	c	1162	VAL	CA-C	5.60	1.67	1.52
15	d	1164	ALA	CA-C	5.55	1.67	1.52
15	f	1066	GLN	N-CA	5.54	1.57	1.46
15	k	1164	ALA	CA-C	5.51	1.67	1.52
15	p	1168	LYS	CA-C	5.46	1.67	1.52
15	l	1168	LYS	CA-C	5.43	1.67	1.52
15	i	1168	LYS	CA-C	5.41	1.67	1.52
15	o	1161	GLY	CA-C	-5.39	1.43	1.51
15	e	1168	LYS	CA-C	5.36	1.66	1.52
15	h	1161	GLY	CA-C	-5.36	1.43	1.51
15	d	1161	GLY	CA-C	5.33	1.60	1.51
15	j	1159	LEU	CA-C	-5.33	1.39	1.52
15	c	1159	LEU	CA-C	-5.32	1.39	1.52
15	k	1161	GLY	CA-C	5.26	1.60	1.51
15	i	1162	VAL	CA-C	5.17	1.66	1.52
15	l	1174	SER	N-CA	-5.16	1.36	1.46
15	n	1175	GLN	N-CA	-5.12	1.36	1.46
15	p	1162	VAL	CA-C	5.10	1.66	1.52
15	e	1174	SER	N-CA	-5.10	1.36	1.46
15	g	1175	GLN	N-CA	-5.07	1.36	1.46
15	m	1067	LEU	N-CA	5.00	1.56	1.46

All (266) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	n	1174	SER	N-CA-CB	-31.23	63.65	110.50
15	g	1174	SER	N-CA-CB	-31.22	63.68	110.50
15	p	1162	VAL	O-C-N	-27.33	78.97	122.70
15	i	1162	VAL	O-C-N	-27.26	79.09	122.70
15	f	1173	GLY	O-C-N	-27.22	79.15	122.70
15	m	1173	GLY	O-C-N	-27.22	79.15	122.70
15	i	1172	GLY	O-C-N	25.26	166.14	123.20
15	p	1172	GLY	O-C-N	25.22	166.08	123.20
15	m	1175	GLN	O-C-N	-23.36	85.33	122.70
15	f	1175	GLN	O-C-N	-23.33	85.37	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	p	1172	GLY	CA-C-N	-23.19	69.82	116.20
15	i	1172	GLY	CA-C-N	-23.18	69.83	116.20
15	l	1175	GLN	O-C-N	-19.81	91.01	122.70
15	e	1175	GLN	O-C-N	-19.78	91.05	122.70
15	p	1162	VAL	CA-C-N	17.28	155.22	117.20
15	i	1162	VAL	CA-C-N	17.27	155.20	117.20
15	p	1172	GLY	C-N-CA	16.87	157.73	122.30
15	i	1172	GLY	C-N-CA	16.85	157.68	122.30
15	f	1173	GLY	N-CA-C	15.14	150.96	113.10
15	m	1173	GLY	N-CA-C	15.10	150.86	113.10
15	m	1172	GLY	C-N-CA	-14.43	91.99	122.30
15	f	1172	GLY	C-N-CA	-14.40	92.06	122.30
15	p	1173	GLY	CA-C-N	-12.67	89.32	117.20
15	i	1173	GLY	CA-C-N	-12.62	89.43	117.20
15	j	1159	LEU	C-N-CA	-11.98	91.76	121.70
15	c	1159	LEU	C-N-CA	-11.94	91.85	121.70
15	g	1168	LYS	CA-C-N	11.36	142.19	117.20
15	h	1171	GLY	O-C-N	-11.35	103.91	123.20
15	o	1171	GLY	O-C-N	-11.34	103.92	123.20
15	n	1168	LYS	CA-C-N	11.34	142.14	117.20
15	o	1170	LYS	O-C-N	-11.22	104.13	123.20
15	h	1170	LYS	O-C-N	-11.20	104.17	123.20
15	n	1171	GLY	N-CA-C	-10.79	86.12	113.10
15	g	1171	GLY	N-CA-C	-10.79	86.13	113.10
15	p	1161	GLY	CA-C-N	-10.39	94.34	117.20
15	i	1161	GLY	CA-C-N	-10.39	94.35	117.20
15	i	1173	GLY	O-C-N	10.06	138.80	122.70
15	p	1173	GLY	O-C-N	10.05	138.78	122.70
15	n	1160	LEU	CB-CA-C	9.96	129.13	110.20
15	g	1160	LEU	CB-CA-C	9.96	129.12	110.20
15	p	1173	GLY	C-N-CA	-9.79	97.22	121.70
15	i	1173	GLY	C-N-CA	-9.75	97.31	121.70
15	d	1160	LEU	CB-CA-C	-9.47	92.21	110.20
15	k	1160	LEU	CB-CA-C	-9.44	92.27	110.20
15	d	1161	GLY	C-N-CA	9.00	144.21	121.70
15	k	1161	GLY	C-N-CA	8.99	144.17	121.70
15	d	1162	VAL	N-CA-C	8.65	134.35	111.00
15	k	1162	VAL	N-CA-C	8.64	134.33	111.00
15	g	1170	LYS	CB-CA-C	8.53	127.47	110.40
15	h	1171	GLY	CA-C-N	8.53	133.26	116.20
15	o	1171	GLY	CA-C-N	8.50	133.20	116.20
15	n	1170	LYS	CB-CA-C	8.49	127.38	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	n	1163	ASP	N-CA-C	8.48	133.90	111.00
15	g	1163	ASP	N-CA-C	8.48	133.88	111.00
15	i	1161	GLY	C-N-CA	8.37	142.63	121.70
15	p	1161	GLY	C-N-CA	8.37	142.62	121.70
15	l	1172	GLY	CA-C-N	-8.24	99.72	116.20
15	e	1172	GLY	CA-C-N	-8.24	99.73	116.20
15	d	1166	SER	N-CA-C	8.12	132.94	111.00
15	k	1166	SER	N-CA-C	8.11	132.91	111.00
15	h	1131	SER	N-CA-C	8.11	132.89	111.00
15	o	1131	SER	N-CA-C	8.08	132.82	111.00
15	o	1169	THR	CA-C-N	7.91	134.61	117.20
15	h	1169	THR	CA-C-N	7.89	134.55	117.20
15	i	1170	LYS	N-CA-C	7.88	132.28	111.00
15	l	1170	LYS	N-CA-C	7.88	132.26	111.00
15	h	1170	LYS	N-CA-C	7.87	132.25	111.00
15	e	1170	LYS	N-CA-C	7.87	132.24	111.00
15	o	1170	LYS	N-CA-C	7.87	132.24	111.00
15	p	1170	LYS	N-CA-C	7.86	132.22	111.00
15	g	1168	LYS	N-CA-C	7.73	131.88	111.00
15	i	1131	SER	N-CA-C	7.73	131.87	111.00
15	k	1131	SER	N-CA-C	7.72	131.85	111.00
15	p	1131	SER	N-CA-C	7.72	131.85	111.00
15	n	1168	LYS	N-CA-C	7.71	131.82	111.00
15	d	1131	SER	N-CA-C	7.70	131.78	111.00
15	i	1174	SER	N-CA-CB	7.54	121.81	110.50
15	h	1169	THR	O-C-N	-7.50	110.69	122.70
15	p	1174	SER	N-CA-CB	7.50	121.75	110.50
15	o	1169	THR	O-C-N	-7.50	110.71	122.70
15	p	1170	LYS	CB-CA-C	-7.41	95.57	110.40
15	i	1170	LYS	CB-CA-C	-7.41	95.58	110.40
15	e	1173	GLY	N-CA-C	-7.39	94.61	113.10
15	e	1170	LYS	CB-CA-C	-7.39	95.62	110.40
15	l	1170	LYS	CB-CA-C	-7.39	95.62	110.40
15	p	1174	SER	O-C-N	-7.37	110.91	122.70
15	n	1131	SER	N-CA-C	7.37	130.89	111.00
15	g	1131	SER	N-CA-C	7.36	130.88	111.00
15	g	1168	LYS	CB-CA-C	-7.36	95.67	110.40
15	n	1168	LYS	CB-CA-C	-7.36	95.68	110.40
15	l	1173	GLY	N-CA-C	-7.34	94.76	113.10
15	i	1174	SER	O-C-N	-7.33	110.98	122.70
15	l	1131	SER	N-CA-C	7.31	130.74	111.00
15	e	1131	SER	N-CA-C	7.31	130.73	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	j	1131	SER	N-CA-C	7.23	130.53	111.00
15	o	1172	GLY	CA-C-N	-7.22	101.76	116.20
15	h	1172	GLY	CA-C-N	-7.22	101.77	116.20
15	c	1131	SER	N-CA-C	7.21	130.48	111.00
15	m	1173	GLY	CA-C-N	7.21	133.06	117.20
15	f	1173	GLY	CA-C-N	7.19	133.01	117.20
15	g	1172	GLY	C-N-CA	-7.16	107.26	122.30
15	n	1172	GLY	C-N-CA	-7.16	107.27	122.30
15	p	1162	VAL	N-CA-CB	-7.14	95.78	111.50
15	i	1162	VAL	N-CA-CB	-7.14	95.79	111.50
15	f	1170	LYS	CB-CA-C	7.13	124.66	110.40
15	h	1160	LEU	C-N-CA	-7.13	107.33	122.30
15	o	1160	LEU	C-N-CA	-7.13	107.33	122.30
15	g	1169	THR	N-CA-CB	7.11	123.81	110.30
15	n	1169	THR	N-CA-CB	7.11	123.81	110.30
15	m	1170	LYS	CB-CA-C	7.10	124.61	110.40
15	l	1171	GLY	C-N-CA	-7.10	107.39	122.30
15	e	1171	GLY	C-N-CA	-7.09	107.42	122.30
15	o	1170	LYS	CA-C-N	7.04	130.27	116.20
15	h	1170	LYS	CA-C-N	7.03	130.25	116.20
15	g	1167	GLY	C-N-CA	7.00	139.20	121.70
15	i	1161	GLY	CA-C-O	7.00	133.20	120.60
15	n	1167	GLY	C-N-CA	6.99	139.16	121.70
15	k	1160	LEU	CA-C-N	6.97	130.14	116.20
15	p	1161	GLY	CA-C-O	6.95	133.12	120.60
15	f	1164	ALA	CA-C-N	6.95	132.48	117.20
15	d	1160	LEU	CA-C-N	6.94	130.09	116.20
15	g	1168	LYS	O-C-N	-6.94	111.60	122.70
15	m	1164	ALA	CA-C-N	6.93	132.44	117.20
15	i	1171	GLY	C-N-CA	-6.90	107.81	122.30
15	p	1171	GLY	C-N-CA	-6.90	107.82	122.30
15	n	1168	LYS	O-C-N	-6.88	111.70	122.70
15	i	1165	GLU	C-N-CA	6.86	138.84	121.70
15	l	1165	GLU	C-N-CA	6.85	138.82	121.70
15	e	1165	GLU	C-N-CA	6.84	138.80	121.70
15	p	1165	GLU	C-N-CA	6.81	138.73	121.70
15	o	1159	LEU	CB-CA-C	-6.81	97.27	110.20
15	h	1159	LEU	CB-CA-C	-6.80	97.27	110.20
15	e	1175	GLN	CA-C-O	6.78	134.33	120.10
15	e	1161	GLY	N-CA-C	6.77	130.03	113.10
15	l	1175	GLN	CA-C-O	6.76	134.30	120.10
15	l	1161	GLY	N-CA-C	6.74	129.96	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	m	1175	GLN	CB-CA-C	6.74	123.89	110.40
15	f	1175	GLN	CB-CA-C	6.74	123.88	110.40
15	d	1130	LYS	C-N-CA	-6.72	104.89	121.70
15	k	1130	LYS	C-N-CA	-6.69	104.98	121.70
15	m	1131	SER	N-CA-C	6.67	129.02	111.00
15	c	1159	LEU	CB-CA-C	-6.67	97.52	110.20
15	n	1168	LYS	CA-C-O	-6.67	106.09	120.10
15	j	1159	LEU	CB-CA-C	-6.67	97.53	110.20
15	f	1131	SER	N-CA-C	6.66	128.98	111.00
15	g	1168	LYS	CA-C-O	-6.64	106.14	120.10
15	n	1173	GLY	N-CA-C	-6.62	96.55	113.10
15	g	1173	GLY	N-CA-C	-6.61	96.56	113.10
15	g	1169	THR	CB-CA-C	-6.54	93.95	111.60
15	n	1169	THR	CB-CA-C	-6.53	93.96	111.60
15	c	1163	ASP	C-N-CA	-6.51	105.43	121.70
15	j	1163	ASP	C-N-CA	-6.48	105.49	121.70
12	Z	4	LEU	CA-CB-CG	6.43	130.09	115.30
15	f	1174	SER	CA-C-N	-6.43	103.06	117.20
15	m	1174	SER	CA-C-N	-6.42	103.07	117.20
15	l	1176	SER	N-CA-CB	-6.41	100.89	110.50
15	e	1176	SER	N-CA-CB	-6.40	100.91	110.50
15	m	1160	LEU	CA-CB-CG	-6.36	100.68	115.30
12	L	4	LEU	CA-CB-CG	6.35	129.90	115.30
15	f	1160	LEU	CA-CB-CG	-6.33	100.75	115.30
15	l	1175	GLN	CA-C-N	6.26	130.97	117.20
15	g	1174	SER	CA-C-N	-6.25	103.45	117.20
15	n	1174	SER	CA-C-N	-6.23	103.49	117.20
15	e	1175	GLN	CA-C-N	6.22	130.88	117.20
15	g	1162	VAL	C-N-CA	-6.21	106.19	121.70
15	n	1162	VAL	C-N-CA	-6.20	106.21	121.70
15	o	1161	GLY	CA-C-N	-6.09	103.81	117.20
15	h	1161	GLY	CA-C-N	-6.07	103.85	117.20
15	p	1161	GLY	O-C-N	6.06	132.39	122.70
15	f	1174	SER	N-CA-C	6.01	127.23	111.00
15	m	1169	THR	C-N-CA	-6.01	106.68	121.70
15	i	1162	VAL	C-N-CA	6.01	136.72	121.70
15	i	1161	GLY	O-C-N	6.00	132.31	122.70
15	m	1171	GLY	C-N-CA	-6.00	109.69	122.30
15	m	1174	SER	N-CA-C	6.00	127.19	111.00
15	f	1171	GLY	C-N-CA	-5.99	109.72	122.30
15	m	1174	SER	O-C-N	5.96	132.23	122.70
15	p	1162	VAL	C-N-CA	5.95	136.57	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	f	1169	THR	C-N-CA	-5.94	106.85	121.70
15	f	1174	SER	O-C-N	5.94	132.21	122.70
15	h	1171	GLY	N-CA-C	-5.76	98.69	113.10
15	o	1171	GLY	N-CA-C	-5.74	98.76	113.10
15	c	1168	LYS	N-CA-C	-5.72	95.54	111.00
15	j	1168	LYS	N-CA-C	-5.72	95.54	111.00
15	g	1163	ASP	CA-C-N	-5.69	104.67	117.20
15	n	1163	ASP	CA-C-N	-5.68	104.70	117.20
15	k	1165	GLU	CA-C-N	5.64	129.60	117.20
15	d	1172	GLY	N-CA-C	5.63	127.18	113.10
15	d	1165	GLU	CA-C-N	5.62	129.56	117.20
15	i	1160	LEU	CA-C-N	-5.62	104.97	116.20
15	p	1173	GLY	CA-C-O	5.62	130.71	120.60
15	p	1160	LEU	CA-C-N	-5.61	104.97	116.20
15	h	1172	GLY	O-C-N	5.61	132.74	123.20
15	k	1172	GLY	N-CA-C	5.61	127.12	113.10
15	o	1172	GLY	O-C-N	5.60	132.72	123.20
15	l	1162	VAL	CA-C-N	-5.59	104.90	117.20
15	e	1162	VAL	CA-C-N	-5.58	104.94	117.20
15	i	1173	GLY	CA-C-O	5.57	130.62	120.60
15	d	1160	LEU	N-CA-C	5.55	125.99	111.00
15	k	1160	LEU	N-CA-C	5.55	125.99	111.00
15	e	1165	GLU	N-CA-C	5.51	125.88	111.00
15	i	1165	GLU	N-CA-C	5.51	125.87	111.00
15	p	1165	GLU	N-CA-C	5.51	125.87	111.00
15	j	1131	SER	CB-CA-C	-5.50	99.65	110.10
15	l	1165	GLU	N-CA-C	5.49	125.83	111.00
15	h	1165	GLU	CA-C-N	-5.49	105.13	117.20
15	c	1131	SER	CB-CA-C	-5.48	99.70	110.10
15	o	1165	GLU	CA-C-N	-5.47	105.17	117.20
15	o	1165	GLU	C-N-CA	5.46	135.36	121.70
15	h	1165	GLU	C-N-CA	5.46	135.35	121.70
15	p	1165	GLU	CA-C-N	-5.46	105.20	117.20
15	e	1165	GLU	CA-C-N	-5.42	105.28	117.20
15	f	1164	ALA	O-C-N	-5.42	114.03	122.70
15	i	1165	GLU	CA-C-N	-5.41	105.29	117.20
15	l	1165	GLU	CA-C-N	-5.41	105.30	117.20
15	g	1165	GLU	C-N-CA	5.40	135.20	121.70
15	m	1164	ALA	O-C-N	-5.40	114.06	122.70
15	n	1165	GLU	C-N-CA	5.38	135.16	121.70
15	p	1167	GLY	N-CA-C	5.38	126.56	113.10
15	e	1170	LYS	CA-C-N	5.38	126.96	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	l	1170	LYS	CA-C-N	5.38	126.95	116.20
15	p	1170	LYS	CA-C-N	5.37	126.95	116.20
10	J	102	TYR	N-CA-C	-5.37	96.50	111.00
15	m	1171	GLY	N-CA-C	-5.37	99.67	113.10
15	i	1170	LYS	CA-C-N	5.37	126.94	116.20
15	h	1162	VAL	CA-C-N	-5.35	105.44	117.20
15	f	1171	GLY	N-CA-C	-5.35	99.73	113.10
15	o	1162	VAL	CA-C-N	-5.32	105.49	117.20
15	h	1169	THR	C-N-CA	5.30	134.94	121.70
15	o	1169	THR	C-N-CA	5.28	134.91	121.70
15	o	1166	SER	CA-C-N	5.27	126.73	116.20
15	h	1166	SER	CA-C-N	5.25	126.71	116.20
15	e	1174	SER	C-N-CA	-5.25	108.57	121.70
15	o	1165	GLU	N-CA-C	5.23	125.13	111.00
15	l	1174	SER	C-N-CA	-5.21	108.67	121.70
15	d	1131	SER	CB-CA-C	-5.21	100.20	110.10
15	l	1172	GLY	C-N-CA	5.21	133.23	122.30
15	k	1131	SER	CB-CA-C	-5.20	100.23	110.10
15	e	1172	GLY	C-N-CA	5.19	133.20	122.30
15	h	1165	GLU	N-CA-C	5.19	125.01	111.00
15	k	1131	SER	CA-C-N	-5.19	105.82	116.20
15	d	1164	ALA	C-N-CA	5.18	134.65	121.70
15	k	1164	ALA	C-N-CA	5.18	134.66	121.70
15	d	1131	SER	CA-C-N	-5.17	105.85	116.20
15	e	1172	GLY	O-C-N	5.17	131.99	123.20
15	l	1172	GLY	O-C-N	5.16	131.96	123.20
15	p	1166	SER	C-N-CA	-5.15	111.49	122.30
15	d	1165	GLU	N-CA-C	5.12	124.82	111.00
15	k	1165	GLU	N-CA-C	5.11	124.80	111.00
10	J	100	GLY	N-CA-C	-5.08	100.39	113.10
6	F	72	LEU	CA-CB-CG	5.08	126.99	115.30
15	e	1131	SER	CB-CA-C	-5.07	100.47	110.10
15	f	1165	GLU	N-CA-C	5.06	124.66	111.00
15	l	1167	GLY	N-CA-C	5.06	125.74	113.10
1	O	12	TYR	CA-C-N	-5.05	106.08	117.20
15	e	1167	GLY	N-CA-C	5.05	125.72	113.10
15	l	1131	SER	CB-CA-C	-5.05	100.51	110.10
1	A	12	TYR	CA-C-N	-5.04	106.11	117.20
15	i	1167	GLY	N-CA-C	5.04	125.69	113.10
15	m	1165	GLU	N-CA-C	5.03	124.59	111.00
10	X	100	GLY	N-CA-C	-5.01	100.56	113.10
15	d	1160	LEU	CA-CB-CG	5.01	126.83	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	i	1166	SER	CA-C-N	5.01	126.23	116.20
15	k	1160	LEU	CA-CB-CG	5.01	126.83	115.30
15	k	1175	GLN	N-CA-C	5.01	124.52	111.00
15	e	1166	SER	CA-C-N	5.00	126.21	116.20

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	TYR	Mainchain
3	C	20	TYR	Sidechain
14	N	76	TYR	Sidechain
1	O	12	TYR	Mainchain
3	Q	20	TYR	Sidechain
15	e	1175	GLN	Mainchain
15	f	1173	GLY	Peptide,Mainchain
15	f	1174	SER	Mainchain
15	f	1175	GLN	Mainchain
15	g	1163	ASP	Mainchain
15	i	1139	PRO	Mainchain
15	i	1162	VAL	Peptide,Mainchain
15	i	1174	SER	Mainchain
15	l	1175	GLN	Mainchain
15	m	1173	GLY	Peptide,Mainchain
15	m	1174	SER	Mainchain
15	m	1175	GLN	Mainchain
15	n	1163	ASP	Mainchain
15	p	1139	PRO	Mainchain
15	p	1162	VAL	Peptide,Mainchain
15	p	1174	SER	Mainchain

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	A	241/252 (96%)	175 (73%)	53 (22%)	13 (5%)	2	13
1	O	241/252 (96%)	174 (72%)	54 (22%)	13 (5%)	2	13
2	B	247/250 (99%)	192 (78%)	39 (16%)	16 (6%)	1	9
2	P	247/250 (99%)	193 (78%)	38 (15%)	16 (6%)	1	9
3	C	241/258 (93%)	192 (80%)	35 (14%)	14 (6%)	1	12
3	Q	241/258 (93%)	192 (80%)	35 (14%)	14 (6%)	1	12
4	D	239/254 (94%)	203 (85%)	28 (12%)	8 (3%)	4	24
4	R	239/254 (94%)	203 (85%)	28 (12%)	8 (3%)	4	24
5	E	243/260 (94%)	204 (84%)	27 (11%)	12 (5%)	2	16
5	S	243/260 (94%)	201 (83%)	30 (12%)	12 (5%)	2	16
6	F	232/234 (99%)	192 (83%)	33 (14%)	7 (3%)	4	27
6	T	232/234 (99%)	191 (82%)	33 (14%)	8 (3%)	3	23
7	G	241/288 (84%)	188 (78%)	37 (15%)	16 (7%)	1	9
7	U	241/288 (84%)	188 (78%)	37 (15%)	16 (7%)	1	9
8	H	194/196 (99%)	143 (74%)	38 (20%)	13 (7%)	1	8
8	V	194/196 (99%)	142 (73%)	37 (19%)	15 (8%)	1	6
9	I	220/222 (99%)	173 (79%)	37 (17%)	10 (4%)	2	17
9	W	220/222 (99%)	174 (79%)	35 (16%)	11 (5%)	2	15
10	J	202/205 (98%)	173 (86%)	24 (12%)	5 (2%)	5	31
10	X	202/205 (98%)	174 (86%)	23 (11%)	5 (2%)	5	31
11	K	196/198 (99%)	171 (87%)	20 (10%)	5 (3%)	5	30
11	Y	196/198 (99%)	170 (87%)	21 (11%)	5 (3%)	5	30
12	L	210/212 (99%)	183 (87%)	24 (11%)	3 (1%)	11	45
12	Z	210/212 (99%)	185 (88%)	22 (10%)	3 (1%)	11	45
13	M	220/222 (99%)	193 (88%)	24 (11%)	3 (1%)	11	45
13	a	220/222 (99%)	192 (87%)	25 (11%)	3 (1%)	11	45
14	N	231/233 (99%)	176 (76%)	39 (17%)	16 (7%)	1	8
14	b	231/233 (99%)	176 (76%)	39 (17%)	16 (7%)	1	8
15	c	228/231 (99%)	207 (91%)	14 (6%)	7 (3%)	4	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	d	228/231 (99%)	206 (90%)	16 (7%)	6 (3%)	5	30
15	e	228/231 (99%)	206 (90%)	16 (7%)	6 (3%)	5	30
15	f	228/231 (99%)	200 (88%)	17 (8%)	11 (5%)	2	16
15	g	228/231 (99%)	202 (89%)	18 (8%)	8 (4%)	3	23
15	h	228/231 (99%)	209 (92%)	15 (7%)	4 (2%)	8	39
15	i	228/231 (99%)	207 (91%)	16 (7%)	5 (2%)	6	34
15	j	228/231 (99%)	207 (91%)	14 (6%)	7 (3%)	4	26
15	k	228/231 (99%)	206 (90%)	16 (7%)	6 (3%)	5	30
15	l	228/231 (99%)	206 (90%)	16 (7%)	6 (3%)	5	30
15	m	228/231 (99%)	199 (87%)	18 (8%)	11 (5%)	2	16
15	n	228/231 (99%)	202 (89%)	18 (8%)	8 (4%)	3	23
15	o	228/231 (99%)	209 (92%)	15 (7%)	4 (2%)	8	39
15	p	228/231 (99%)	207 (91%)	16 (7%)	5 (2%)	6	34
All	All	9506/9802 (97%)	7986 (84%)	1140 (12%)	380 (4%)	3	20

All (380) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	150	LEU
1	A	168	ALA
1	A	221	ASN
1	A	232	LYS
2	B	123	GLN
2	B	124	SER
2	B	244	ASN
3	C	4	ARG
3	C	20	TYR
3	C	183	ASP
3	C	203	SER
3	C	221	ASN
4	D	40	ASN
4	D	56	ASP
4	D	205	THR
5	E	61	SER
5	E	127	ALA
5	E	130	GLU
5	E	209	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	E	249	ALA
6	F	142	ALA
6	F	218	LYS
6	F	228	GLU
7	G	182	HIS
7	G	183	PRO
7	G	184	GLU
8	H	17	ASP
8	H	97	ILE
8	H	105	LYS
8	H	106	ASN
8	H	137	TYR
8	H	138	CYS
9	I	91	GLN
9	I	189	ASN
10	J	193	GLU
11	K	193	ASP
12	L	209	ASN
14	N	25	ASP
14	N	81	ALA
14	N	130	VAL
14	N	211	ASN
14	N	221	PHE
1	O	150	LEU
1	O	168	ALA
1	O	221	ASN
1	O	232	LYS
2	P	123	GLN
2	P	124	SER
2	P	244	ASN
3	Q	4	ARG
3	Q	20	TYR
3	Q	183	ASP
3	Q	203	SER
3	Q	221	ASN
4	R	40	ASN
4	R	56	ASP
4	R	205	THR
5	S	127	ALA
5	S	130	GLU
5	S	209	GLU
5	S	249	ALA

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	T	142	ALA
6	T	218	LYS
6	T	228	GLU
7	U	182	HIS
7	U	183	PRO
7	U	184	GLU
8	V	17	ASP
8	V	97	ILE
8	V	105	LYS
8	V	106	ASN
8	V	137	TYR
8	V	138	CYS
9	W	189	ASN
10	X	193	GLU
11	Y	193	ASP
12	Z	209	ASN
14	b	25	ASP
14	b	81	ALA
14	b	130	VAL
14	b	211	ASN
14	b	221	PHE
15	c	1133	SER
15	c	1139	PRO
15	c	1162	VAL
15	c	1164	ALA
15	d	1133	SER
15	d	1139	PRO
15	e	1133	SER
15	e	1139	PRO
15	f	1133	SER
15	f	1139	PRO
15	f	1162	VAL
15	f	1174	SER
15	g	1133	SER
15	g	1139	PRO
15	g	1162	VAL
15	g	1163	ASP
15	g	1164	ALA
15	g	1170	LYS
15	h	1133	SER
15	h	1139	PRO
15	i	1133	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
15	i	1139	PRO
15	i	1162	VAL
15	j	1133	SER
15	j	1139	PRO
15	j	1162	VAL
15	j	1164	ALA
15	k	1133	SER
15	k	1139	PRO
15	l	1133	SER
15	l	1139	PRO
15	m	1133	SER
15	m	1139	PRO
15	m	1162	VAL
15	m	1174	SER
15	m	1175	GLN
15	n	1133	SER
15	n	1139	PRO
15	n	1162	VAL
15	n	1163	ASP
15	n	1164	ALA
15	n	1170	LYS
15	o	1133	SER
15	o	1139	PRO
15	p	1133	SER
15	p	1139	PRO
15	p	1162	VAL
1	A	37	GLN
1	A	151	GLY
1	A	164	VAL
1	A	190	LYS
1	A	243	GLU
2	B	20	GLN
2	B	31	GLY
2	B	182	GLU
2	B	242	GLU
2	B	243	ILE
3	C	184	MET
3	C	223	GLY
5	E	131	GLU
5	E	134	MET
5	E	206	GLN
5	E	244	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	F	118	LYS
6	F	159	THR
7	G	71	ARG
7	G	72	HIS
7	G	186	LEU
7	G	188	ALA
7	G	204	GLU
7	G	207	LYS
8	H	74	SER
9	I	22	GLN
9	I	95	GLY
9	I	221	CYS
13	M	81	ASP
14	N	24	ALA
14	N	132	LEU
14	N	152	ASN
14	N	189	ALA
1	O	37	GLN
1	O	151	GLY
1	O	164	VAL
1	O	175	GLN
1	O	190	LYS
1	O	243	GLU
2	P	20	GLN
2	P	31	GLY
2	P	182	GLU
2	P	242	GLU
2	P	243	ILE
3	Q	184	MET
3	Q	223	GLY
3	Q	236	LYS
5	S	61	SER
5	S	131	GLU
5	S	134	MET
5	S	206	GLN
5	S	244	LYS
6	T	118	LYS
6	T	159	THR
7	U	71	ARG
7	U	72	HIS
7	U	152	PRO
7	U	185	GLY

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	U	186	LEU
7	U	188	ALA
7	U	204	GLU
7	U	207	LYS
8	V	74	SER
9	W	22	GLN
9	W	91	GLN
9	W	95	GLY
9	W	221	CYS
13	a	81	ASP
14	b	24	ALA
14	b	132	LEU
14	b	152	ASN
14	b	189	ALA
15	c	1163	ASP
15	c	1166	SER
15	e	1174	SER
15	f	1164	ALA
15	f	1170	LYS
15	f	1175	GLN
15	j	1163	ASP
15	j	1166	SER
15	l	1174	SER
15	m	1164	ALA
15	m	1170	LYS
1	A	175	GLN
1	A	189	SER
3	C	80	LEU
3	C	209	ASP
3	C	236	LYS
5	E	189	SER
7	G	70	ASP
7	G	152	PRO
7	G	185	GLY
7	G	224	ASN
8	H	9	LYS
8	H	33	LYS
8	H	191	ASP
9	I	48	THR
9	I	145	ASP
10	J	5	SER
11	K	141	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
14	N	76	TYR
14	N	151	ALA
14	N	170	VAL
1	O	77	ARG
1	O	189	SER
3	Q	80	LEU
3	Q	209	ASP
7	U	224	ASN
8	V	9	LYS
9	W	145	ASP
10	X	5	SER
11	Y	141	PHE
13	a	37	SER
14	b	76	TYR
14	b	151	ALA
14	b	170	VAL
15	d	1162	VAL
15	d	1176	SER
15	f	1166	SER
15	f	1173	GLY
15	f	1176	SER
15	g	1166	SER
15	k	1162	VAL
15	k	1176	SER
15	m	1166	SER
15	m	1173	GLY
15	m	1176	SER
15	n	1166	SER
1	A	77	ARG
1	A	200	GLU
2	B	29	LYS
2	B	79	GLY
3	C	233	GLN
4	D	58	ARG
4	D	78	LEU
5	E	214	GLU
6	F	117	GLN
6	F	232	LYS
8	H	68	SER
8	H	145	ASN
9	I	17	ASP
9	I	49	ALA

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	K	50	ALA
12	L	97	MET
12	L	165	ALA
13	M	37	SER
13	M	58	ALA
1	O	200	GLU
2	P	79	GLY
3	Q	195	LYS
3	Q	233	GLN
4	R	58	ARG
4	R	78	LEU
4	R	122	GLN
5	S	189	SER
5	S	214	GLU
6	T	232	LYS
7	U	70	ASP
7	U	210	ASP
8	V	33	LYS
8	V	68	SER
8	V	145	ASN
8	V	191	ASP
9	W	17	ASP
9	W	48	THR
9	W	49	ALA
11	Y	192	VAL
12	Z	97	MET
12	Z	165	ALA
13	a	58	ALA
14	b	9	THR
2	B	69	PRO
2	B	122	THR
2	B	208	THR
2	B	219	PRO
3	C	177	GLN
3	C	234	GLU
4	D	122	GLN
7	G	210	ASP
11	K	192	VAL
2	P	29	LYS
2	P	122	THR
2	P	208	THR
2	P	219	PRO

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	Q	234	GLU
4	R	200	LEU
6	T	117	GLN
8	V	50	ALA
11	Y	50	ALA
15	d	1226	SER
15	e	1226	SER
15	i	1226	SER
15	k	1226	SER
15	l	1226	SER
15	p	1226	SER
2	B	191	ILE
3	C	195	LYS
4	D	200	LEU
5	E	62	ASP
7	G	241	PHE
9	I	39	PRO
10	J	2	ASP
14	N	9	THR
2	P	69	PRO
2	P	158	PRO
2	P	191	ILE
3	Q	30	SER
5	S	62	ASP
6	T	5	ASN
7	U	241	PHE
9	W	21	THR
9	W	39	PRO
10	X	2	ASP
15	h	1226	SER
15	o	1226	SER
2	B	158	PRO
11	K	9	VAL
11	Y	9	VAL
15	i	1064	PRO
15	p	1064	PRO
4	D	202	VAL
7	G	84	GLY
10	J	100	GLY
10	J	107	VAL
14	N	177	ILE
4	R	202	VAL

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Mol	Chain	Res	Type
8	V	30	VAL
14	b	11	VAL
14	b	22	ILE
14	b	177	ILE
15	c	1064	PRO
15	d	1064	PRO
15	e	1162	VAL
15	f	1064	PRO
15	h	1064	PRO
15	j	1064	PRO
15	k	1064	PRO
15	l	1162	VAL
15	m	1064	PRO
15	o	1064	PRO
8	H	30	VAL
14	N	11	VAL
7	U	84	GLY
10	X	100	GLY
10	X	107	VAL
15	e	1064	PRO
15	l	1064	PRO
15	n	1064	PRO
14	N	22	ILE
8	V	189	TYR
15	g	1064	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	A	207/210 (99%)	185 (89%)	22 (11%)	6 27
1	O	207/210 (99%)	186 (90%)	21 (10%)	7 29
2	B	208/209 (100%)	188 (90%)	20 (10%)	8 31
2	P	208/209 (100%)	189 (91%)	19 (9%)	9 33
3	C	203/216 (94%)	181 (89%)	22 (11%)	6 26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Q	203/216 (94%)	181 (89%)	22 (11%)	6	26
4	D	213/226 (94%)	196 (92%)	17 (8%)	12	42
4	R	213/226 (94%)	196 (92%)	17 (8%)	12	42
5	E	201/215 (94%)	188 (94%)	13 (6%)	17	50
5	S	201/215 (94%)	187 (93%)	14 (7%)	15	47
6	F	193/193 (100%)	174 (90%)	19 (10%)	8	30
6	T	193/193 (100%)	173 (90%)	20 (10%)	7	28
7	G	201/239 (84%)	182 (90%)	19 (10%)	8	31
7	U	201/239 (84%)	183 (91%)	18 (9%)	9	34
8	H	162/162 (100%)	145 (90%)	17 (10%)	7	27
8	V	162/162 (100%)	144 (89%)	18 (11%)	6	25
9	I	181/181 (100%)	164 (91%)	17 (9%)	8	32
9	W	181/181 (100%)	164 (91%)	17 (9%)	8	32
10	J	172/173 (99%)	163 (95%)	9 (5%)	23	58
10	X	172/173 (99%)	163 (95%)	9 (5%)	23	58
11	K	175/175 (100%)	157 (90%)	18 (10%)	7	28
11	Y	175/175 (100%)	158 (90%)	17 (10%)	8	31
12	L	169/169 (100%)	159 (94%)	10 (6%)	19	54
12	Z	169/169 (100%)	158 (94%)	11 (6%)	17	50
13	M	185/185 (100%)	164 (89%)	21 (11%)	5	24
13	a	185/185 (100%)	163 (88%)	22 (12%)	5	22
14	N	199/199 (100%)	185 (93%)	14 (7%)	15	47
14	b	199/199 (100%)	184 (92%)	15 (8%)	13	44
15	c	188/189 (100%)	182 (97%)	6 (3%)	39	70
15	d	188/189 (100%)	186 (99%)	2 (1%)	73	88
15	e	188/189 (100%)	186 (99%)	2 (1%)	73	88
15	f	188/189 (100%)	182 (97%)	6 (3%)	39	70
15	g	188/189 (100%)	184 (98%)	4 (2%)	53	79
15	h	188/189 (100%)	186 (99%)	2 (1%)	73	88
15	i	188/189 (100%)	186 (99%)	2 (1%)	73	88
15	j	188/189 (100%)	182 (97%)	6 (3%)	39	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	k	188/189 (100%)	186 (99%)	2 (1%)	73	88
15	l	188/189 (100%)	186 (99%)	2 (1%)	73	88
15	m	188/189 (100%)	182 (97%)	6 (3%)	39	70
15	n	188/189 (100%)	184 (98%)	4 (2%)	53	79
15	o	188/189 (100%)	186 (99%)	2 (1%)	73	88
15	p	188/189 (100%)	186 (99%)	2 (1%)	73	88
All	All	7970/8150 (98%)	7444 (93%)	526 (7%)	16	50

All (526) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	56	GLN
1	A	65	ASP
1	A	73	PHE
1	A	117	LEU
1	A	124	LEU
1	A	126	GLN
1	A	128	TYR
1	A	131	ARG
1	A	133	TYR
1	A	150	LEU
1	A	153	SER
1	A	163	TYR
1	A	167	LYS
1	A	193	HIS
1	A	195	ASN
1	A	212	ASP
1	A	220	LYS
1	A	221	ASN
1	A	230	LYS
1	A	234	PHE
1	A	250	GLU
2	B	10	THR
2	B	26	THR
2	B	28	VAL
2	B	35	LEU
2	B	55	LEU
2	B	59	GLU
2	B	68	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	118	MET
2	B	134	LEU
2	B	150	VAL
2	B	157	PHE
2	B	173	THR
2	B	178	ARG
2	B	182	GLU
2	B	184	GLU
2	B	204	PHE
2	B	211	LEU
2	B	220	ASP
2	B	244	ASN
2	B	245	ASP
3	C	10	THR
3	C	26	LEU
3	C	53	THR
3	C	70	ASN
3	C	81	THR
3	C	86	ILE
3	C	111	LEU
3	C	115	LEU
3	C	120	GLN
3	C	134	SER
3	C	142	ASP
3	C	150	THR
3	C	158	THR
3	C	175	LEU
3	C	183	ASP
3	C	185	LYS
3	C	190	ILE
3	C	192	LEU
3	C	202	ASP
3	C	217	ARG
3	C	221	ASN
3	C	224	GLU
4	D	9	SER
4	D	24	LEU
4	D	29	ARG
4	D	49	ARG
4	D	52	LEU
4	D	54	LEU
4	D	59	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	D	105	THR
4	D	118	GLN
4	D	132	SER
4	D	162	GLN
4	D	166	ARG
4	D	208	LYS
4	D	211	GLU
4	D	215	VAL
4	D	218	ASP
4	D	239	GLU
5	E	48	LEU
5	E	76	CYS
5	E	78	MET
5	E	110	GLU
5	E	119	LEU
5	E	154	GLN
5	E	184	LEU
5	E	221	CYS
5	E	222	ILE
5	E	226	ASP
5	E	232	ASP
5	E	233	ASN
5	E	245	GLU
6	F	3	ARG
6	F	10	THR
6	F	31	GLN
6	F	62	LYS
6	F	72	LEU
6	F	90	GLN
6	F	93	ASN
6	F	94	TYR
6	F	100	ASN
6	F	107	ARG
6	F	117	GLN
6	F	147	PHE
6	F	166	GLN
6	F	171	TYR
6	F	176	LEU
6	F	185	ASN
6	F	189	LEU
6	F	206	LEU
6	F	228	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	G	19	ARG
7	G	27	VAL
7	G	28	LYS
7	G	42	ASN
7	G	72	HIS
7	G	76	VAL
7	G	80	LEU
7	G	81	ILE
7	G	97	SER
7	G	120	GLN
7	G	126	ASN
7	G	127	SER
7	G	147	LEU
7	G	152	PRO
7	G	189	ARG
7	G	208	GLU
7	G	217	TRP
7	G	224	ASN
7	G	243	GLN
8	H	8	PHE
8	H	21	THR
8	H	36	ARG
8	H	39	ASP
8	H	72	THR
8	H	82	PHE
8	H	83	LYS
8	H	84	GLU
8	H	88	GLU
8	H	92	ASN
8	H	104	ASP
8	H	118	SER
8	H	132	THR
8	H	137	TYR
8	H	149	GLU
8	H	153	ASP
8	H	172	VAL
9	I	10	ASN
9	I	21	THR
9	I	33	LYS
9	I	39	PRO
9	I	41	ILE
9	I	72	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	I	81	GLN
9	I	82	MET
9	I	85	GLN
9	I	98	LEU
9	I	104	ASP
9	I	132	LEU
9	I	144	GLN
9	I	146	LEU
9	I	153	LYS
9	I	177	VAL
9	I	178	MET
10	J	37	ASN
10	J	64	GLU
10	J	90	VAL
10	J	123	PHE
10	J	125	LEU
10	J	133	LYS
10	J	138	SER
10	J	171	LEU
10	J	191	LYS
11	K	7	ILE
11	K	8	ARG
11	K	11	ASP
11	K	22	THR
11	K	28	LEU
11	K	36	ARG
11	K	75	LEU
11	K	78	GLN
11	K	86	GLN
11	K	91	SER
11	K	110	LYS
11	K	111	LYS
11	K	136	SER
11	K	162	LYS
11	K	194	ASP
11	K	195	PHE
11	K	196	GLN
11	K	198	GLN
12	L	4	LEU
12	L	9	GLN
12	L	21	THR
12	L	25	TRP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
12	L	33	ARG
12	L	86	LEU
12	L	104	TYR
12	L	105	THR
12	L	111	THR
12	L	211	ILE
13	M	3	ASN
13	M	18	GLU
13	M	23	LEU
13	M	27	THR
13	M	31	THR
13	M	48	ASP
13	M	49	ASN
13	M	52	MET
13	M	67	ARG
13	M	85	SER
13	M	109	THR
13	M	135	GLN
13	M	144	SER
13	M	151	ASP
13	M	152	ASN
13	M	165	ASN
13	M	172	LEU
13	M	174	TYR
13	M	175	LEU
13	M	214	LYS
13	M	221	ARG
14	N	34	LEU
14	N	48	ASN
14	N	85	GLU
14	N	102	GLN
14	N	104	ARG
14	N	111	TRP
14	N	132	LEU
14	N	138	SER
14	N	140	PRO
14	N	171	GLN
14	N	184	LEU
14	N	212	LEU
14	N	216	ASN
14	N	226	LYS
1	O	39	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	O	56	GLN
1	O	65	ASP
1	O	73	PHE
1	O	117	LEU
1	O	124	LEU
1	O	126	GLN
1	O	128	TYR
1	O	131	ARG
1	O	133	TYR
1	O	150	LEU
1	O	153	SER
1	O	163	TYR
1	O	167	LYS
1	O	193	HIS
1	O	195	ASN
1	O	220	LYS
1	O	221	ASN
1	O	230	LYS
1	O	234	PHE
1	O	250	GLU
2	P	10	THR
2	P	26	THR
2	P	28	VAL
2	P	35	LEU
2	P	55	LEU
2	P	59	GLU
2	P	68	THR
2	P	118	MET
2	P	134	LEU
2	P	150	VAL
2	P	157	PHE
2	P	173	THR
2	P	178	ARG
2	P	182	GLU
2	P	184	GLU
2	P	204	PHE
2	P	220	ASP
2	P	244	ASN
2	P	245	ASP
3	Q	10	THR
3	Q	26	LEU
3	Q	53	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	Q	70	ASN
3	Q	81	THR
3	Q	86	ILE
3	Q	111	LEU
3	Q	115	LEU
3	Q	120	GLN
3	Q	134	SER
3	Q	142	ASP
3	Q	150	THR
3	Q	158	THR
3	Q	175	LEU
3	Q	183	ASP
3	Q	185	LYS
3	Q	190	ILE
3	Q	192	LEU
3	Q	202	ASP
3	Q	217	ARG
3	Q	221	ASN
3	Q	224	GLU
4	R	9	SER
4	R	24	LEU
4	R	29	ARG
4	R	49	ARG
4	R	52	LEU
4	R	54	LEU
4	R	59	ILE
4	R	105	THR
4	R	118	GLN
4	R	132	SER
4	R	162	GLN
4	R	166	ARG
4	R	208	LYS
4	R	211	GLU
4	R	215	VAL
4	R	218	ASP
4	R	239	GLU
5	S	48	LEU
5	S	76	CYS
5	S	78	MET
5	S	110	GLU
5	S	119	LEU
5	S	154	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	S	180	GLN
5	S	184	LEU
5	S	221	CYS
5	S	222	ILE
5	S	226	ASP
5	S	232	ASP
5	S	233	ASN
5	S	245	GLU
6	T	3	ARG
6	T	10	THR
6	T	31	GLN
6	T	62	LYS
6	T	72	LEU
6	T	90	GLN
6	T	93	ASN
6	T	94	TYR
6	T	100	ASN
6	T	107	ARG
6	T	117	GLN
6	T	147	PHE
6	T	157	TYR
6	T	166	GLN
6	T	171	TYR
6	T	176	LEU
6	T	185	ASN
6	T	189	LEU
6	T	206	LEU
6	T	228	GLU
7	U	19	ARG
7	U	27	VAL
7	U	42	ASN
7	U	72	HIS
7	U	76	VAL
7	U	80	LEU
7	U	81	ILE
7	U	97	SER
7	U	120	GLN
7	U	126	ASN
7	U	127	SER
7	U	147	LEU
7	U	152	PRO
7	U	189	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	U	208	GLU
7	U	217	TRP
7	U	224	ASN
7	U	243	GLN
8	V	4	MET
8	V	8	PHE
8	V	21	THR
8	V	36	ARG
8	V	39	ASP
8	V	72	THR
8	V	82	PHE
8	V	83	LYS
8	V	84	GLU
8	V	88	GLU
8	V	92	ASN
8	V	104	ASP
8	V	118	SER
8	V	132	THR
8	V	137	TYR
8	V	149	GLU
8	V	153	ASP
8	V	172	VAL
9	W	10	ASN
9	W	21	THR
9	W	33	LYS
9	W	39	PRO
9	W	41	ILE
9	W	72	ARG
9	W	81	GLN
9	W	82	MET
9	W	85	GLN
9	W	98	LEU
9	W	104	ASP
9	W	132	LEU
9	W	144	GLN
9	W	146	LEU
9	W	153	LYS
9	W	177	VAL
9	W	178	MET
10	X	37	ASN
10	X	64	GLU
10	X	90	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
10	X	123	PHE
10	X	125	LEU
10	X	133	LYS
10	X	138	SER
10	X	171	LEU
10	X	191	LYS
11	Y	7	ILE
11	Y	8	ARG
11	Y	11	ASP
11	Y	22	THR
11	Y	36	ARG
11	Y	75	LEU
11	Y	78	GLN
11	Y	86	GLN
11	Y	91	SER
11	Y	110	LYS
11	Y	111	LYS
11	Y	136	SER
11	Y	162	LYS
11	Y	194	ASP
11	Y	195	PHE
11	Y	196	GLN
11	Y	198	GLN
12	Z	4	LEU
12	Z	9	GLN
12	Z	21	THR
12	Z	25	TRP
12	Z	33	ARG
12	Z	86	LEU
12	Z	104	TYR
12	Z	105	THR
12	Z	111	THR
12	Z	152	ASP
12	Z	211	ILE
13	a	3	ASN
13	a	18	GLU
13	a	23	LEU
13	a	27	THR
13	a	31	THR
13	a	48	ASP
13	a	49	ASN
13	a	51	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
13	a	52	MET
13	a	67	ARG
13	a	85	SER
13	a	103	PHE
13	a	109	THR
13	a	135	GLN
13	a	151	ASP
13	a	152	ASN
13	a	165	ASN
13	a	172	LEU
13	a	174	TYR
13	a	175	LEU
13	a	214	LYS
13	a	221	ARG
14	b	9	THR
14	b	34	LEU
14	b	48	ASN
14	b	72	THR
14	b	85	GLU
14	b	102	GLN
14	b	104	ARG
14	b	111	TRP
14	b	132	LEU
14	b	138	SER
14	b	140	PRO
14	b	171	GLN
14	b	212	LEU
14	b	216	ASN
14	b	226	LYS
15	c	1130	LYS
15	c	1162	VAL
15	c	1165	GLU
15	c	1168	LYS
15	c	1170	LYS
15	c	1227	ASP
15	d	1130	LYS
15	d	1227	ASP
15	e	1174	SER
15	e	1227	ASP
15	f	1130	LYS
15	f	1165	GLU
15	f	1166	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
15	f	1168	LYS
15	f	1174	SER
15	f	1227	ASP
15	g	1130	LYS
15	g	1166	SER
15	g	1170	LYS
15	g	1227	ASP
15	h	1130	LYS
15	h	1227	ASP
15	i	1174	SER
15	i	1227	ASP
15	j	1130	LYS
15	j	1162	VAL
15	j	1165	GLU
15	j	1168	LYS
15	j	1170	LYS
15	j	1227	ASP
15	k	1130	LYS
15	k	1227	ASP
15	l	1174	SER
15	l	1227	ASP
15	m	1130	LYS
15	m	1165	GLU
15	m	1166	SER
15	m	1168	LYS
15	m	1174	SER
15	m	1227	ASP
15	n	1130	LYS
15	n	1166	SER
15	n	1170	LYS
15	n	1227	ASP
15	o	1130	LYS
15	o	1227	ASP
15	p	1174	SER
15	p	1227	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (259) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	39	ASN
1	A	92	ASN
1	A	123	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	126	GLN
1	A	130	GLN
1	A	176	GLN
1	A	184	ASN
1	A	193	HIS
1	A	195	ASN
1	A	209	HIS
1	A	251	GLN
2	B	94	HIS
2	B	139	HIS
2	B	218	ASN
2	B	241	GLN
2	B	244	ASN
3	C	70	ASN
3	C	94	HIS
3	C	96	GLN
3	C	97	ASN
3	C	103	ASN
3	C	120	GLN
3	C	124	GLN
3	C	156	ASN
3	C	177	GLN
3	C	221	ASN
3	C	227	GLN
4	D	94	GLN
4	D	162	GLN
4	D	178	ASN
4	D	209	ASN
4	D	241	GLN
4	D	243	GLN
5	E	99	HIS
5	E	108	ASN
5	E	154	GLN
5	E	168	ASN
5	E	215	ASN
5	E	233	ASN
6	F	100	ASN
6	F	110	HIS
6	F	121	GLN
6	F	152	ASN
6	F	185	ASN
7	G	72	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	G	86	HIS
7	G	122	HIS
7	G	126	ASN
7	G	194	GLN
7	G	206	ASN
7	G	224	ASN
8	H	38	HIS
8	H	60	GLN
8	H	69	GLN
8	H	157	HIS
9	I	22	GLN
9	I	62	ASN
9	I	66	HIS
9	I	116	HIS
9	I	144	GLN
9	I	160	GLN
9	I	165	ASN
10	J	37	ASN
10	J	71	ASN
10	J	88	GLN
10	J	156	ASN
11	K	37	GLN
11	K	118	GLN
11	K	147	HIS
11	K	191	GLN
11	K	196	GLN
11	K	198	GLN
12	L	9	GLN
12	L	66	HIS
12	L	85	ASN
12	L	133	GLN
12	L	176	ASN
12	L	188	HIS
12	L	190	ASN
12	L	191	HIS
12	L	208	ASN
13	M	3	ASN
13	M	49	ASN
13	M	70	ASN
13	M	80	ASN
13	M	108	HIS
13	M	152	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
13	M	158	ASN
13	M	165	ASN
13	M	195	HIS
14	N	3	GLN
14	N	18	ASN
14	N	48	ASN
14	N	62	HIS
14	N	108	ASN
14	N	149	HIS
14	N	152	ASN
14	N	171	GLN
14	N	179	ASN
14	N	211	ASN
14	N	216	ASN
1	O	39	ASN
1	O	92	ASN
1	O	123	ASN
1	O	126	GLN
1	O	130	GLN
1	O	176	GLN
1	O	184	ASN
1	O	193	HIS
1	O	195	ASN
1	O	209	HIS
1	O	251	GLN
2	P	94	HIS
2	P	139	HIS
2	P	218	ASN
2	P	241	GLN
2	P	244	ASN
3	Q	70	ASN
3	Q	94	HIS
3	Q	96	GLN
3	Q	97	ASN
3	Q	103	ASN
3	Q	120	GLN
3	Q	124	GLN
3	Q	156	ASN
3	Q	177	GLN
3	Q	221	ASN
3	Q	227	GLN
4	R	94	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	R	162	GLN
4	R	178	ASN
4	R	209	ASN
4	R	241	GLN
4	R	243	GLN
5	S	99	HIS
5	S	108	ASN
5	S	154	GLN
5	S	168	ASN
5	S	215	ASN
5	S	233	ASN
6	T	69	HIS
6	T	100	ASN
6	T	110	HIS
6	T	121	GLN
6	T	152	ASN
6	T	185	ASN
7	U	72	HIS
7	U	86	HIS
7	U	122	HIS
7	U	126	ASN
7	U	194	GLN
7	U	206	ASN
7	U	224	ASN
8	V	38	HIS
8	V	60	GLN
8	V	69	GLN
8	V	157	HIS
9	W	22	GLN
9	W	62	ASN
9	W	66	HIS
9	W	144	GLN
9	W	160	GLN
9	W	165	ASN
10	X	37	ASN
10	X	88	GLN
10	X	156	ASN
11	Y	37	GLN
11	Y	118	GLN
11	Y	147	HIS
11	Y	191	GLN
11	Y	196	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	Y	198	GLN
12	Z	9	GLN
12	Z	66	HIS
12	Z	85	ASN
12	Z	133	GLN
12	Z	176	ASN
12	Z	188	HIS
12	Z	190	ASN
12	Z	191	HIS
13	a	3	ASN
13	a	49	ASN
13	a	70	ASN
13	a	80	ASN
13	a	108	HIS
13	a	152	ASN
13	a	158	ASN
13	a	165	ASN
13	a	195	HIS
14	b	3	GLN
14	b	18	ASN
14	b	48	ASN
14	b	62	HIS
14	b	108	ASN
14	b	149	HIS
14	b	152	ASN
14	b	171	GLN
14	b	179	ASN
14	b	211	ASN
14	b	216	ASN
15	c	1047	HIS
15	c	1072	GLN
15	c	1099	HIS
15	d	1047	HIS
15	d	1072	GLN
15	d	1079	HIS
15	d	1099	HIS
15	e	1047	HIS
15	e	1072	GLN
15	e	1079	HIS
15	e	1099	HIS
15	e	1111	HIS
15	f	1047	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
15	f	1072	GLN
15	f	1079	HIS
15	f	1099	HIS
15	g	1047	HIS
15	g	1072	GLN
15	g	1079	HIS
15	g	1099	HIS
15	g	1111	HIS
15	h	1047	HIS
15	h	1072	GLN
15	h	1079	HIS
15	h	1099	HIS
15	h	1111	HIS
15	i	1047	HIS
15	i	1072	GLN
15	i	1079	HIS
15	i	1099	HIS
15	j	1047	HIS
15	j	1072	GLN
15	j	1099	HIS
15	k	1047	HIS
15	k	1072	GLN
15	k	1079	HIS
15	k	1099	HIS
15	l	1047	HIS
15	l	1072	GLN
15	l	1079	HIS
15	l	1099	HIS
15	l	1111	HIS
15	m	1047	HIS
15	m	1072	GLN
15	m	1079	HIS
15	m	1099	HIS
15	n	1047	HIS
15	n	1072	GLN
15	n	1079	HIS
15	n	1099	HIS
15	n	1111	HIS
15	o	1047	HIS
15	o	1072	GLN
15	o	1079	HIS
15	o	1111	HIS

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Mol	Chain	Res	Type
15	p	1047	HIS
15	p	1072	GLN
15	p	1079	HIS
15	p	1099	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
15	i	2
15	p	2
15	f	1
15	m	1
15	e	1
15	l	1
15	h	1
15	o	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	i	1172:GLY	C	1173:GLY	N	1.91
1	p	1172:GLY	C	1173:GLY	N	1.91
1	i	1173:GLY	C	1174:SER	N	1.16
1	p	1173:GLY	C	1174:SER	N	1.16
1	f	1175:GLN	C	1176:SER	N	1.15
1	m	1175:GLN	C	1176:SER	N	1.15
1	e	1175:GLN	C	1176:SER	N	1.14
1	l	1175:GLN	C	1176:SER	N	1.14
1	h	1170:LYS	C	1171:GLY	N	1.10
1	o	1170:LYS	C	1171:GLY	N	1.10

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	243/252 (96%)	0.27	10 (4%) 37 25	47, 82, 112, 124	0
1	O	243/252 (96%)	0.24	11 (4%) 33 21	47, 82, 112, 125	0
2	B	249/250 (99%)	0.14	8 (3%) 47 33	45, 67, 102, 123	0
2	P	249/250 (99%)	0.01	9 (3%) 42 29	46, 68, 102, 123	0
3	C	243/258 (94%)	-0.01	5 (2%) 63 50	32, 60, 108, 122	0
3	Q	243/258 (94%)	0.07	10 (4%) 37 25	32, 62, 108, 122	0
4	D	241/254 (94%)	-0.01	5 (2%) 63 50	34, 58, 105, 135	0
4	R	241/254 (94%)	-0.05	7 (2%) 51 37	35, 61, 104, 133	0
5	E	245/260 (94%)	0.10	15 (6%) 21 12	31, 55, 108, 133	0
5	S	245/260 (94%)	0.08	13 (5%) 26 15	33, 57, 108, 134	0
6	F	234/234 (100%)	-0.16	1 (0%) 92 89	34, 58, 78, 111	0
6	T	234/234 (100%)	-0.07	2 (0%) 84 76	36, 59, 79, 111	0
7	G	243/288 (84%)	0.14	4 (1%) 72 60	48, 69, 112, 121	0
7	U	243/288 (84%)	0.24	13 (5%) 26 15	50, 70, 112, 121	0
8	H	196/196 (100%)	0.01	5 (2%) 56 42	46, 66, 91, 98	0
8	V	196/196 (100%)	0.06	6 (3%) 49 34	46, 66, 91, 98	0
9	I	222/222 (100%)	-0.09	4 (1%) 68 56	40, 60, 84, 128	0
9	W	222/222 (100%)	-0.02	5 (2%) 60 48	39, 59, 84, 127	0
10	J	204/205 (99%)	-0.40	2 (0%) 82 73	28, 43, 63, 76	0
10	X	204/205 (99%)	-0.39	1 (0%) 91 86	27, 43, 62, 76	0
11	K	198/198 (100%)	-0.24	5 (2%) 57 44	23, 40, 61, 126	0
11	Y	198/198 (100%)	-0.35	3 (1%) 73 62	24, 41, 62, 126	0
12	L	212/212 (100%)	-0.40	0 100 100	17, 37, 55, 72	0
12	Z	212/212 (100%)	-0.50	0 100 100	18, 38, 54, 70	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	222/222 (100%)	-0.31	1 (0%) 91 86	24, 47, 65, 80	0
13	a	222/222 (100%)	-0.28	1 (0%) 91 86	24, 48, 66, 80	0
14	N	233/233 (100%)	-0.12	2 (0%) 84 76	34, 60, 87, 98	0
14	b	233/233 (100%)	0.02	7 (3%) 50 36	36, 61, 87, 98	0
15	c	195/231 (84%)	0.30	8 (4%) 37 25	46, 79, 110, 123	0
15	d	195/231 (84%)	0.15	6 (3%) 49 34	46, 75, 109, 125	0
15	e	195/231 (84%)	0.19	11 (5%) 24 14	40, 70, 104, 122	0
15	f	195/231 (84%)	-0.02	2 (1%) 82 73	38, 69, 103, 130	0
15	g	195/231 (84%)	0.12	7 (3%) 42 29	47, 75, 110, 159	0
15	h	195/231 (84%)	0.48	12 (6%) 20 12	55, 85, 119, 168	0
15	i	192/231 (83%)	0.55	16 (8%) 11 6	56, 86, 112, 159	1 (0%)
15	j	195/231 (84%)	0.49	12 (6%) 20 12	61, 96, 124, 134	0
15	k	195/231 (84%)	0.59	22 (11%) 5 3	66, 100, 130, 138	0
15	l	195/231 (84%)	0.46	15 (7%) 13 7	64, 98, 127, 136	0
15	m	195/231 (84%)	0.32	14 (7%) 15 9	56, 96, 129, 140	0
15	n	195/231 (84%)	0.37	19 (9%) 7 5	58, 92, 130, 169	0
15	o	195/231 (84%)	0.37	16 (8%) 11 7	64, 93, 122, 167	0
15	p	192/231 (83%)	0.41	8 (4%) 36 24	57, 93, 119, 165	1 (0%)
All	All	9094/9802 (92%)	0.06	323 (3%) 42 29	17, 66, 113, 169	2 (0%)

All (323) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	p	1231	SER	9.4
15	h	1227	ASP	8.5
3	Q	245	THR	8.5
15	h	1231	SER	7.0
3	Q	244	ILE	6.9
3	C	245	THR	6.4
5	S	126	GLY	6.3
15	j	1002	PRO	5.9
5	S	129	GLY	5.9
5	S	125	GLU	5.8
15	h	1226	SER	5.7
15	o	1231	SER	5.3
5	S	128	SER	5.2

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Mol	Chain	Res	Type	RSRZ
15	i	1231	SER	5.2
5	E	128	SER	5.2
4	D	52	LEU	5.2
15	p	1227	ASP	5.1
15	p	1229	MET	5.1
15	c	1159	LEU	5.1
11	K	196	GLN	5.1
15	l	1179	LEU	5.0
5	S	250	GLU	4.9
15	m	1055	TYR	4.9
15	n	1157	ASP	4.7
15	i	1229	MET	4.7
1	A	251	GLN	4.6
15	m	1159	LEU	4.6
15	i	1228	HIS	4.6
11	Y	198	GLN	4.6
15	k	1055	TYR	4.5
15	o	1227	ASP	4.5
11	K	198	GLN	4.5
8	V	11	GLY	4.5
4	R	51	THR	4.4
15	m	1227	ASP	4.4
5	E	124	GLY	4.4
15	p	1228	HIS	4.4
15	k	1002	PRO	4.4
15	o	1226	SER	4.3
5	E	247	GLU	4.3
15	o	1229	MET	4.3
15	o	1228	HIS	4.3
15	l	1055	TYR	4.2
7	U	5	THR	4.2
15	p	1230	VAL	4.2
1	O	252	ASP	4.2
15	k	1182	GLU	4.2
15	k	1159	LEU	4.2
15	o	1159	LEU	4.1
14	b	1	THR	4.1
15	h	1228	HIS	4.1
15	k	1057	ARG	4.1
15	f	1227	ASP	4.1
5	E	127	ALA	4.1
8	V	10	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
5	S	127	ALA	4.0
15	l	1177	PRO	4.0
15	g	1231	SER	4.0
15	n	1159	LEU	3.9
15	i	1055	TYR	3.9
15	m	1231	SER	3.9
15	d	1159	LEU	3.8
5	E	125	GLU	3.8
15	m	1179	LEU	3.8
4	D	51	THR	3.7
2	P	249	ALA	3.7
15	k	1152	ARG	3.7
2	B	52	SER	3.7
15	n	1002	PRO	3.7
15	n	1231	SER	3.6
15	k	1060	ALA	3.6
15	k	1056	GLY	3.6
1	O	249	ALA	3.5
15	j	1055	TYR	3.5
15	c	1231	SER	3.5
15	o	1230	VAL	3.5
3	Q	42	ASP	3.5
6	T	1	MET	3.5
8	H	11	GLY	3.5
15	h	1230	VAL	3.5
15	m	1183	LEU	3.4
8	H	10	ASP	3.4
11	K	197	ALA	3.4
15	i	1179	LEU	3.4
15	h	1159	LEU	3.3
9	W	222	ASP	3.3
15	i	1227	ASP	3.3
7	U	201	LEU	3.3
11	Y	196	GLN	3.3
15	o	1002	PRO	3.3
15	o	1183	LEU	3.2
15	g	1227	ASP	3.2
15	g	1157	ASP	3.2
14	N	203	ASN	3.2
15	m	1057	ARG	3.2
15	h	1002	PRO	3.2
5	S	131	GLU	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	R	52	LEU	3.2
7	G	186	LEU	3.2
8	H	8	PHE	3.2
15	n	1228	HIS	3.2
3	C	219	GLY	3.2
3	Q	41	SER	3.1
7	U	205	ASP	3.1
5	E	244	LYS	3.1
2	P	39	ALA	3.1
4	D	242	GLU	3.1
15	n	1226	SER	3.1
15	h	1158	LYS	3.1
3	Q	221	ASN	3.1
15	d	1063	SER	3.1
15	n	1158	LYS	3.1
15	n	1229	MET	3.1
9	W	219	ASN	3.0
7	U	220	LEU	3.0
9	I	221	CYS	3.0
15	k	1071	LEU	3.0
5	S	130	GLU	3.0
15	n	1053	SER	3.0
5	E	240	ILE	3.0
7	G	207	LYS	3.0
15	l	1157	ASP	3.0
15	h	1055	TYR	3.0
15	l	1231	SER	3.0
5	E	129	GLY	3.0
3	Q	205	ALA	3.0
14	N	1	THR	3.0
1	A	252	ASP	2.9
3	Q	204	SER	2.9
4	R	205	THR	2.9
15	e	1158	LYS	2.9
15	e	1157	ASP	2.9
7	U	184	GLU	2.9
15	c	1179	LEU	2.9
15	i	1159	LEU	2.9
15	n	1155	VAL	2.9
15	j	1157	ASP	2.9
15	d	1180	LEU	2.8
3	Q	184	MET	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	50	CYS	2.8
5	S	132	ARG	2.8
15	m	1158	LYS	2.8
15	c	1052	ASN	2.8
8	H	9	LYS	2.8
8	V	9	LYS	2.8
15	i	1003	PRO	2.8
15	k	1143	TYR	2.8
15	o	1055	TYR	2.8
15	p	1159	LEU	2.8
15	e	1055	TYR	2.8
15	m	1061	GLU	2.8
15	k	1231	SER	2.8
9	W	220	ILE	2.7
5	S	124	GLY	2.7
15	h	1229	MET	2.7
15	j	1180	LEU	2.7
7	U	44	GLY	2.7
15	m	1178	SER	2.7
4	R	40	ASN	2.7
15	l	1003	PRO	2.7
8	V	8	PHE	2.7
15	k	1158	LYS	2.7
2	P	250	LEU	2.7
15	e	1231	SER	2.7
2	B	247	LEU	2.7
15	g	1063	SER	2.7
14	b	18	ASN	2.7
15	e	1002	PRO	2.7
3	C	220	ALA	2.7
5	E	131	GLU	2.7
15	k	1061	GLU	2.7
15	j	1067	LEU	2.7
1	O	189	SER	2.7
9	W	221	CYS	2.7
1	A	222	ASP	2.7
3	C	60	ASP	2.7
15	e	1159	LEU	2.7
13	a	1	GLN	2.7
15	i	1157	ASP	2.6
15	l	1149	LEU	2.6
4	R	236	ILE	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	214	LEU	2.6
1	A	213	ALA	2.6
7	U	207	LYS	2.6
15	f	1159	LEU	2.6
15	g	1159	LEU	2.6
1	O	39	ASN	2.6
15	i	1230	VAL	2.6
15	h	1050	ILE	2.6
15	l	1050	ILE	2.6
11	K	195	PHE	2.6
15	d	1181	LEU	2.6
7	U	246	ILE	2.5
15	p	1002	PRO	2.5
15	n	1060	ALA	2.5
15	l	1180	LEU	2.5
11	Y	197	ALA	2.5
15	n	1182	GLU	2.5
15	d	1179	LEU	2.5
2	P	208	THR	2.5
5	E	207	VAL	2.5
15	j	1047	HIS	2.5
15	k	1181	LEU	2.5
15	c	1063	SER	2.5
15	i	1002	PRO	2.5
15	g	1228	HIS	2.5
1	A	197	GLU	2.5
15	k	1183	LEU	2.5
15	j	1061	GLU	2.5
9	W	218	VAL	2.5
2	P	247	LEU	2.5
14	b	202	LYS	2.5
15	k	1016	TYR	2.5
4	D	241	GLN	2.5
1	O	218	PHE	2.4
7	U	217	TRP	2.4
3	Q	220	ALA	2.4
10	J	191	LYS	2.4
15	c	1062	LYS	2.4
15	l	1159	LEU	2.4
7	G	244	LYS	2.4
15	m	1228	HIS	2.4
15	o	1157	ASP	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	P	216	ASP	2.4
15	n	1227	ASP	2.4
1	A	198	SER	2.4
15	j	1147	GLU	2.4
5	E	132	ARG	2.4
2	B	178	ARG	2.4
4	R	60	THR	2.4
14	b	16	TYR	2.4
15	e	1061	GLU	2.4
15	m	1187	ASP	2.4
15	e	1179	LEU	2.4
15	i	1178	SER	2.4
15	c	1067	LEU	2.4
2	B	177	LYS	2.4
15	i	1182	GLU	2.4
4	R	241	GLN	2.3
10	X	194	VAL	2.3
9	I	175	VAL	2.3
15	i	1057	ARG	2.3
5	E	133	LEU	2.3
2	B	206	GLY	2.3
6	F	1	MET	2.3
15	o	1143	TYR	2.3
15	e	1056	GLY	2.3
2	B	201	GLU	2.3
15	m	1064	PRO	2.3
2	B	250	LEU	2.3
15	l	1187	ASP	2.3
15	h	1011	ASN	2.3
15	k	1058	ALA	2.3
15	n	1057	ARG	2.3
1	O	217	GLU	2.3
5	E	130	GLU	2.3
8	V	179	THR	2.3
15	k	1227	ASP	2.3
15	j	1091	VAL	2.3
4	D	124	GLY	2.3
14	b	201	ASP	2.3
2	P	201	GLU	2.2
15	m	1182	GLU	2.2
9	I	222	ASP	2.2
5	S	249	ALA	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
15	l	1058	ALA	2.2
15	o	1178	SER	2.2
15	l	1185	GLN	2.2
15	k	1179	LEU	2.2
10	J	18	ASP	2.2
2	P	219	PRO	2.2
15	o	1152	ARG	2.2
15	k	1157	ASP	2.2
15	i	1183	LEU	2.2
8	H	12	VAL	2.2
15	g	1055	TYR	2.2
11	K	194	ASP	2.2
7	U	187	SER	2.2
15	k	1063	SER	2.2
14	b	47	ASP	2.2
3	C	236	LYS	2.2
15	k	1059	GLN	2.2
15	l	1184	ARG	2.2
8	V	182	GLY	2.2
7	U	174	GLU	2.2
1	O	188	LYS	2.2
5	S	212	LEU	2.2
13	M	1	GLN	2.2
7	G	185	GLY	2.2
5	E	126	GLY	2.1
15	n	1183	LEU	2.1
9	I	182	LYS	2.1
15	o	1003	PRO	2.1
15	o	1158	LYS	2.1
3	Q	56	LEU	2.1
7	U	238	ALA	2.1
15	e	1228	HIS	2.1
1	O	191	ILE	2.1
15	j	1068	LEU	2.1
5	S	248	ALA	2.1
15	j	1158	LYS	2.1
1	O	195	ASN	2.1
1	O	198	SER	2.1
15	c	1182	GLU	2.1
15	e	1183	LEU	2.1
2	B	174	PHE	2.1
15	n	1189	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
15	n	1156	GLU	2.1
15	l	1057	ARG	2.1
1	A	215	GLY	2.1
6	T	42	THR	2.1
1	O	194	ILE	2.1
1	A	168	ALA	2.1
5	E	248	ALA	2.1
7	U	242	ALA	2.1
15	p	1003	PRO	2.1
15	i	1036	ILE	2.0
15	d	1187	ASP	2.0
15	n	1063	SER	2.0
2	P	52	SER	2.0
14	b	198	ALA	2.0
15	j	1074	TYR	2.0
15	n	1003	PRO	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.