



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 12:08 pm BST

PDB ID : 1YA7  
Title : Implications for interactions of proteasome with PAN and PA700 from the 1.9 Å structure of a proteasome-11S activator complex  
Authors : Forster, A.; Masters, E.I.; Whitby, F.G.; Robinson, H.; Hill, C.P.  
Deposited on : 2004-12-17  
Resolution : 2.30 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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

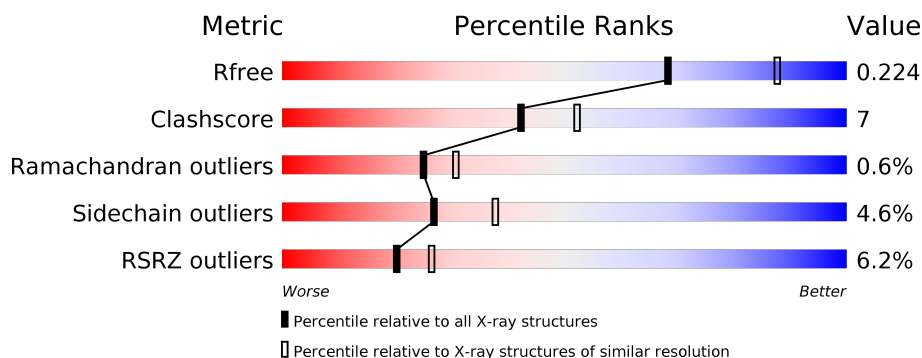
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 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	233	<div> <div>9%</div> <div>78% 16% ...</div> </div>
1	B	233	<div> <div>8%</div> <div>79% 16% ..</div> </div>
1	C	233	<div> <div>8%</div> <div>81% 13% ..</div> </div>
1	D	233	<div> <div>9%</div> <div>80% 14% ..</div> </div>
1	E	233	<div> <div>7%</div> <div>80% 14% ..</div> </div>
1	F	233	<div> <div>8%</div> <div>75% 20% ..</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	233	
2	H	217	
2	I	217	
2	J	217	
2	K	217	
2	L	217	
2	M	217	
2	N	217	
3	O	237	
3	P	237	
3	Q	237	
3	R	237	
3	S	237	
3	T	237	
3	U	237	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 37185 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 alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	2	0
			1787	1134	304	346	3			
1	B	227	Total	C	N	O	S	0	2	0
			1787	1134	304	346	3			
1	C	227	Total	C	N	O	S	0	2	0
			1787	1134	304	346	3			
1	D	227	Total	C	N	O	S	0	2	0
			1787	1134	304	346	3			
1	E	227	Total	C	N	O	S	0	2	0
			1787	1134	304	346	3			
1	F	227	Total	C	N	O	S	0	1	0
			1780	1129	303	345	3			
1	G	227	Total	C	N	O	S	0	1	0
			1780	1129	303	345	3			

- Molecule 2 is a protein called Proteasome beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	203	Total	C	N	O	S	0	4	0
			1594	1008	270	304	12			
2	I	203	Total	C	N	O	S	0	3	0
			1585	1003	268	302	12			
2	J	203	Total	C	N	O	S	0	4	0
			1591	1006	269	304	12			
2	K	203	Total	C	N	O	S	0	4	0
			1594	1008	270	304	12			
2	L	203	Total	C	N	O	S	0	4	0
			1591	1006	269	304	12			
2	M	203	Total	C	N	O	S	0	3	0
			1585	1003	268	302	12			
2	N	203	Total	C	N	O	S	0	4	0
			1591	1006	269	304	12			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	204	HIS	-	EXPRESSION TAG	UNP P28061
H	205	HIS	-	EXPRESSION TAG	UNP P28061
H	206	HIS	-	EXPRESSION TAG	UNP P28061
H	207	HIS	-	EXPRESSION TAG	UNP P28061
H	208	HIS	-	EXPRESSION TAG	UNP P28061
H	209	HIS	-	EXPRESSION TAG	UNP P28061
I	204	HIS	-	EXPRESSION TAG	UNP P28061
I	205	HIS	-	EXPRESSION TAG	UNP P28061
I	206	HIS	-	EXPRESSION TAG	UNP P28061
I	207	HIS	-	EXPRESSION TAG	UNP P28061
I	208	HIS	-	EXPRESSION TAG	UNP P28061
I	209	HIS	-	EXPRESSION TAG	UNP P28061
J	204	HIS	-	EXPRESSION TAG	UNP P28061
J	205	HIS	-	EXPRESSION TAG	UNP P28061
J	206	HIS	-	EXPRESSION TAG	UNP P28061
J	207	HIS	-	EXPRESSION TAG	UNP P28061
J	208	HIS	-	EXPRESSION TAG	UNP P28061
J	209	HIS	-	EXPRESSION TAG	UNP P28061
K	204	HIS	-	EXPRESSION TAG	UNP P28061
K	205	HIS	-	EXPRESSION TAG	UNP P28061
K	206	HIS	-	EXPRESSION TAG	UNP P28061
K	207	HIS	-	EXPRESSION TAG	UNP P28061
K	208	HIS	-	EXPRESSION TAG	UNP P28061
K	209	HIS	-	EXPRESSION TAG	UNP P28061
L	204	HIS	-	EXPRESSION TAG	UNP P28061
L	205	HIS	-	EXPRESSION TAG	UNP P28061
L	206	HIS	-	EXPRESSION TAG	UNP P28061
L	207	HIS	-	EXPRESSION TAG	UNP P28061
L	208	HIS	-	EXPRESSION TAG	UNP P28061
L	209	HIS	-	EXPRESSION TAG	UNP P28061
M	204	HIS	-	EXPRESSION TAG	UNP P28061
M	205	HIS	-	EXPRESSION TAG	UNP P28061
M	206	HIS	-	EXPRESSION TAG	UNP P28061
M	207	HIS	-	EXPRESSION TAG	UNP P28061
M	208	HIS	-	EXPRESSION TAG	UNP P28061
M	209	HIS	-	EXPRESSION TAG	UNP P28061
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N	205	HIS	-	EXPRESSION TAG	UNP P28061
N	206	HIS	-	EXPRESSION TAG	UNP P28061
N	207	HIS	-	EXPRESSION TAG	UNP P28061
N	208	HIS	-	EXPRESSION TAG	UNP P28061
N	209	HIS	-	EXPRESSION TAG	UNP P28061

- Molecule 3 is a protein called proteasome activator protein PA26.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	O	218	Total 1679	C 1051	N 296	O 326	S 6	0	0	0
3	P	218	Total 1679	C 1051	N 296	O 326	S 6	0	0	0
3	Q	218	Total 1679	C 1051	N 296	O 326	S 6	0	0	0
3	R	218	Total 1679	C 1051	N 296	O 326	S 6	0	0	0
3	S	218	Total 1679	C 1051	N 296	O 326	S 6	0	0	0
3	T	218	Total 1679	C 1051	N 296	O 326	S 6	0	0	0
3	U	218	Total 1679	C 1051	N 296	O 326	S 6	0	0	0

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	-5	MET	-	INITIATING METHIONINE	GB 5757773
O	-4	HIS	-	EXPRESSION TAG	GB 5757773
O	-3	HIS	-	EXPRESSION TAG	GB 5757773
O	-2	HIS	-	EXPRESSION TAG	GB 5757773
O	-1	HIS	-	EXPRESSION TAG	GB 5757773
O	0	HIS	-	EXPRESSION TAG	GB 5757773
O	1	HIS	-	EXPRESSION TAG	GB 5757773
O	49	VAL	THR	VARIANT	GB 5757773
P	-5	MET	-	INITIATING METHIONINE	GB 5757773
P	-4	HIS	-	EXPRESSION TAG	GB 5757773
P	-3	HIS	-	EXPRESSION TAG	GB 5757773
P	-2	HIS	-	EXPRESSION TAG	GB 5757773
P	-1	HIS	-	EXPRESSION TAG	GB 5757773
P	0	HIS	-	EXPRESSION TAG	GB 5757773
P	1	HIS	-	EXPRESSION TAG	GB 5757773
P	49	VAL	THR	VARIANT	GB 5757773
Q	-5	MET	-	INITIATING METHIONINE	GB 5757773
Q	-4	HIS	-	EXPRESSION TAG	GB 5757773
Q	-3	HIS	-	EXPRESSION TAG	GB 5757773
Q	-2	HIS	-	EXPRESSION TAG	GB 5757773
Q	-1	HIS	-	EXPRESSION TAG	GB 5757773
Q	0	HIS	-	EXPRESSION TAG	GB 5757773
Q	1	HIS	-	EXPRESSION TAG	GB 5757773
Q	49	VAL	THR	VARIANT	GB 5757773

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-5	MET	-	INITIATING METHIONINE	GB 5757773
R	-4	HIS	-	EXPRESSION TAG	GB 5757773
R	-3	HIS	-	EXPRESSION TAG	GB 5757773
R	-2	HIS	-	EXPRESSION TAG	GB 5757773
R	-1	HIS	-	EXPRESSION TAG	GB 5757773
R	0	HIS	-	EXPRESSION TAG	GB 5757773
R	1	HIS	-	EXPRESSION TAG	GB 5757773
R	49	VAL	THR	VARIANT	GB 5757773
S	-5	MET	-	INITIATING METHIONINE	GB 5757773
S	-4	HIS	-	EXPRESSION TAG	GB 5757773
S	-3	HIS	-	EXPRESSION TAG	GB 5757773
S	-2	HIS	-	EXPRESSION TAG	GB 5757773
S	-1	HIS	-	EXPRESSION TAG	GB 5757773
S	0	HIS	-	EXPRESSION TAG	GB 5757773
S	1	HIS	-	EXPRESSION TAG	GB 5757773
S	49	VAL	THR	VARIANT	GB 5757773
T	-5	MET	-	INITIATING METHIONINE	GB 5757773
T	-4	HIS	-	EXPRESSION TAG	GB 5757773
T	-3	HIS	-	EXPRESSION TAG	GB 5757773
T	-2	HIS	-	EXPRESSION TAG	GB 5757773
T	-1	HIS	-	EXPRESSION TAG	GB 5757773
T	0	HIS	-	EXPRESSION TAG	GB 5757773
T	1	HIS	-	EXPRESSION TAG	GB 5757773
T	49	VAL	THR	VARIANT	GB 5757773
U	-5	MET	-	INITIATING METHIONINE	GB 5757773
U	-4	HIS	-	EXPRESSION TAG	GB 5757773
U	-3	HIS	-	EXPRESSION TAG	GB 5757773
U	-2	HIS	-	EXPRESSION TAG	GB 5757773
U	-1	HIS	-	EXPRESSION TAG	GB 5757773
U	0	HIS	-	EXPRESSION TAG	GB 5757773
U	1	HIS	-	EXPRESSION TAG	GB 5757773
U	49	VAL	THR	VARIANT	GB 5757773

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	K	1	Total	O	S	0	0
			5	4	1		

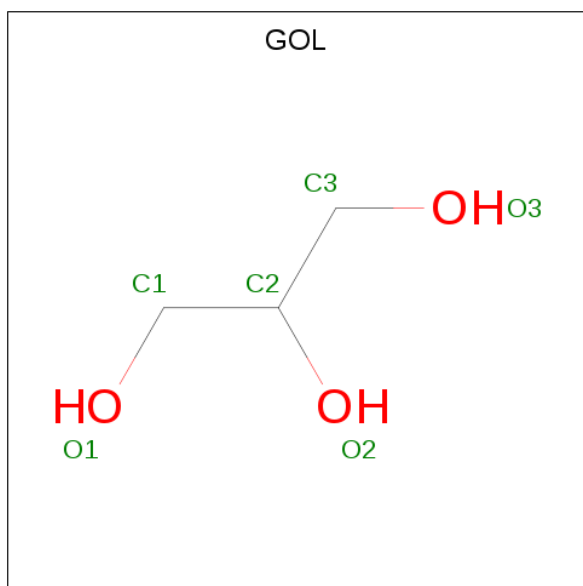
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	K	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		
4	M	1	Total	O	S	0	0
			5	4	1		
4	M	1	Total	O	S	0	0
			5	4	1		
4	N	1	Total	O	S	0	0
			5	4	1		
4	N	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	H	1	Total	C	O	0	0
			6	3	3		
5	I	1	Total	C	O	0	0
			6	3	3		
5	J	1	Total	C	O	0	0
			6	3	3		
5	K	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	L	1	Total	C	O	0	0
			6	3	3		
5	M	1	Total	C	O	0	0
			6	3	3		
5	N	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	75	Total	O	0	0
			75	75		
6	B	70	Total	O	0	0
			70	70		
6	C	67	Total	O	0	0
			67	67		
6	D	77	Total	O	0	0
			77	77		
6	E	65	Total	O	0	0
			65	65		
6	F	60	Total	O	0	0
			60	60		
6	G	65	Total	O	0	0
			65	65		
6	H	94	Total	O	0	0
			94	94		
6	I	91	Total	O	0	0
			91	91		
6	J	88	Total	O	0	0
			88	88		
6	K	86	Total	O	0	0
			86	86		
6	L	86	Total	O	0	0
			86	86		
6	M	96	Total	O	0	0
			96	96		
6	N	92	Total	O	0	0
			92	92		
6	O	72	Total	O	0	0
			72	72		
6	P	54	Total	O	0	0
			54	54		

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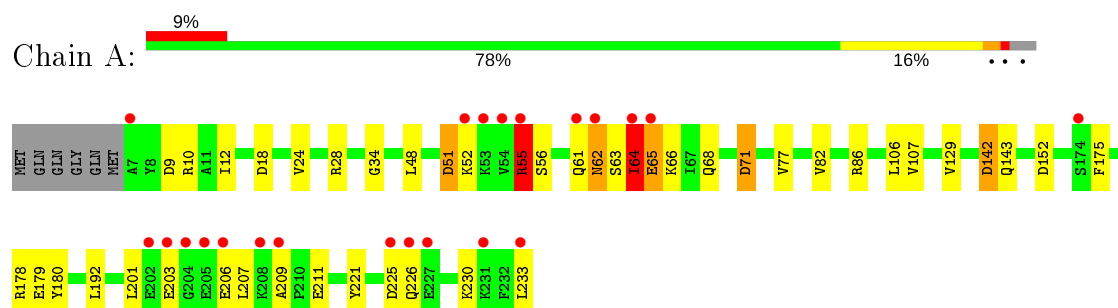
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	Q	63	Total 63	O 63	0	0
6	R	67	Total 67	O 67	0	0
6	S	103	Total 103	O 103	0	0
6	T	90	Total 90	O 90	0	0
6	U	98	Total 98	O 98	0	0

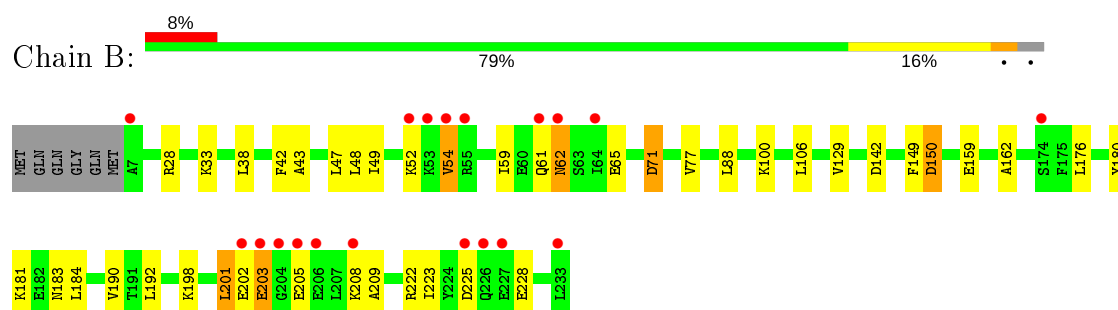
### 3 Residue-property plots [i](#)

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.

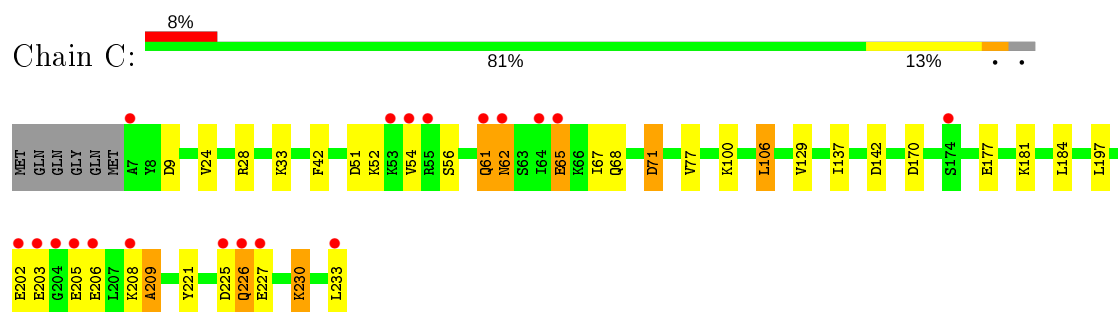
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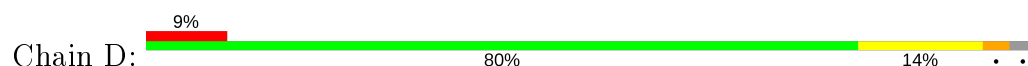
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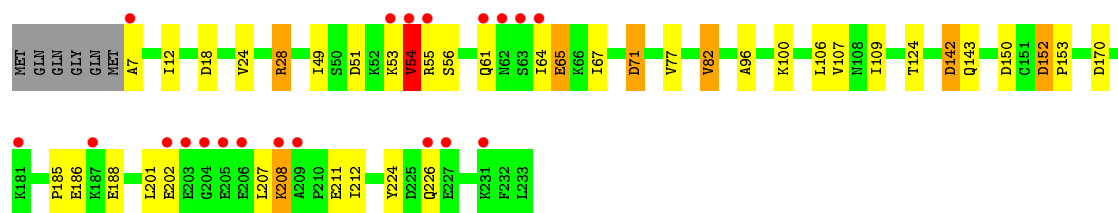


#### • Molecule 1: Proteasome alpha subunit

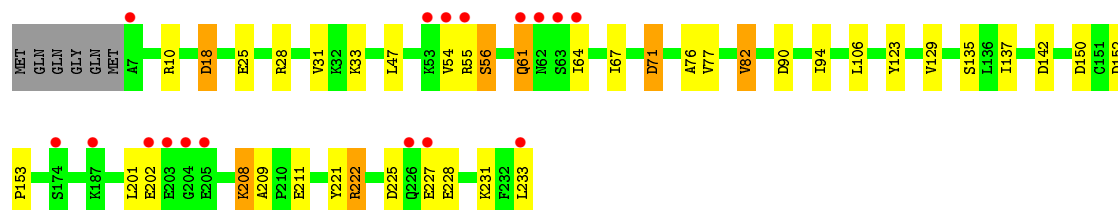
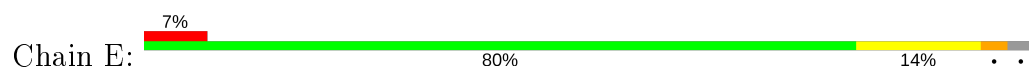


#### • Molecule 1: Proteasome alpha subunit

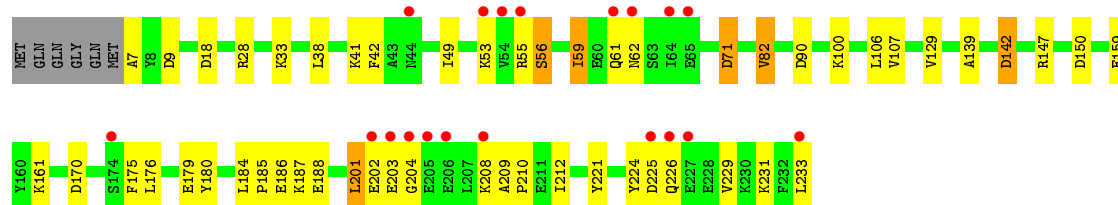
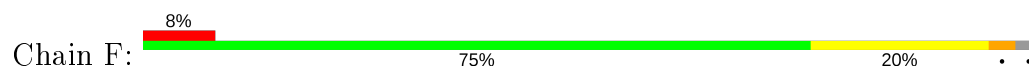




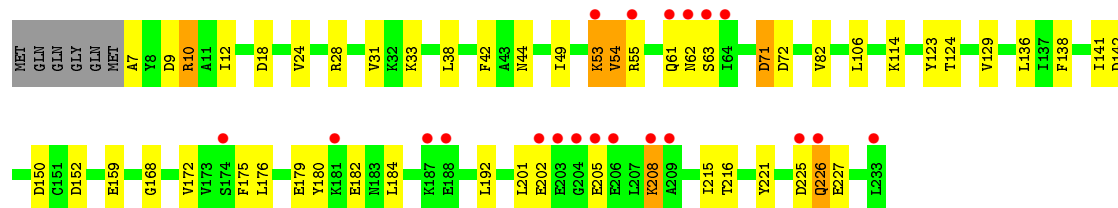
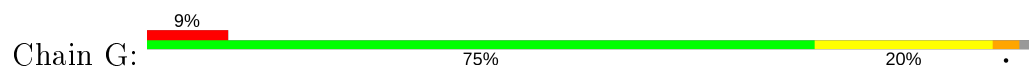
• Molecule 1: Proteasome alpha subunit



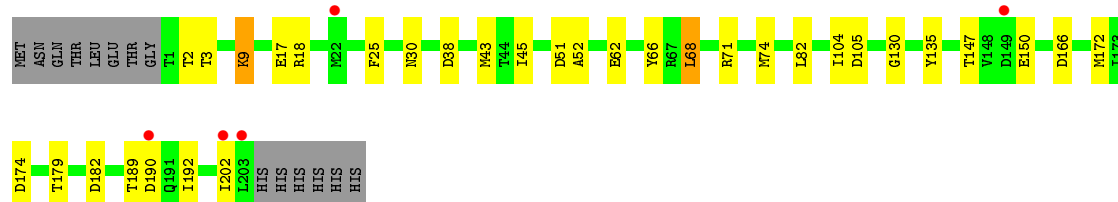
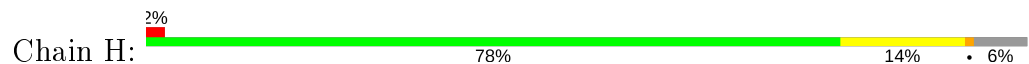
• Molecule 1: Proteasome alpha subunit



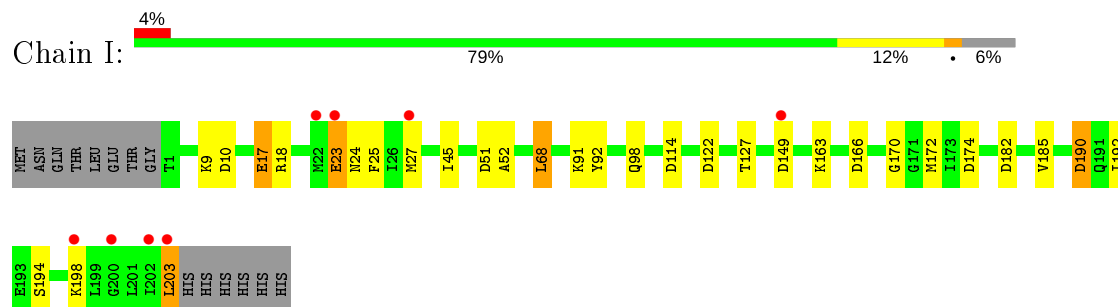
• Molecule 1: Proteasome alpha subunit



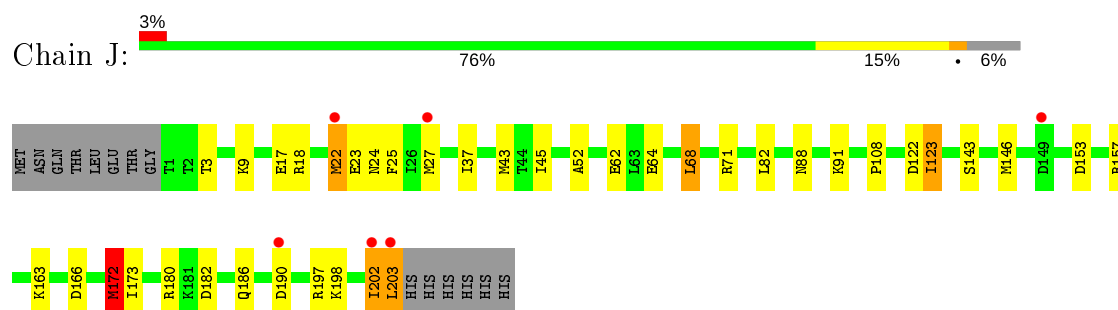
• Molecule 2: Proteasome beta subunit



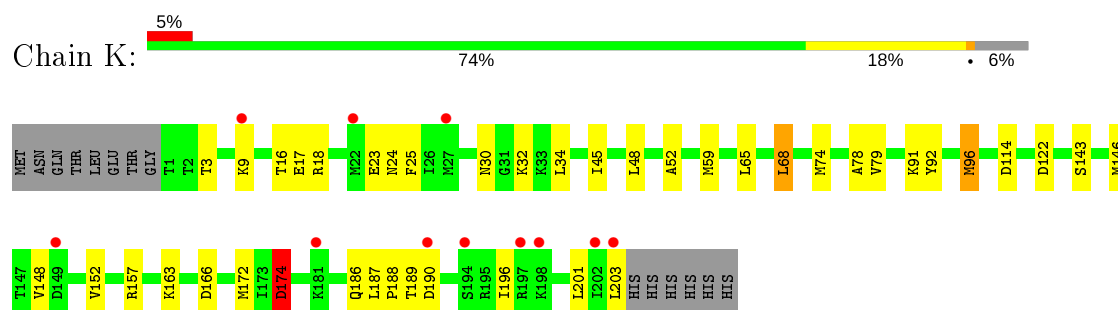
- Molecule 2: Proteasome beta subunit



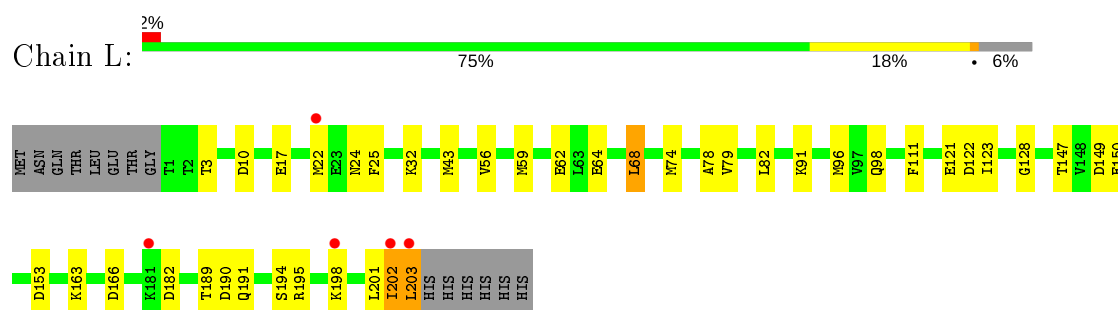
- Molecule 2: Proteasome beta subunit



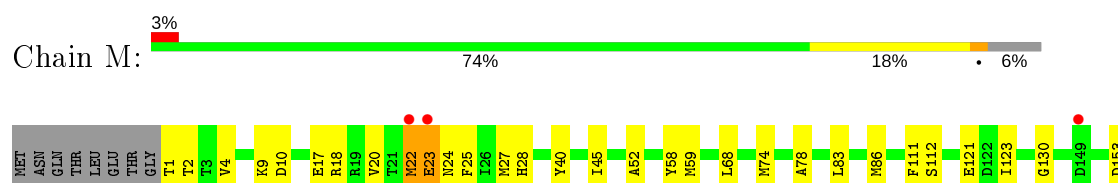
- Molecule 2: Proteasome beta subunit

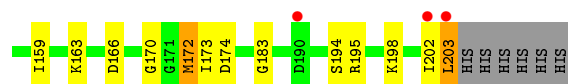


- Molecule 2: Proteasome beta subunit

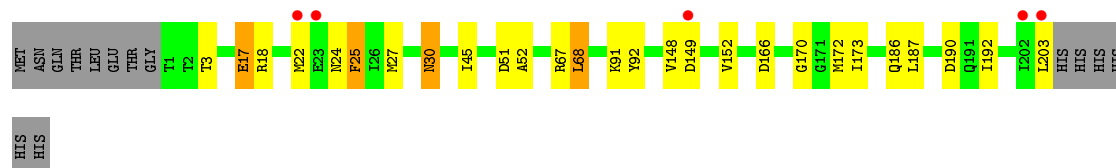
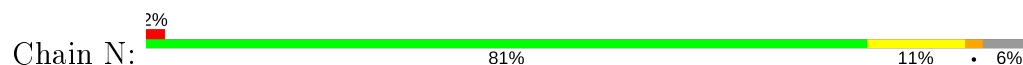


- Molecule 2: Proteasome beta subunit

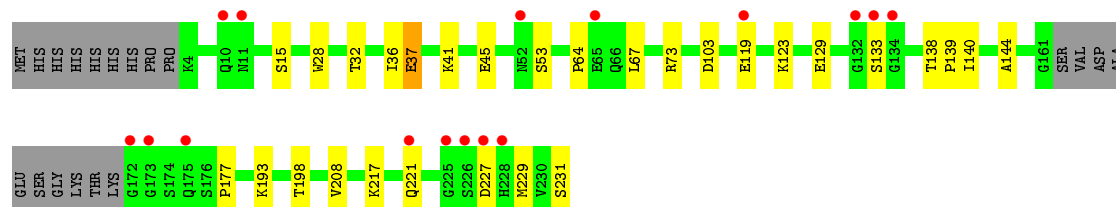
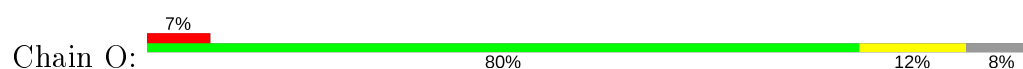




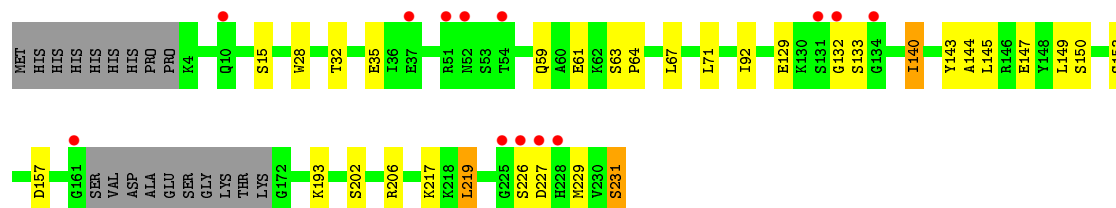
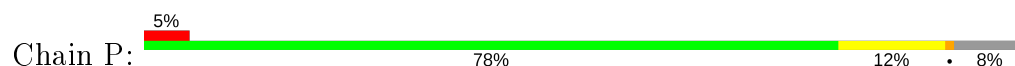
- Molecule 2: Proteasome beta subunit



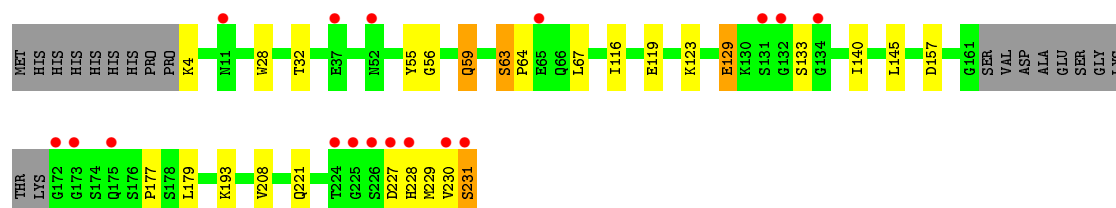
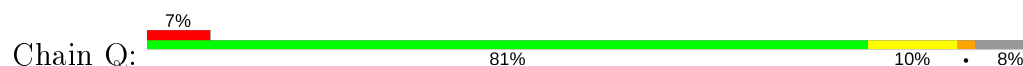
- Molecule 3: proteasome activator protein PA26



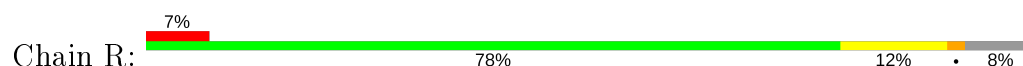
- Molecule 3: proteasome activator protein PA26

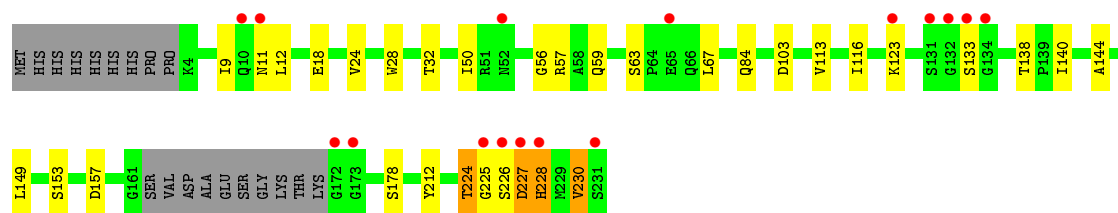


- Molecule 3: proteasome activator protein PA26

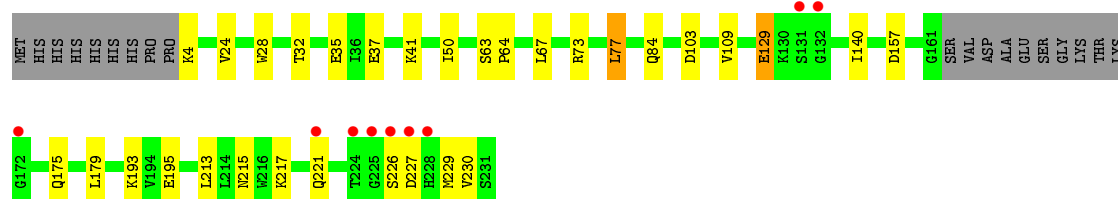
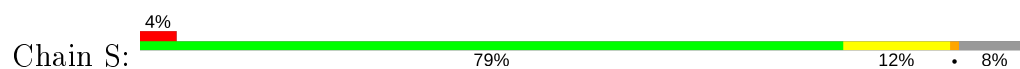


- Molecule 3: proteasome activator protein PA26

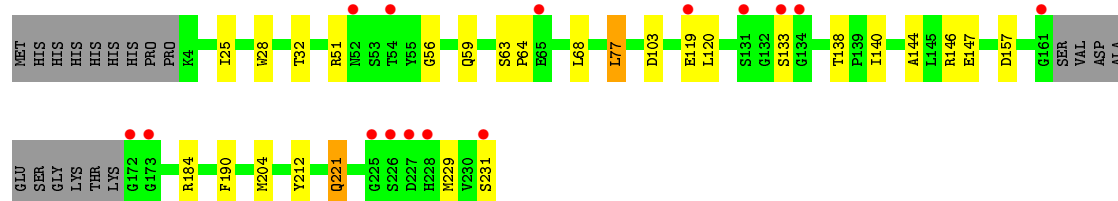
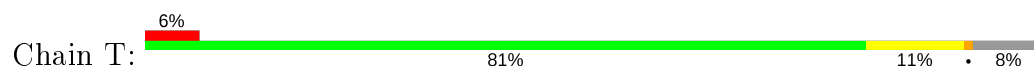




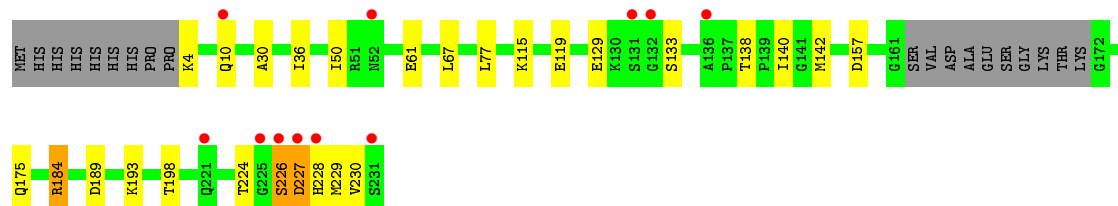
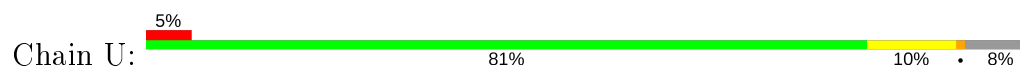
- Molecule 3: proteasome activator protein PA26



- Molecule 3: proteasome activator protein PA26



- Molecule 3: proteasome activator protein PA26





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	255.71Å 126.96Å 181.49Å 90.00° 92.63° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 8.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.30) 100.0 (8.00-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.59 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.180 , 0.224 0.179 , 0.224	Depositor DCC
$R_{free}$ test set	991 reflections (0.40%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.9	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.51 , 70.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	37185	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4

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	0.74	0/1811	0.87	5/2440 (0.2%)
1	B	0.76	0/1811	0.84	3/2440 (0.1%)
1	C	0.74	0/1811	0.83	5/2440 (0.2%)
1	D	0.73	0/1811	0.87	9/2440 (0.4%)
1	E	0.75	0/1811	0.83	4/2440 (0.2%)
1	F	0.69	0/1804	0.84	5/2430 (0.2%)
1	G	0.72	0/1804	0.84	6/2430 (0.2%)
2	H	0.75	0/1614	0.89	5/2180 (0.2%)
2	I	0.76	0/1605	0.93	8/2168 (0.4%)
2	J	0.71	0/1611	0.87	4/2176 (0.2%)
2	K	0.72	0/1614	0.92	7/2180 (0.3%)
2	L	0.73	0/1611	0.92	5/2176 (0.2%)
2	M	0.77	0/1605	0.94	5/2168 (0.2%)
2	N	0.72	0/1611	0.89	5/2176 (0.2%)
3	O	0.62	0/1702	0.76	2/2299 (0.1%)
3	P	0.61	0/1702	0.73	1/2299 (0.0%)
3	Q	0.62	0/1702	0.75	1/2299 (0.0%)
3	R	0.67	0/1702	0.77	2/2299 (0.1%)
3	S	0.73	0/1702	0.78	3/2299 (0.1%)
3	T	0.76	1/1702 (0.1%)	0.77	1/2299 (0.0%)
3	U	0.72	0/1702	0.78	2/2299 (0.1%)
All	All	0.72	1/35848 (0.0%)	0.84	88/48377 (0.2%)

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	G	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	R	0	1
3	U	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	221	GLN	CG-CD	5.42	1.63	1.51

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	174	ASP	CB-CG-OD2	8.88	126.29	118.30
1	A	71	ASP	CB-CG-OD2	8.74	126.17	118.30
1	E	71	ASP	CB-CG-OD2	8.40	125.86	118.30
2	N	166	ASP	CB-CG-OD2	8.13	125.62	118.30
1	B	71	ASP	CB-CG-OD2	8.12	125.61	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	64	ILE	Peptide
1	G	53	LYS	Peptide
3	R	230	VAL	Peptide
3	U	226	SER	Peptide

## 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	1787	0	1820	40	0
1	B	1787	0	1820	36	0
1	C	1787	0	1820	24	0
1	D	1787	0	1820	36	0
1	E	1787	0	1820	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1780	0	1812	36	0
1	G	1780	0	1812	45	0
2	H	1594	0	1637	29	0
2	I	1585	0	1630	21	0
2	J	1591	0	1634	25	0
2	K	1594	0	1637	25	0
2	L	1591	0	1634	18	0
2	M	1585	0	1630	32	0
2	N	1591	0	1634	17	0
3	O	1679	0	1700	24	0
3	P	1679	0	1700	23	0
3	Q	1679	0	1700	25	0
3	R	1679	0	1700	19	0
3	S	1679	0	1700	21	0
3	T	1679	0	1700	21	0
3	U	1679	0	1700	23	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
4	G	10	0	0	0	0
4	H	10	0	0	0	0
4	I	10	0	0	1	0
4	J	10	0	0	0	0
4	K	10	0	0	0	0
4	L	10	0	0	1	0
4	M	10	0	0	2	0
4	N	10	0	0	0	0
5	H	6	0	8	0	0
5	I	6	0	8	0	0
5	J	6	0	8	0	0
5	K	6	0	8	0	0
5	L	6	0	8	0	0
5	M	6	0	8	0	0
5	N	6	0	8	0	0
6	A	75	0	0	6	0
6	B	70	0	0	3	0
6	C	67	0	0	3	0
6	D	77	0	0	2	0
6	E	65	0	0	1	0
6	F	60	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	65	0	0	2	0
6	H	94	0	0	6	0
6	I	91	0	0	4	0
6	J	88	0	0	9	0
6	K	86	0	0	4	0
6	L	86	0	0	2	0
6	M	96	0	0	4	0
6	N	92	0	0	3	0
6	O	72	0	0	2	0
6	P	54	0	0	3	0
6	Q	63	0	0	0	0
6	R	67	0	0	1	0
6	S	103	0	0	3	0
6	T	90	0	0	0	0
6	U	98	0	0	3	0
All	All	37185	0	36116	495	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 7.

The worst 5 of 495 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)
1:D:28[A]:ARG:NH2	3:U:229:MET:HG3	1.31	1.39
1:D:28[A]:ARG:HH22	3:U:229:MET:CG	1.47	1.28
1:F:28[A]:ARG:NH2	3:P:229:MET:HG3	1.57	1.20
2:M:59:MET:HE1	2:M:86:MET:HE1	1.26	1.12
1:G:28[A]:ARG:HH22	3:Q:229:MET:HG3	1.06	1.11

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	227/233 (97%)	213 (94%)	10 (4%)	4 (2%)	8	7
1	B	227/233 (97%)	216 (95%)	9 (4%)	2 (1%)	17	20
1	C	227/233 (97%)	216 (95%)	8 (4%)	3 (1%)	12	12
1	D	227/233 (97%)	216 (95%)	9 (4%)	2 (1%)	17	20
1	E	227/233 (97%)	218 (96%)	7 (3%)	2 (1%)	17	20
1	F	226/233 (97%)	215 (95%)	8 (4%)	3 (1%)	12	12
1	G	226/233 (97%)	207 (92%)	16 (7%)	3 (1%)	12	12
2	H	205/217 (94%)	201 (98%)	4 (2%)	0	100	100
2	I	204/217 (94%)	199 (98%)	5 (2%)	0	100	100
2	J	205/217 (94%)	197 (96%)	8 (4%)	0	100	100
2	K	205/217 (94%)	200 (98%)	5 (2%)	0	100	100
2	L	205/217 (94%)	199 (97%)	5 (2%)	1 (0%)	29	35
2	M	204/217 (94%)	197 (97%)	7 (3%)	0	100	100
2	N	205/217 (94%)	198 (97%)	7 (3%)	0	100	100
3	O	214/237 (90%)	210 (98%)	4 (2%)	0	100	100
3	P	214/237 (90%)	210 (98%)	3 (1%)	1 (0%)	29	35
3	Q	214/237 (90%)	206 (96%)	7 (3%)	1 (0%)	29	35
3	R	214/237 (90%)	207 (97%)	4 (2%)	3 (1%)	11	11
3	S	214/237 (90%)	209 (98%)	4 (2%)	1 (0%)	29	35
3	T	214/237 (90%)	209 (98%)	5 (2%)	0	100	100
3	U	214/237 (90%)	211 (99%)	1 (0%)	2 (1%)	17	20
All	All	4518/4809 (94%)	4354 (96%)	136 (3%)	28 (1%)	25	31

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	GLU
1	C	203	GLU
1	D	56	SER
1	E	56	SER
1	F	56	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	190/193 (98%)	184 (97%)	6 (3%)	39	54
1	B	190/193 (98%)	183 (96%)	7 (4%)	34	48
1	C	190/193 (98%)	177 (93%)	13 (7%)	16	21
1	D	190/193 (98%)	183 (96%)	7 (4%)	34	48
1	E	190/193 (98%)	179 (94%)	11 (6%)	20	27
1	F	189/193 (98%)	181 (96%)	8 (4%)	30	42
1	G	189/193 (98%)	181 (96%)	8 (4%)	30	42
2	H	174/183 (95%)	166 (95%)	8 (5%)	27	38
2	I	173/183 (94%)	165 (95%)	8 (5%)	27	38
2	J	174/183 (95%)	157 (90%)	17 (10%)	8	9
2	K	174/183 (95%)	166 (95%)	8 (5%)	27	38
2	L	174/183 (95%)	160 (92%)	14 (8%)	12	15
2	M	173/183 (94%)	163 (94%)	10 (6%)	20	27
2	N	174/183 (95%)	167 (96%)	7 (4%)	31	44
3	O	179/196 (91%)	172 (96%)	7 (4%)	32	46
3	P	179/196 (91%)	172 (96%)	7 (4%)	32	46
3	Q	179/196 (91%)	172 (96%)	7 (4%)	32	46
3	R	179/196 (91%)	173 (97%)	6 (3%)	37	51
3	S	179/196 (91%)	175 (98%)	4 (2%)	52	69
3	T	179/196 (91%)	175 (98%)	4 (2%)	52	69
3	U	179/196 (91%)	172 (96%)	7 (4%)	32	46
All	All	3797/4004 (95%)	3623 (95%)	174 (5%)	27	38

5 of 174 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	17	GLU
2	K	96[A]	MET

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Mol	Chain	Res	Type
3	S	63	SER
2	J	25	PHE
2	J	190	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	98	GLN
3	P	75	GLN
3	U	47	HIS
2	L	191	GLN
2	N	191	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](#)

28 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	SO4	N	3021	-	4,4,4	0.23	0	6,6,6	0.28	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	H	3008	-	4,4,4	0.23	0	6,6,6	0.46	0
5	GOL	K	2007	-	5,5,5	0.68	0	5,5,5	1.26	1 (20%)
4	SO4	J	3017	-	4,4,4	0.17	0	6,6,6	0.67	0
5	GOL	I	2005	-	5,5,5	0.37	0	5,5,5	0.50	0
4	SO4	G	3007	-	4,4,4	0.15	0	6,6,6	0.18	0
5	GOL	H	2004	-	5,5,5	0.30	0	5,5,5	0.55	0
4	SO4	M	3020	-	4,4,4	0.10	0	6,6,6	0.40	0
4	SO4	E	3004	-	4,4,4	0.16	0	6,6,6	0.22	0
5	GOL	L	2001	-	5,5,5	0.55	0	5,5,5	0.39	0
4	SO4	M	3010	-	4,4,4	0.22	0	6,6,6	0.45	0
4	SO4	G	3006	-	4,4,4	0.14	0	6,6,6	0.24	0
4	SO4	L	3014	-	4,4,4	0.18	0	6,6,6	0.34	0
4	SO4	L	3019	-	4,4,4	0.13	0	6,6,6	0.46	0
5	GOL	J	2006	-	5,5,5	0.64	0	5,5,5	0.96	0
4	SO4	I	3011	-	4,4,4	0.22	0	6,6,6	0.38	0
4	SO4	F	3005	-	4,4,4	0.17	0	6,6,6	0.40	0
4	SO4	J	3012	-	4,4,4	0.17	0	6,6,6	0.59	0
4	SO4	C	3002	-	4,4,4	0.13	0	6,6,6	0.15	0
4	SO4	D	3003	-	4,4,4	0.16	0	6,6,6	0.27	0
5	GOL	N	2003	-	5,5,5	0.36	0	5,5,5	0.24	0
4	SO4	H	3015	-	4,4,4	0.18	0	6,6,6	0.63	0
4	SO4	B	3001	-	4,4,4	0.18	0	6,6,6	0.22	0
4	SO4	K	3018	-	4,4,4	0.23	0	6,6,6	0.57	0
4	SO4	K	3013	-	4,4,4	0.23	0	6,6,6	0.52	0
5	GOL	M	2002	-	5,5,5	0.27	0	5,5,5	0.27	0
4	SO4	N	3009	-	4,4,4	0.20	0	6,6,6	0.36	0
4	SO4	I	3016	-	4,4,4	0.17	0	6,6,6	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	N	2003	-	-	2/4/4/4	-
5	GOL	H	2004	-	-	2/4/4/4	-
5	GOL	K	2007	-	-	2/4/4/4	-
5	GOL	L	2001	-	-	2/4/4/4	-
5	GOL	J	2006	-	-	0/4/4/4	-
5	GOL	M	2002	-	-	2/4/4/4	-
5	GOL	I	2005	-	-	4/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
5	K	2007	GOL	O3-C3-C2	-2.03	100.48	110.20

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	2004	GOL	O1-C1-C2-O2
5	H	2004	GOL	O1-C1-C2-C3
5	K	2007	GOL	C1-C2-C3-O3
5	N	2003	GOL	O1-C1-C2-C3
5	M	2002	GOL	O1-C1-C2-C3

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	3020	SO4	1	0
4	M	3010	SO4	1	0
4	L	3019	SO4	1	0
4	I	3016	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	227/233 (97%)	-0.04	22 (9%) 7 10	28, 41, 78, 91	0
1	B	227/233 (97%)	-0.09	19 (8%) 11 15	28, 40, 75, 91	0
1	C	227/233 (97%)	-0.10	19 (8%) 11 15	28, 39, 76, 88	0
1	D	227/233 (97%)	-0.05	20 (8%) 10 13	30, 43, 78, 87	0
1	E	227/233 (97%)	-0.09	17 (7%) 14 19	29, 41, 74, 84	0
1	F	227/233 (97%)	0.02	19 (8%) 11 15	31, 44, 81, 91	0
1	G	227/233 (97%)	-0.01	20 (8%) 10 13	30, 41, 76, 87	0
2	H	203/217 (93%)	-0.45	5 (2%) 57 64	29, 35, 53, 81	0
2	I	203/217 (93%)	-0.42	8 (3%) 39 46	30, 37, 55, 76	0
2	J	203/217 (93%)	-0.37	6 (2%) 50 57	31, 39, 56, 78	0
2	K	203/217 (93%)	-0.34	11 (5%) 25 32	32, 38, 57, 82	0
2	L	203/217 (93%)	-0.38	5 (2%) 57 64	31, 38, 56, 78	0
2	M	203/217 (93%)	-0.45	6 (2%) 50 57	29, 36, 52, 74	0
2	N	203/217 (93%)	-0.39	5 (2%) 57 64	29, 36, 56, 80	0
3	O	218/237 (91%)	0.09	16 (7%) 15 20	36, 48, 68, 74	0
3	P	218/237 (91%)	0.18	13 (5%) 21 28	37, 52, 70, 79	0
3	Q	218/237 (91%)	0.17	17 (7%) 13 17	36, 51, 72, 87	0
3	R	218/237 (91%)	0.09	16 (7%) 15 20	30, 47, 69, 77	0
3	S	218/237 (91%)	-0.14	9 (4%) 37 44	29, 42, 66, 78	0
3	T	218/237 (91%)	-0.11	15 (6%) 16 22	30, 42, 63, 72	0
3	U	218/237 (91%)	-0.10	11 (5%) 28 35	32, 43, 67, 78	0
All	All	4536/4809 (94%)	-0.13	279 (6%) 20 26	28, 42, 70, 91	0

The worst 5 of 279 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	203	LEU	12.0
3	Q	227	ASP	11.3
2	N	203	LEU	11.0
3	R	226	SER	9.6
3	O	225	GLY	9.3

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	J	2006	6/6	0.84	0.17	46,47,51,54	0
4	SO4	F	3005	5/5	0.92	0.19	86,87,87,87	0
4	SO4	D	3003	5/5	0.93	0.19	86,87,88,88	0
4	SO4	E	3004	5/5	0.94	0.27	97,97,98,98	0
4	SO4	M	3020	5/5	0.94	0.17	66,67,68,69	0
4	SO4	H	3015	5/5	0.94	0.18	51,52,53,54	0
4	SO4	K	3018	5/5	0.94	0.21	64,64,65,67	0
5	GOL	K	2007	6/6	0.95	0.10	50,51,53,53	0
5	GOL	I	2005	6/6	0.96	0.10	48,50,53,54	0
5	GOL	H	2004	6/6	0.96	0.08	48,49,50,51	0
4	SO4	N	3021	5/5	0.96	0.18	58,59,59,61	0
4	SO4	J	3017	5/5	0.96	0.15	57,57,60,60	0
4	SO4	M	3010	5/5	0.96	0.17	61,62,64,66	0
4	SO4	B	3001	5/5	0.96	0.12	83,84,85,85	0
4	SO4	L	3019	5/5	0.96	0.17	62,62,62,64	0
5	GOL	M	2002	6/6	0.96	0.07	47,48,49,51	0
4	SO4	G	3006	5/5	0.97	0.15	83,84,84,84	0
5	GOL	N	2003	6/6	0.97	0.07	43,46,46,47	0
4	SO4	J	3012	5/5	0.97	0.17	54,55,57,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	G	3007	5/5	0.97	0.19	88,88,89,89	0
5	GOL	L	2001	6/6	0.97	0.08	40,44,47,48	0
4	SO4	H	3008	5/5	0.97	0.18	56,58,59,60	0
4	SO4	I	3016	5/5	0.97	0.15	63,63,65,65	0
4	SO4	N	3009	5/5	0.98	0.14	54,55,57,57	0
4	SO4	C	3002	5/5	0.98	0.20	78,78,78,79	0
4	SO4	L	3014	5/5	0.99	0.12	56,56,57,58	0
4	SO4	I	3011	5/5	0.99	0.14	54,55,58,59	0
4	SO4	K	3013	5/5	0.99	0.15	48,48,51,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.