



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2018 – 02:38 pm GMT

PDB ID : 1G0U  
Title : A GATED CHANNEL INTO THE PROTEASOME CORE PARTICLE  
Authors : Groll, M.; Bajorek, M.; Kohler, A.; Moroder, L.; Rubin, D.M.; Huber, R.;  
Glickman, M.H.; Finley, D.  
Deposited on : 2000-10-09  
Resolution : 2.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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.

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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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30686

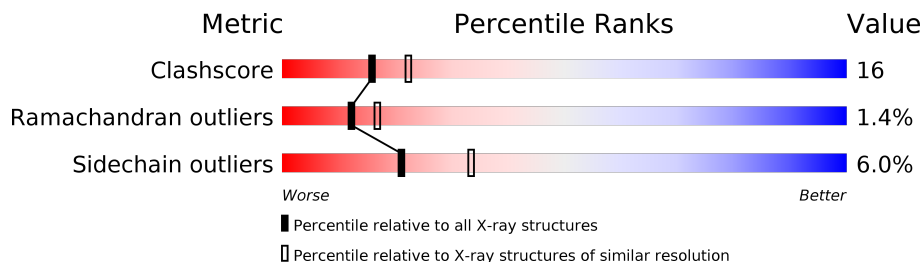
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
Clashscore	122078	3953 (2.40-2.40)
Ramachandran outliers	120005	3894 (2.40-2.40)
Sidechain outliers	119972	3895 (2.40-2.40)











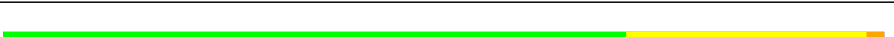

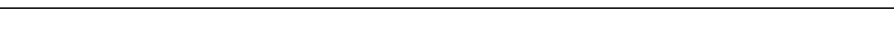
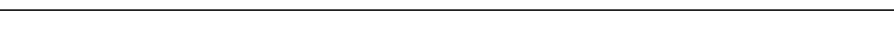
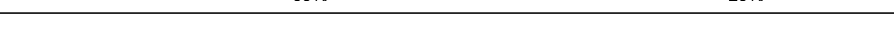
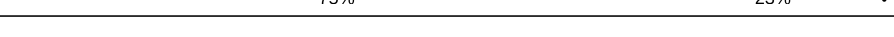

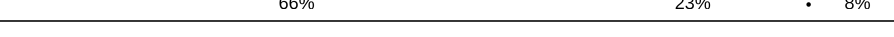


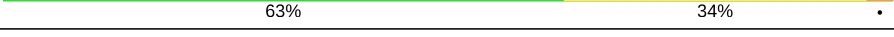
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	250	
1	O	250	
2	B	245	
2	P	245	
3	C	243	
3	Q	243	
4	D	241	

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Mol	Chain	Length	Quality of chain
4	R	241	
5	E	234	
5	S	234	
6	F	248	
6	T	248	
7	G	252	
7	U	252	
8	H	222	
8	V	222	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	241	
12	Z	241	
13	1	266	
13	M	266	
14	2	196	
14	N	196	

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 51834 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 Y7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	0	0	0
			1881	1200	308	370	3			
1	O	246	Total	C	N	O	S	0	0	0
			1881	1200	308	370	3			

- Molecule 2 is a protein called PROTEASOME COMPONENT Y13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	235	Total	C	N	O	S	0	0	0
			1827	1157	303	364	3			
2	P	235	Total	C	N	O	S	0	0	0
			1827	1157	303	364	3			

- Molecule 3 is a protein called PROTEASOME COMPONENT PRE6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	238	Total	C	N	O	S	0	0	0
			1861	1163	325	369	4			
3	Q	238	Total	C	N	O	S	0	0	0
			1861	1163	325	369	4			

- Molecule 4 is a protein called PROTEASOME COMPONENT PUP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	230	Total	C	N	O	S	0	0	0
			1758	1100	293	358	7			
4	R	230	Total	C	N	O	S	0	0	0
			1758	1100	293	358	7			

- Molecule 5 is a protein called PROTEASOME COMPONENT PRE5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	230	Total	C	N	O	S	0	0	0
			1755	1103	304	344	4			
5	S	230	Total	C	N	O	S	0	0	0
			1755	1103	304	344	4			

- Molecule 6 is a protein called PROTEASOME COMPONENT C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	242	Total	C	N	O	S	0	0	0
			1886	1199	328	355	4			
6	T	242	Total	C	N	O	S	0	0	0
			1886	1199	328	355	4			

- Molecule 7 is a protein called PROTEASOME COMPONENT C7-ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	240	Total	C	N	O	S	0	0	0
			1897	1206	319	364	8			
7	U	240	Total	C	N	O	S	0	0	0
			1897	1206	319	364	8			

- Molecule 8 is a protein called PROTEASOME COMPONENT PUP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			
8	V	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			

- Molecule 9 is a protein called PROTEASOME COMPONENT PUP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			
9	W	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

- Molecule 10 is a protein called PROTEASOME COMPONENT C11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

- Molecule 11 is a protein called PROTEASOME COMPONENT PRE2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			

- Molecule 12 is a protein called PROTEASOME COMPONENT C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
12	Z	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

- Molecule 13 is a protein called PROTEASOME COMPONENT PRE4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	1	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

- Molecule 14 is a protein called PROTEASOME COMPONENT PRE3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
14	2	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	G	2	Total	Mg	0	0
			2	2		
15	K	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	H	1	Total 1	Mg 1	0	0
15	I	2	Total 2	Mg 2	0	0
15	V	1	Total 1	Mg 1	0	0
15	W	2	Total 2	Mg 2	0	0
15	Z	2	Total 2	Mg 2	0	0
15	T	1	Total 1	Mg 1	0	0
15	N	1	Total 1	Mg 1	0	0
15	U	2	Total 2	Mg 2	0	0
15	2	1	Total 1	Mg 1	0	0
15	Y	1	Total 1	Mg 1	0	0
15	L	2	Total 2	Mg 2	0	0
15	F	1	Total 1	Mg 1	0	0

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	102	Total 102	O 102	0	0
16	B	74	Total 74	O 74	0	0
16	C	73	Total 73	O 73	0	0
16	D	82	Total 82	O 82	0	0
16	E	63	Total 63	O 63	0	0
16	F	97	Total 97	O 97	0	0
16	G	110	Total 110	O 110	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	H	132	Total 132	O 132	0	0
16	I	107	Total 107	O 107	0	0
16	J	107	Total 107	O 107	0	0
16	K	107	Total 107	O 107	0	0
16	L	141	Total 141	O 141	0	0
16	M	151	Total 151	O 151	0	0
16	N	115	Total 115	O 115	0	0
16	O	98	Total 98	O 98	0	0
16	P	78	Total 78	O 78	0	0
16	Q	62	Total 62	O 62	0	0
16	R	79	Total 79	O 79	0	0
16	S	66	Total 66	O 66	0	0
16	T	94	Total 94	O 94	0	0
16	U	110	Total 110	O 110	0	0
16	V	131	Total 131	O 131	0	0
16	W	114	Total 114	O 114	0	0
16	X	110	Total 110	O 110	0	0
16	Y	104	Total 104	O 104	0	0
16	Z	137	Total 137	O 137	0	0
16	1	151	Total 151	O 151	0	0
16	2	113	Total 113	O 113	0	0

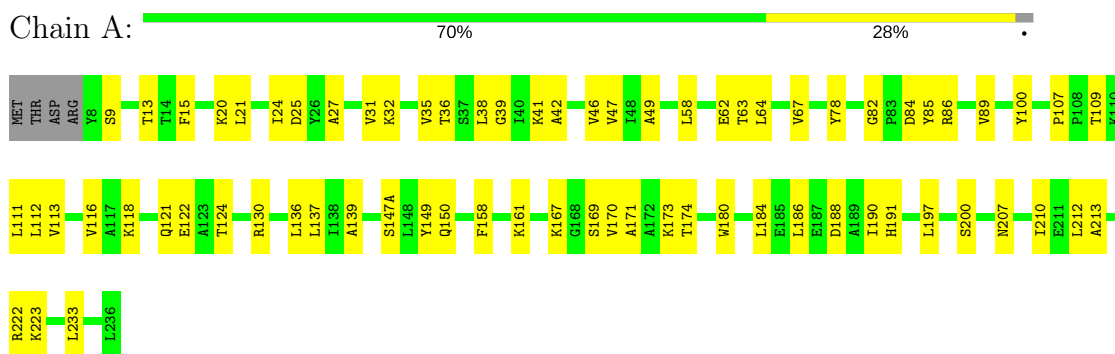


### 3 Residue-property plots

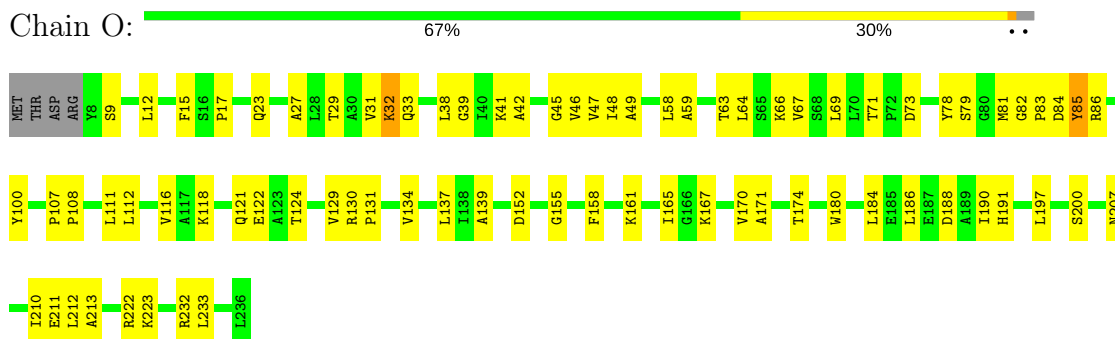
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

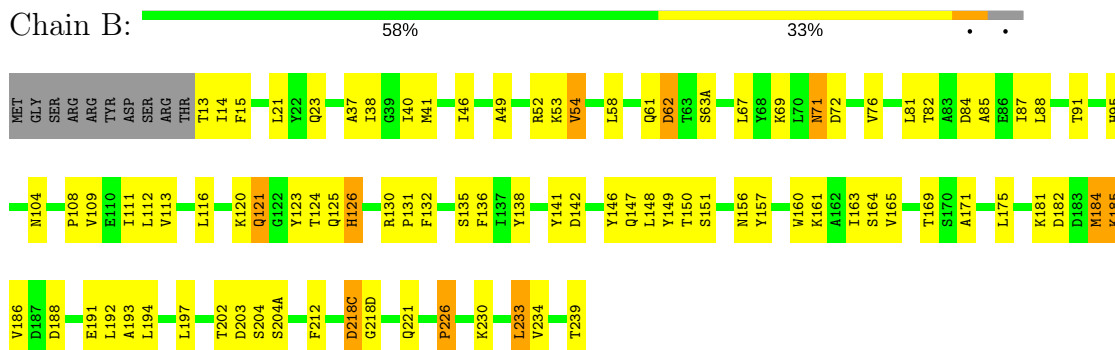
#### • Molecule 1: PROTEASOME COMPONENT Y7



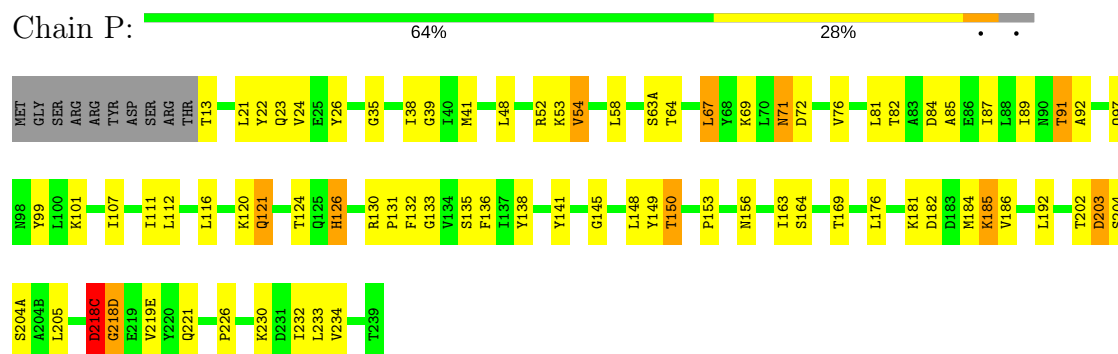
#### • Molecule 1: PROTEASOME COMPONENT Y7



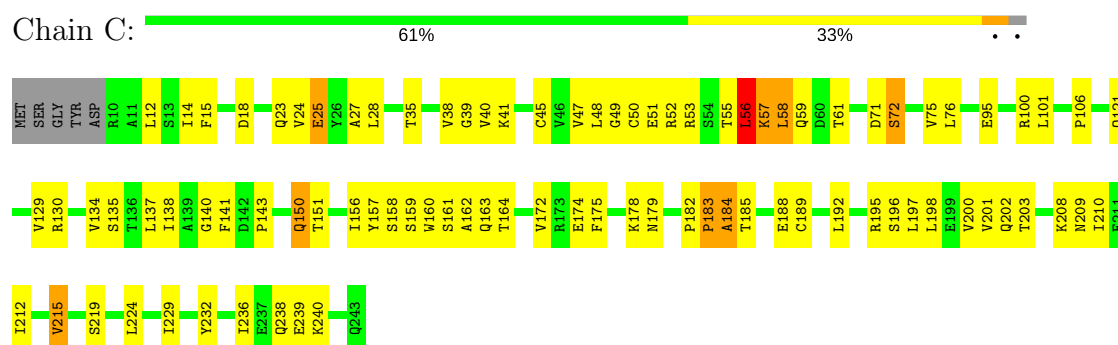
#### • Molecule 2: PROTEASOME COMPONENT Y13



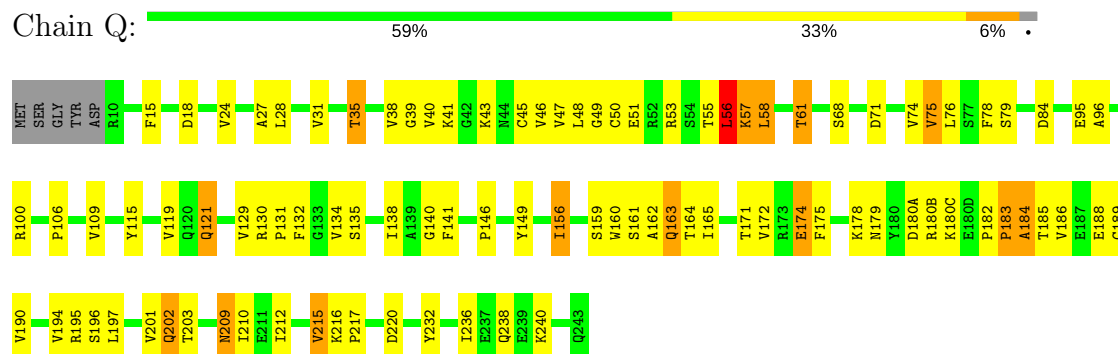
- Molecule 2: PROTEASOME COMPONENT Y13



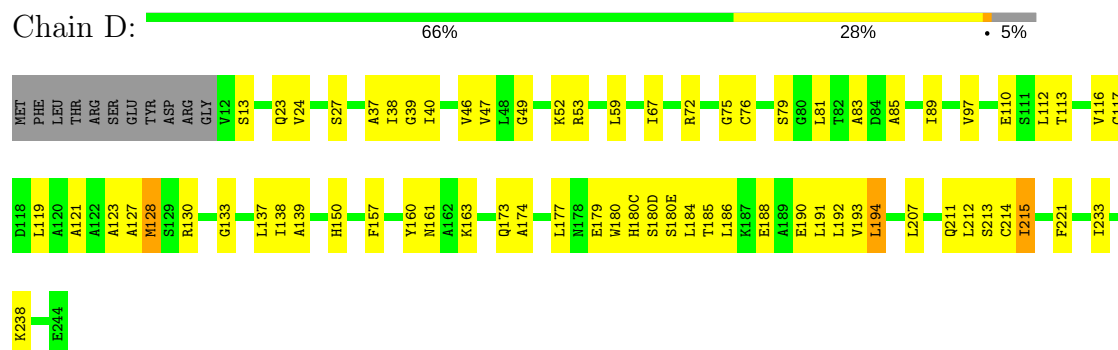
- Molecule 3: PROTEASOME COMPONENT PRE6



- Molecule 3: PROTEASOME COMPONENT PRE6



- Molecule 4: PROTEASOME COMPONENT PUP2



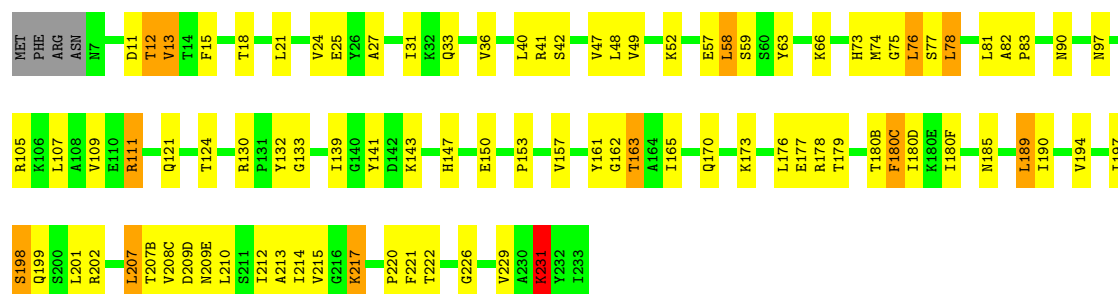
- Molecule 4: PROTEASOME COMPONENT PUP2

Chain R: 



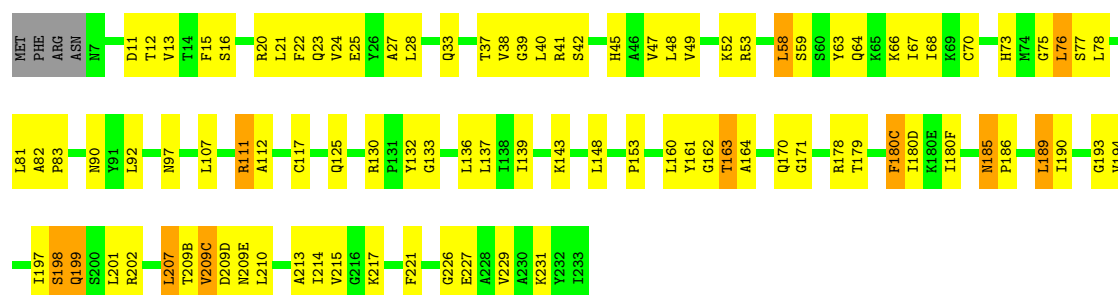
- Molecule 5: PROTEASOME COMPONENT PRE5

Chain E: 



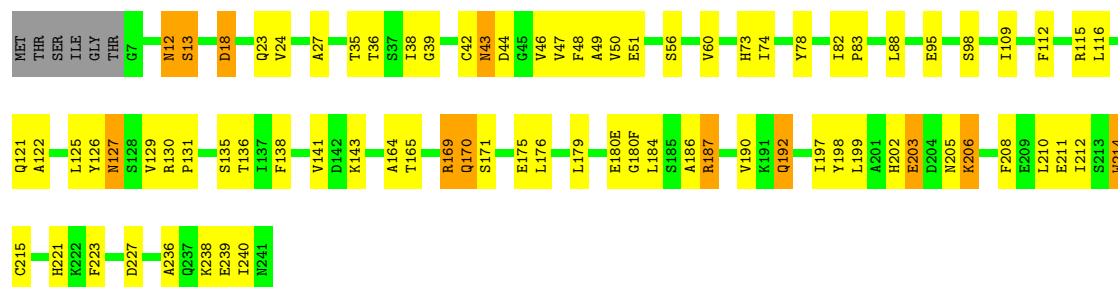
- Molecule 5: PROTEASOME COMPONENT PRE5

Chain S: 

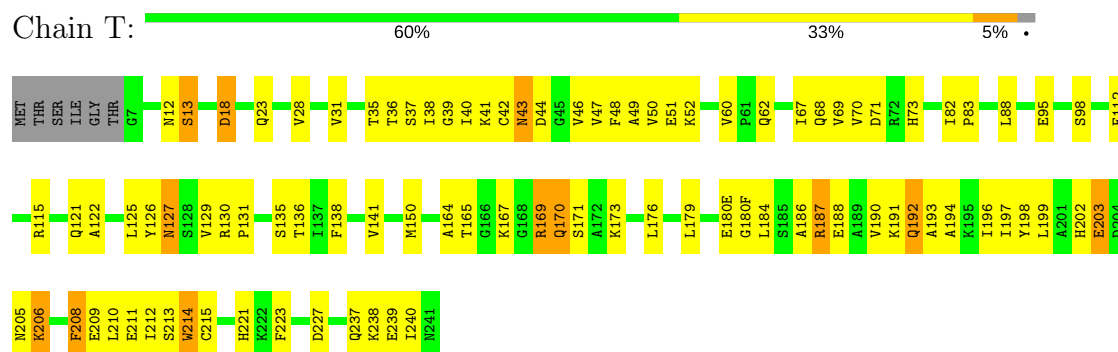


- Molecule 6: PROTEASOME COMPONENT C1

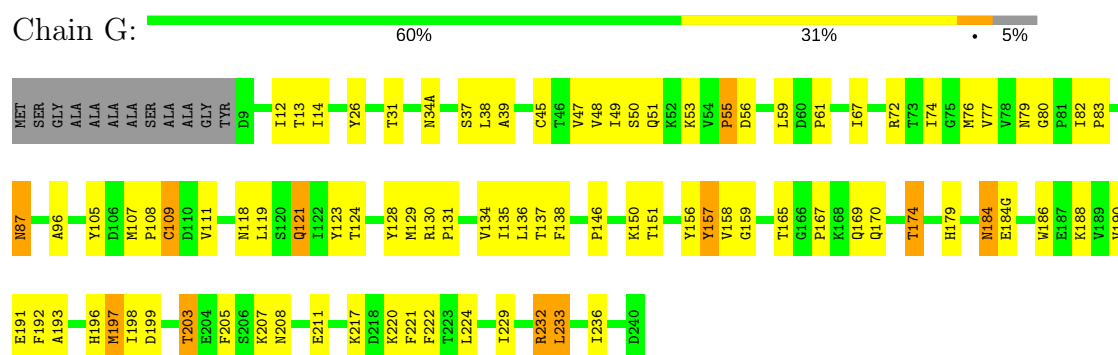
Chain F: 



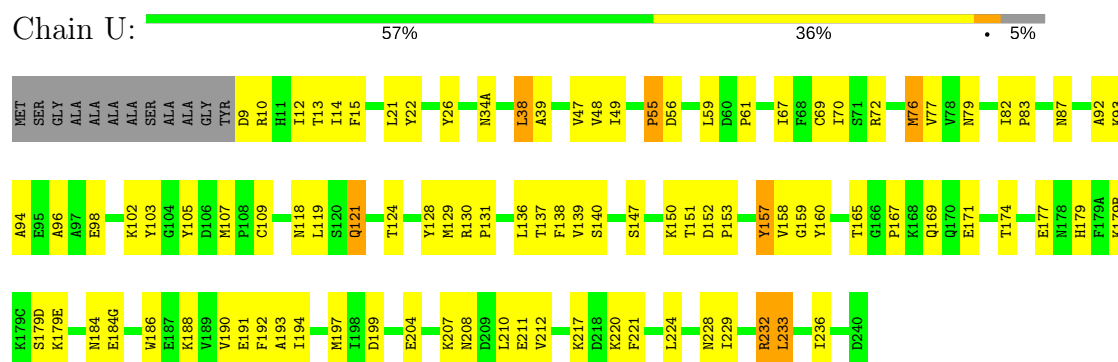
- Molecule 6: PROTEASOME COMPONENT C1



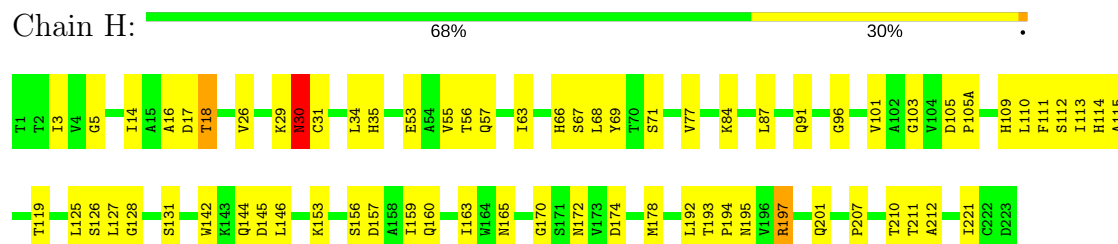
- Molecule 7: PROTEASOME COMPONENT C7-ALPHA



- Molecule 7: PROTEASOME COMPONENT C7-ALPHA

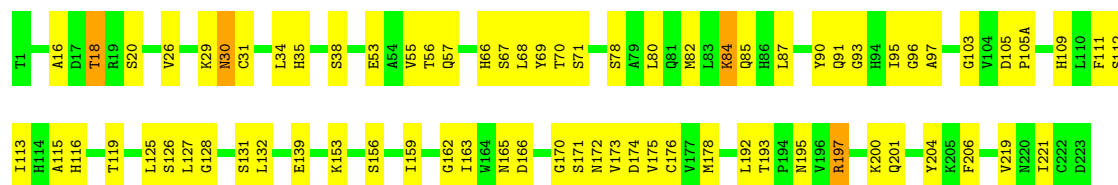


- Molecule 8: PROTEASOME COMPONENT PUP1



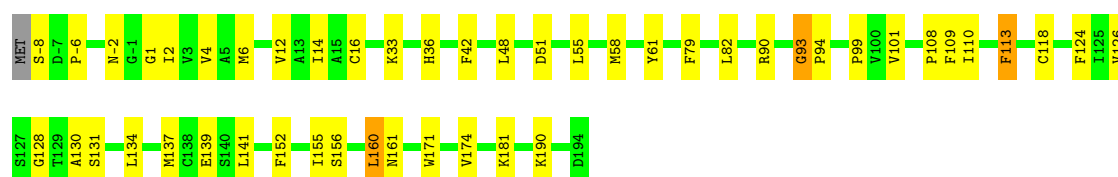
- Molecule 8: PROTEASOME COMPONENT PUP1

Chain V:  67% 32% .



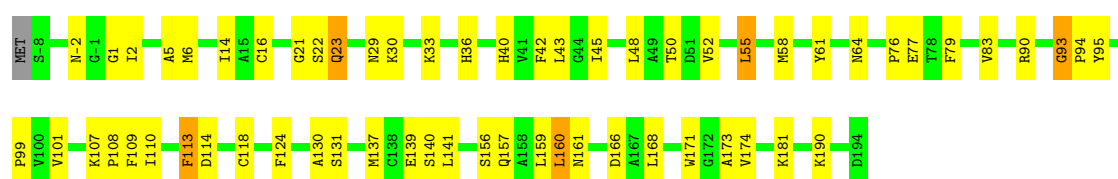
• Molecule 9: PROTEASOME COMPONENT PUP3

Chain I:  76% 22% .



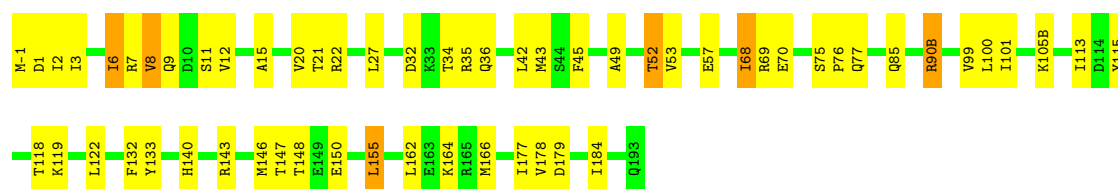
• Molecule 9: PROTEASOME COMPONENT PUP3

Chain W:  70% 27% .



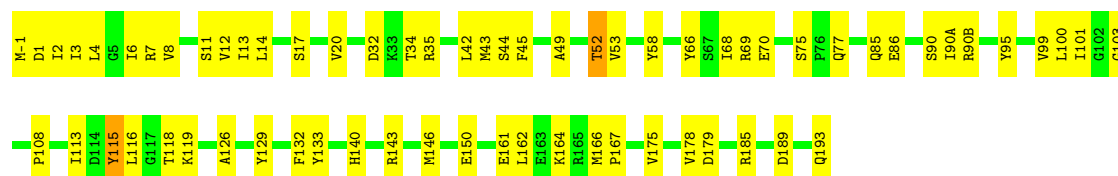
• Molecule 10: PROTEASOME COMPONENT C11

Chain J:  70% 27% .



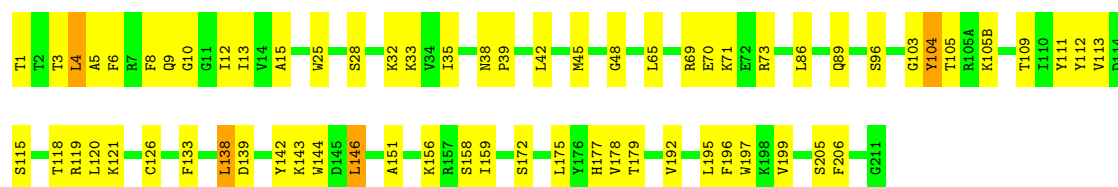
• Molecule 10: PROTEASOME COMPONENT C11

Chain X:  67% 32% .



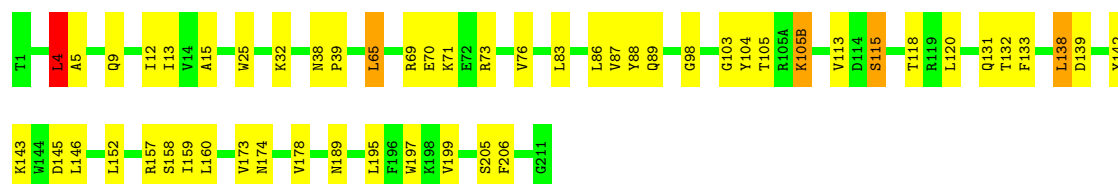
• Molecule 11: PROTEASOME COMPONENT PRE2

Chain K:  69% 29% .



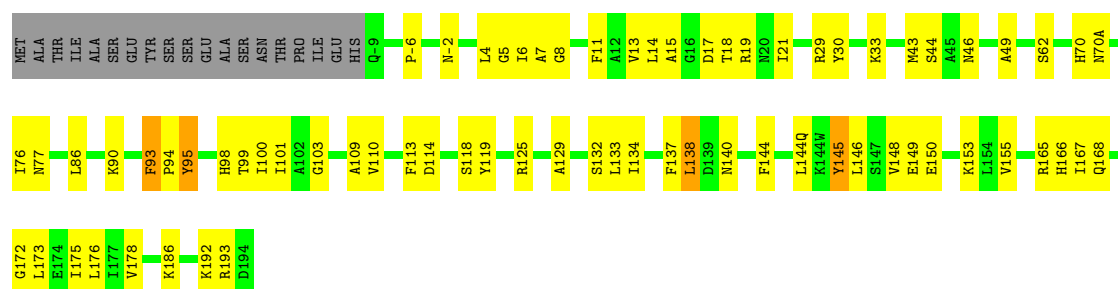
• Molecule 11: PROTEASOME COMPONENT PRE2

Chain Y: 75% 23%



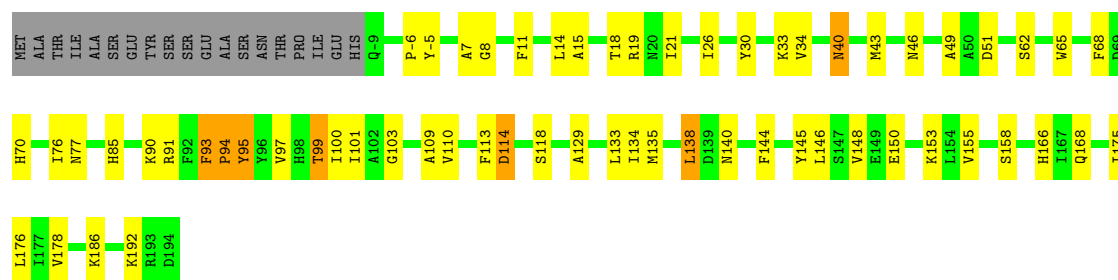
• Molecule 12: PROTEASOME COMPONENT C5

Chain L: 62% 28% 8%



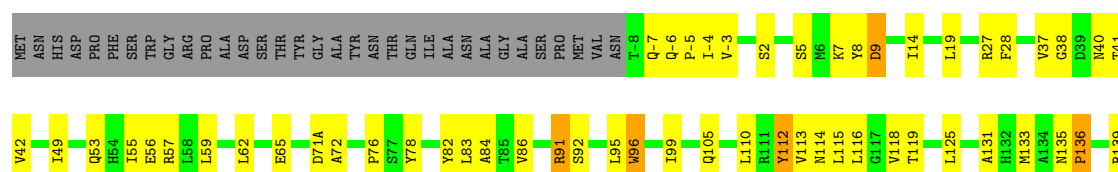
• Molecule 12: PROTEASOME COMPONENT C5

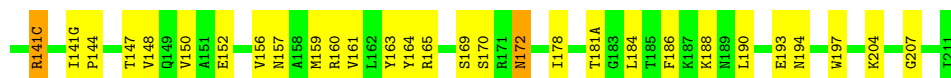
Chain Z: 66% 23% 8%



• Molecule 13: PROTEASOME COMPONENT PRE4

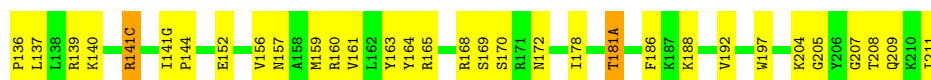
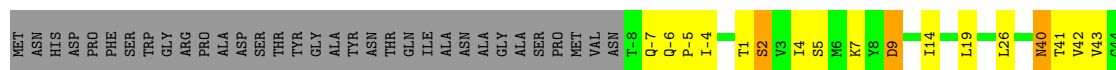
Chain M: 56% 29% 12%





• Molecule 13: PROTEASOME COMPONENT PRE4

Chain 1: 55% 30% 12%



• Molecule 14: PROTEASOME COMPONENT PRE3

Chain N: 70% 29%



• Molecule 14: PROTEASOME COMPONENT PRE3

Chain 2: 63% 34%



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.18Å 301.10Å 144.10Å 90.00° 113.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.40)	Depositor
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.250 , 0.303	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	51834	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP



## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.62	0/1918	0.78	1/2597 (0.0%)
1	O	0.58	0/1918	0.78	1/2597 (0.0%)
2	B	0.58	0/1856	0.75	0/2513
2	P	0.61	0/1856	0.76	0/2513
3	C	0.58	0/1889	0.75	1/2557 (0.0%)
3	Q	0.61	0/1889	0.77	1/2557 (0.0%)
4	D	0.63	0/1782	0.83	2/2404 (0.1%)
4	R	0.64	0/1782	0.81	2/2404 (0.1%)
5	E	0.52	0/1781	0.73	0/2407
5	S	0.54	0/1781	0.73	0/2407
6	F	0.56	0/1926	0.75	0/2599
6	T	0.60	0/1926	0.79	0/2599
7	G	0.61	0/1934	0.75	0/2618
7	U	0.62	0/1934	0.77	0/2618
8	H	0.61	0/1716	0.78	0/2326
8	V	0.61	0/1716	0.78	0/2326
9	I	0.64	0/1611	0.79	0/2174
9	W	0.67	0/1611	0.82	0/2174
10	J	0.61	0/1613	0.79	0/2173
10	X	0.64	0/1613	0.79	0/2173
11	K	0.62	0/1681	0.80	0/2274
11	Y	0.61	0/1681	0.78	2/2274 (0.1%)
12	L	0.63	0/1795	0.79	2/2420 (0.1%)
12	Z	0.63	0/1795	0.78	1/2420 (0.0%)
13	1	0.66	0/1855	0.82	1/2514 (0.0%)
13	M	0.63	0/1855	0.79	1/2514 (0.0%)
14	2	0.66	0/1541	0.78	0/2087
14	N	0.65	0/1541	0.78	0/2087
All	All	0.61	0/49796	0.78	15/67326 (0.0%)

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	O	0	1
12	L	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	128	MET	N-CA-C	-6.85	92.50	111.00
11	Y	4	LEU	CA-CB-CG	6.44	130.12	115.30
4	D	128	MET	N-CA-C	-6.08	94.59	111.00
13	M	95	LEU	N-CA-C	-5.95	94.93	111.00
12	L	95	TYR	N-CA-C	-5.92	95.03	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	L	145	TYR	Sidechain
1	O	85	TYR	Sidechain

## 5.2 Too-close contacts ⓘ

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	A	1881	0	1893	50	0
1	O	1881	0	1893	61	0
2	B	1827	0	1824	67	0
2	P	1827	0	1824	58	0
3	C	1861	0	1873	79	0
3	Q	1861	0	1873	82	0
4	D	1758	0	1735	62	0
4	R	1758	0	1735	65	0
5	E	1755	0	1761	73	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	S	1755	0	1761	84	0
6	F	1886	0	1876	61	0
6	T	1886	0	1876	74	0
7	G	1897	0	1891	75	0
7	U	1897	0	1891	76	0
8	H	1685	0	1688	49	0
8	V	1685	0	1688	54	0
9	I	1581	0	1574	33	0
9	W	1581	0	1574	43	0
10	J	1585	0	1590	46	0
10	X	1585	0	1590	52	0
11	K	1644	0	1595	51	0
11	Y	1644	0	1595	38	0
12	L	1757	0	1711	62	0
12	Z	1757	0	1711	56	0
13	1	1824	0	1832	70	0
13	M	1824	0	1832	57	0
14	2	1512	0	1481	52	0
14	N	1512	0	1481	43	0
15	2	1	0	0	0	0
15	F	1	0	0	0	0
15	G	2	0	0	0	0
15	H	1	0	0	0	0
15	I	2	0	0	0	0
15	K	1	0	0	0	0
15	L	2	0	0	0	0
15	N	1	0	0	0	0
15	T	1	0	0	0	0
15	U	2	0	0	0	0
15	V	1	0	0	0	0
15	W	2	0	0	0	0
15	Y	1	0	0	0	0
15	Z	2	0	0	0	0
16	1	151	0	0	5	0
16	2	113	0	0	1	0
16	A	102	0	0	2	0
16	B	74	0	0	3	0
16	C	73	0	0	0	0
16	D	82	0	0	2	0
16	E	63	0	0	2	0
16	F	97	0	0	0	0
16	G	110	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	H	132	0	0	2	0
16	I	107	0	0	1	0
16	J	107	0	0	3	0
16	K	107	0	0	2	0
16	L	141	0	0	4	0
16	M	151	0	0	3	0
16	N	115	0	0	1	0
16	O	98	0	0	4	0
16	P	78	0	0	2	0
16	Q	62	0	0	2	0
16	R	79	0	0	4	0
16	S	66	0	0	3	0
16	T	94	0	0	1	0
16	U	110	0	0	2	0
16	V	131	0	0	1	0
16	W	114	0	0	2	0
16	X	110	0	0	4	0
16	Y	104	0	0	2	0
16	Z	137	0	0	4	0
All	All	51834	0	48648	1521	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 16.

The worst 5 of 1521 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:G:151:THR:HG22	7:G:157:TYR:HB2	1.28	1.09
7:G:96:ALA:HA	7:G:107:MET:HE2	1.36	1.03
3:C:163:GLN:HE21	3:C:164:THR:H	1.09	1.01
3:Q:163:GLN:HE21	3:Q:164:THR:H	1.10	0.99
10:J:113:ILE:HG12	10:J:119:LYS:HG3	1.48	0.95

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	244/250 (98%)	225 (92%)	17 (7%)	2 (1%)	21	31
1	O	244/250 (98%)	225 (92%)	17 (7%)	2 (1%)	21	31
2	B	233/245 (95%)	209 (90%)	18 (8%)	6 (3%)	6	5
2	P	233/245 (95%)	212 (91%)	14 (6%)	7 (3%)	5	4
3	C	236/243 (97%)	210 (89%)	20 (8%)	6 (2%)	6	6
3	Q	236/243 (97%)	211 (89%)	18 (8%)	7 (3%)	5	4
4	D	228/241 (95%)	205 (90%)	21 (9%)	2 (1%)	19	27
4	R	228/241 (95%)	204 (90%)	20 (9%)	4 (2%)	9	11
5	E	228/234 (97%)	208 (91%)	15 (7%)	5 (2%)	7	8
5	S	228/234 (97%)	203 (89%)	20 (9%)	5 (2%)	7	8
6	F	240/248 (97%)	218 (91%)	18 (8%)	4 (2%)	10	13
6	T	240/248 (97%)	214 (89%)	24 (10%)	2 (1%)	21	31
7	G	238/252 (94%)	217 (91%)	20 (8%)	1 (0%)	36	51
7	U	238/252 (94%)	222 (93%)	15 (6%)	1 (0%)	36	51
8	H	220/222 (99%)	203 (92%)	12 (6%)	5 (2%)	7	7
8	V	220/222 (99%)	206 (94%)	10 (4%)	4 (2%)	9	11
9	I	202/205 (98%)	189 (94%)	12 (6%)	1 (0%)	31	44
9	W	202/205 (98%)	190 (94%)	10 (5%)	2 (1%)	17	25
10	J	196/198 (99%)	180 (92%)	14 (7%)	2 (1%)	17	25
10	X	196/198 (99%)	183 (93%)	11 (6%)	2 (1%)	17	25
11	K	210/212 (99%)	195 (93%)	14 (7%)	1 (0%)	31	44
11	Y	210/212 (99%)	198 (94%)	11 (5%)	1 (0%)	31	44
12	L	220/241 (91%)	200 (91%)	18 (8%)	2 (1%)	19	27
12	Z	220/241 (91%)	203 (92%)	16 (7%)	1 (0%)	31	44
13	1	231/266 (87%)	208 (90%)	19 (8%)	4 (2%)	10	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	M	231/266 (87%)	210 (91%)	15 (6%)	6 (3%)	6	5
14	2	194/196 (99%)	185 (95%)	9 (5%)	0	100	100
14	N	194/196 (99%)	185 (95%)	9 (5%)	0	100	100
All	All	6240/6506 (96%)	5718 (92%)	437 (7%)	85 (1%)	12	17

5 of 85 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	LYS
2	B	54	VAL
2	B	218(C)	ASP
3	C	58	LEU
4	D	180(E)	SER

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	205/209 (98%)	198 (97%)	7 (3%)	40	60
1	O	205/209 (98%)	195 (95%)	10 (5%)	27	44
2	B	194/204 (95%)	179 (92%)	15 (8%)	14	22
2	P	194/204 (95%)	176 (91%)	18 (9%)	10	14
3	C	210/215 (98%)	196 (93%)	14 (7%)	18	28
3	Q	210/215 (98%)	197 (94%)	13 (6%)	20	32
4	D	186/197 (94%)	178 (96%)	8 (4%)	32	49
4	R	186/197 (94%)	179 (96%)	7 (4%)	36	55
5	E	187/192 (97%)	166 (89%)	21 (11%)	6	9
5	S	187/192 (97%)	168 (90%)	19 (10%)	8	11
6	F	200/205 (98%)	180 (90%)	20 (10%)	8	12
6	T	200/205 (98%)	181 (90%)	19 (10%)	9	14
7	G	205/210 (98%)	190 (93%)	15 (7%)	15	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	U	205/210 (98%)	187 (91%)	18 (9%)	11	16
8	H	181/181 (100%)	173 (96%)	8 (4%)	31	48
8	V	181/181 (100%)	173 (96%)	8 (4%)	31	48
9	I	172/173 (99%)	166 (96%)	6 (4%)	39	59
9	W	172/173 (99%)	166 (96%)	6 (4%)	39	59
10	J	175/175 (100%)	166 (95%)	9 (5%)	26	42
10	X	175/175 (100%)	167 (95%)	8 (5%)	29	46
11	K	169/169 (100%)	163 (96%)	6 (4%)	38	58
11	Y	169/169 (100%)	161 (95%)	8 (5%)	29	45
12	L	185/201 (92%)	179 (97%)	6 (3%)	42	63
12	Z	185/201 (92%)	177 (96%)	8 (4%)	32	49
13	1	199/224 (89%)	190 (96%)	9 (4%)	30	47
13	M	199/224 (89%)	188 (94%)	11 (6%)	24	37
14	2	162/162 (100%)	151 (93%)	11 (7%)	17	27
14	N	162/162 (100%)	154 (95%)	8 (5%)	27	44
All	All	5260/5434 (97%)	4944 (94%)	316 (6%)	21	33

5 of 316 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	M	141(C)	ARG
2	P	185	LYS
12	Z	99	THR
14	N	22	THR
1	O	170	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 171 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	149	GLN
4	R	23	GLN
12	Z	144(B)	ASN
14	N	38	HIS
2	P	125	GLN

### 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 20 ligands modelled in this entry, 20 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.