wwPDB X-ray Structure Validation Summary Report (i)

Aug 16, 2023 – 05:12 AM EDT

PDB ID	:	1YAR
Title	:	Structure of Archeabacterial 20S proteasome mutant D9S- PA26 complex
Authors	:	Forster, A.; Masters, E.I.; Whitby, F.G.; Robinson, H.; Hill, C.P.
Deposited on	:	2004-12-17
Resolution	:	1.90 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

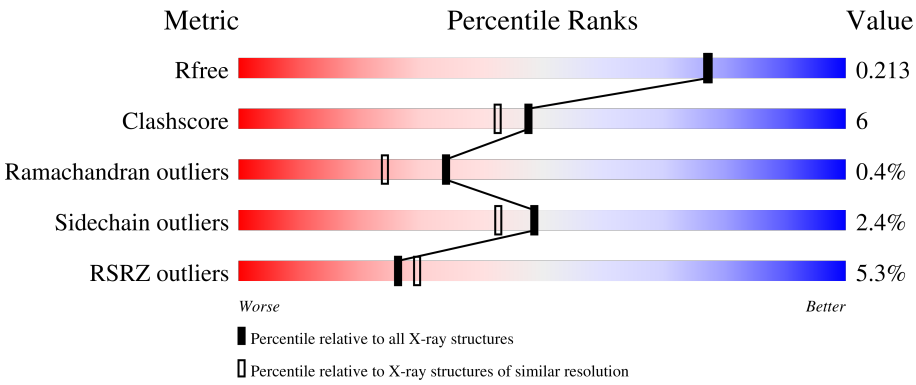
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	6% 80% 13% • 5%
1	B	233	8% 85% 9% • 5%
1	C	233	8% 82% 12% 5%
1	D	233	8% 84% 10% • 5%
1	E	233	6% 83% 10% • 5%

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Mol	Chain	Length	Quality of chain
1	F	233	9% 80% 13% • 5%
1	G	233	7% 79% 13% • 5%
2	H	217	2% 85% 8% • 6%
2	I	217	2% 82% 11% 6%
2	J	217	5% 79% 12% • 6%
2	K	217	4% 82% 10% • 6%
2	L	217	3% 80% 12% • 6%
2	M	217	3% 78% 15% • 6%
2	N	217	2% 79% 15% 6%
3	O	237	5% 81% 10% • 8%
3	P	237	3% 81% 11% • 8%
3	Q	237	5% 78% 13% • 8%
3	R	237	5% 79% 12% • 8%
3	S	237	4% 82% 9% • 8%
3	T	237	3% 80% 11% • 8%
3	U	237	3% 80% 11% • 8%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	G	4007	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 39593 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
			Total	C	N	O	S			
1	A	221	1777	1127	302	345	3	0	7	0
1	B	221	1777	1127	302	345	3	0	7	0
1	C	221	1771	1124	301	343	3	0	6	0
1	D	221	1777	1127	302	345	3	0	7	0
1	E	221	1771	1124	301	343	3	0	6	0
1	F	221	1771	1124	301	343	3	0	6	0
1	G	221	1771	1124	301	343	3	0	6	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	SER	ASP	engineered mutation	UNP P25156
B	9	SER	ASP	engineered mutation	UNP P25156
C	9	SER	ASP	engineered mutation	UNP P25156
D	9	SER	ASP	engineered mutation	UNP P25156
E	9	SER	ASP	engineered mutation	UNP P25156
F	9	SER	ASP	engineered mutation	UNP P25156
G	9	SER	ASP	engineered mutation	UNP P25156

- Molecule 2 is a protein called Proteasome beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	203	1613	1019	271	311	12	0	7	0
2	I	203	1613	1019	271	311	12	0	7	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	J	203	1613	1019	271	311	12	0	7	0
			Total	C	N	O	S			
2	K	203	1613	1019	271	311	12	0	7	0
			Total	C	N	O	S			
2	L	203	1613	1019	271	311	12	0	7	0
			Total	C	N	O	S			
2	M	203	1613	1019	271	311	12	0	7	0
			Total	C	N	O	S			
2	N	203	1613	1019	271	311	12	0	7	0

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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
N	204	HIS	-	expression tag	UNP P28061
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
			Total	C	N	O	S			
3	O	218	1754	1094	309	343	8	0	10	0
3	P	218	1754	1094	309	343	8	0	10	0
3	Q	218	1754	1094	309	343	8	0	10	0
3	R	218	1754	1094	309	343	8	0	10	0
3	S	218	1754	1094	309	343	8	0	10	0
3	T	218	1746	1089	308	342	7	0	9	0
3	U	218	1754	1094	309	343	8	0	10	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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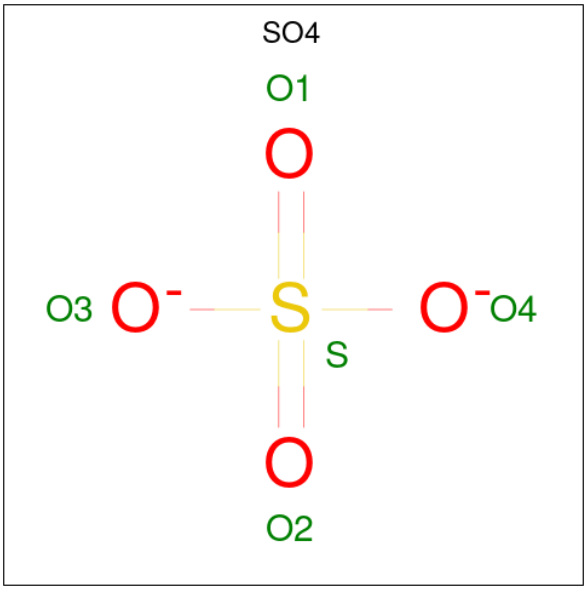
Chain	Residue	Modelled	Actual	Comment	Reference
U	-4	HIS	-	expression tag	GB 5757773
U	-3	HIS	-	expression tag	GB 5757773
U	-2	HIS	-	expression tag	GB 5757773
U	-1	HIS	-	expression tag	GB 5757773
U	0	HIS	-	expression tag	GB 5757773
U	1	HIS	-	expression tag	GB 5757773
U	49	VAL	THR	variant	GB 5757773

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
4	A	1	5	4	1	0	0
4	B	1	5	4	1	0	0
4	B	1	5	4	1	0	0
4	C	1	5	4	1	0	0
4	D	1	5	4	1	0	0
4	F	1	5	4	1	0	0
4	F	1	5	4	1	0	0
4	G	1	5	4	1	0	0

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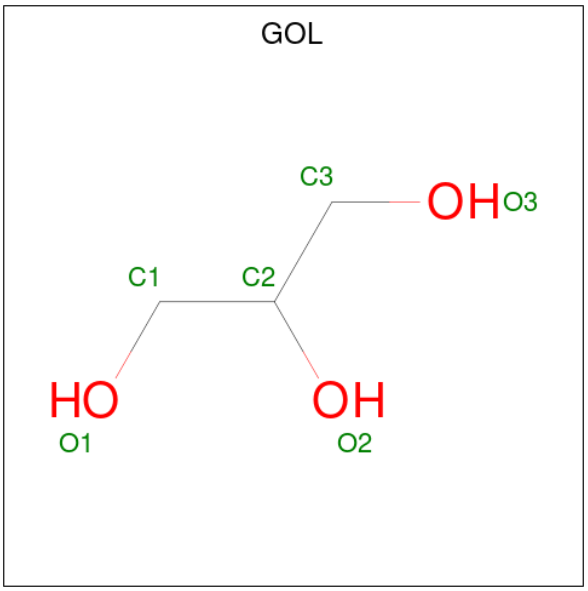
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
4	H	1	5	4	1	0	0
			Total	O	S		
4	H	1	5	4	1	0	0
			Total	O	S		
4	I	1	5	4	1	0	0
			Total	O	S		
4	J	1	5	4	1	0	0
			Total	O	S		
4	J	1	5	4	1	0	0
			Total	O	S		
4	K	1	5	4	1	0	0
			Total	O	S		
4	K	1	5	4	1	0	0
			Total	O	S		
4	L	1	5	4	1	0	0
			Total	O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

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



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	153	153	153	0	0
6	B	145	145	145	0	0
6	C	128	128	128	0	0
6	D	130	130	130	0	0
6	E	153	153	153	0	0

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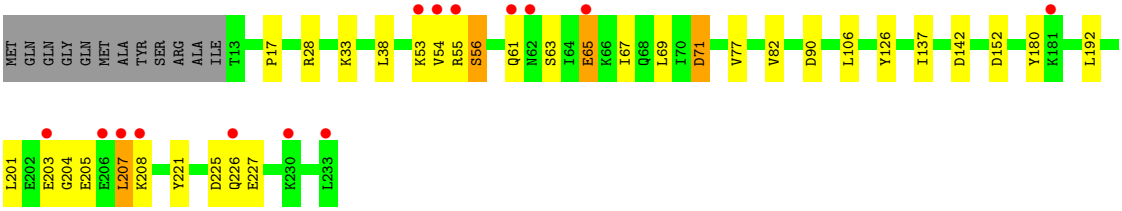
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	F	122	122	122	0	0
			Total	O		
6	G	133	133	133	0	0
			Total	O		
6	H	165	165	165	0	0
			Total	O		
6	I	165	165	165	0	0
			Total	O		
6	J	159	159	159	0	0
			Total	O		
6	K	177	177	177	0	0
			Total	O		
6	L	153	153	153	0	0
			Total	O		
6	M	180	180	180	0	0
			Total	O		
6	N	179	179	179	0	0
			Total	O		
6	O	178	178	178	0	0
			Total	O		
6	P	162	162	162	0	0
			Total	O		
6	Q	161	161	161	0	0
			Total	O		
6	R	189	189	189	0	0
			Total	O		
6	S	221	221	221	0	0
			Total	O		
6	T	207	207	207	0	0
			Total	O		
6	U	210	210	210	0	0

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.

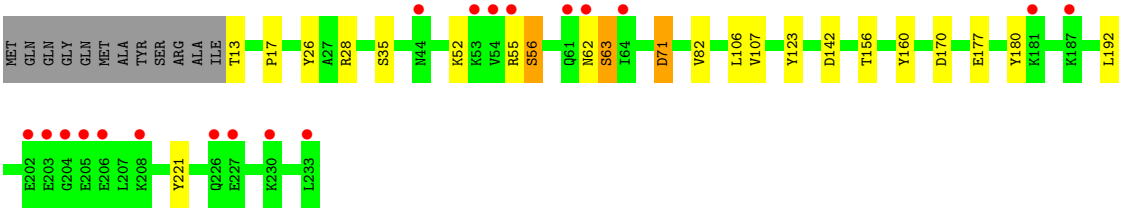
• Molecule 1: Proteasome alpha subunit

Chain A:



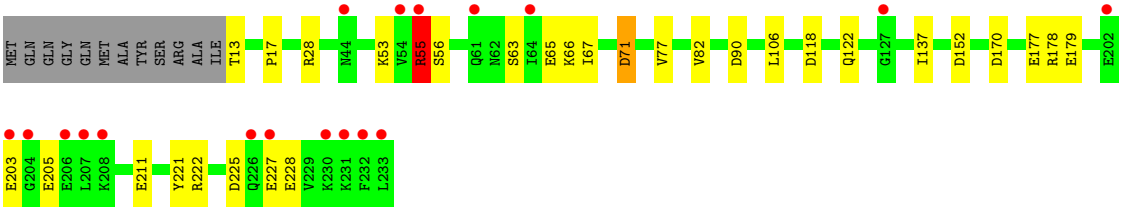
• Molecule 1: Proteasome alpha subunit

Chain B:



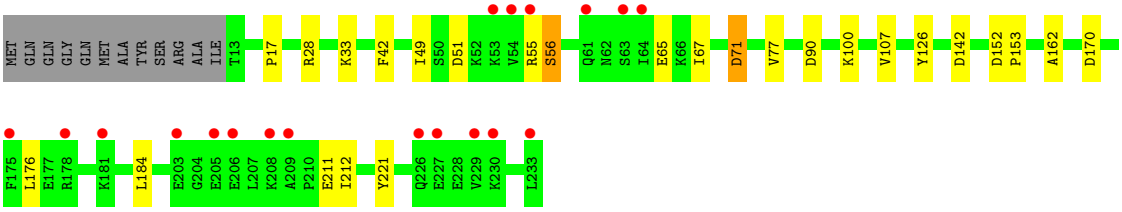
• Molecule 1: Proteasome alpha subunit

Chain C:



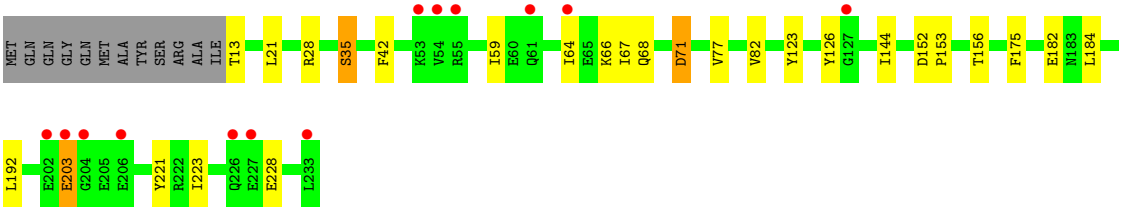
• Molecule 1: Proteasome alpha subunit

Chain D:



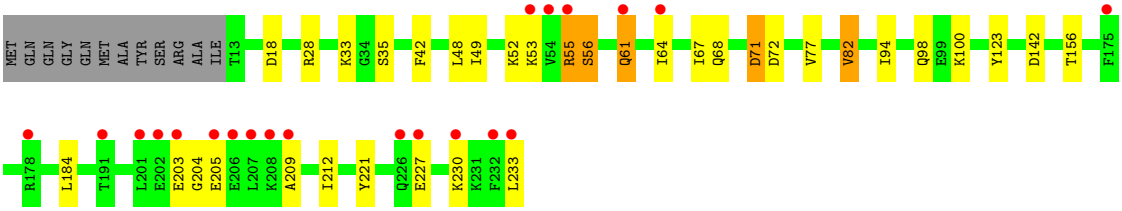
• Molecule 1: Proteasome alpha subunit

Chain E:



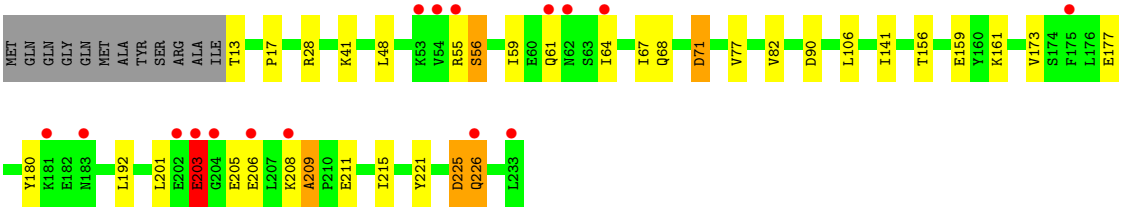
• Molecule 1: Proteasome alpha subunit

Chain F:



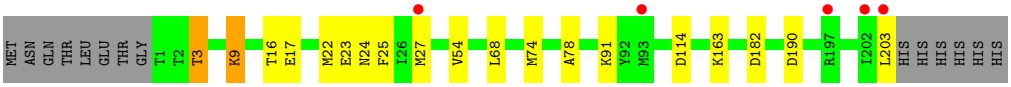
• Molecule 1: Proteasome alpha subunit

Chain G:



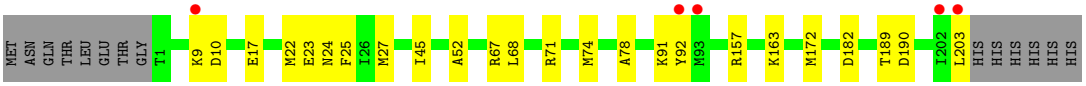
• Molecule 2: Proteasome beta subunit

Chain H:



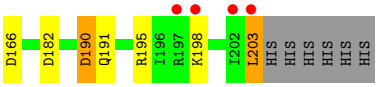
• Molecule 2: Proteasome beta subunit

Chain I:



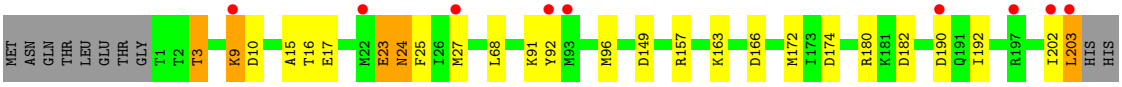
• Molecule 2: Proteasome beta subunit

Chain J:



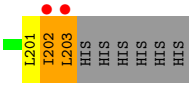
• Molecule 2: Proteasome beta subunit

Chain K:



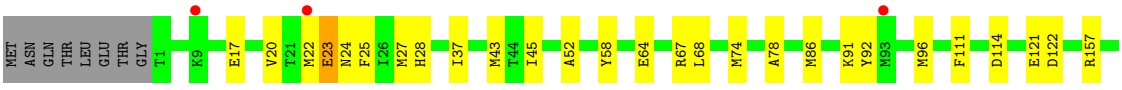
• Molecule 2: Proteasome beta subunit

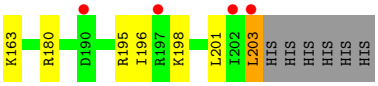
Chain L:



• Molecule 2: Proteasome beta subunit

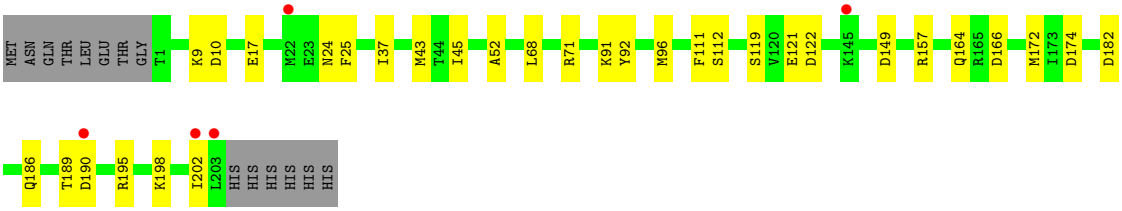
Chain M:





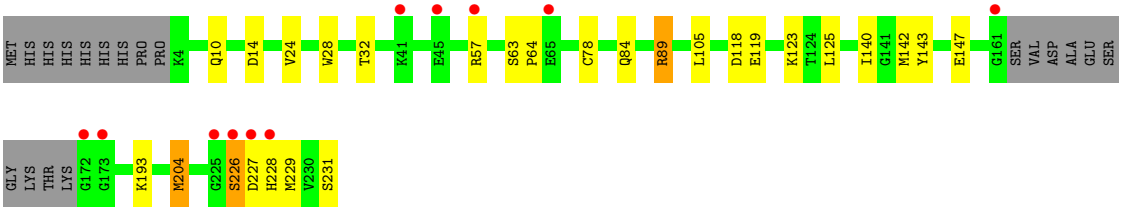
• Molecule 2: Proteasome beta subunit

Chain N:



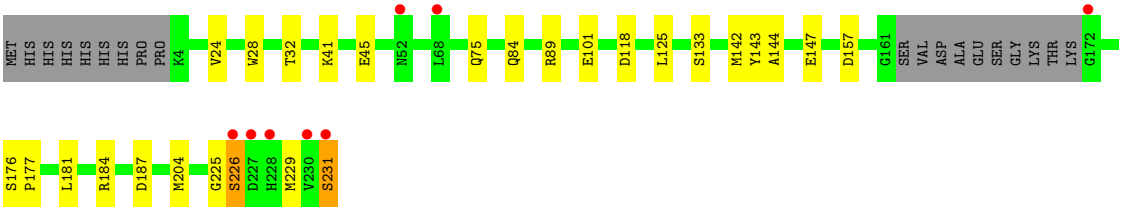
• Molecule 3: proteasome activator protein PA26

Chain O:



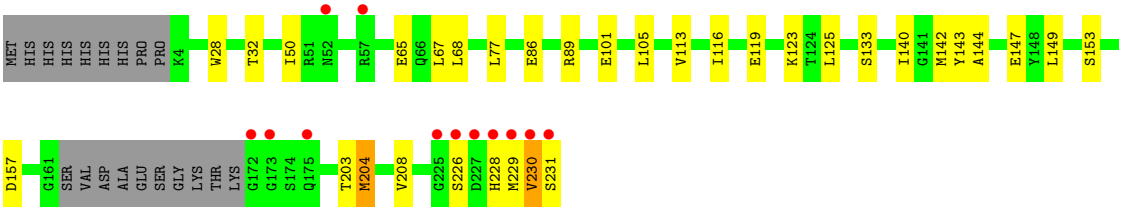
• Molecule 3: proteasome activator protein PA26

Chain P:



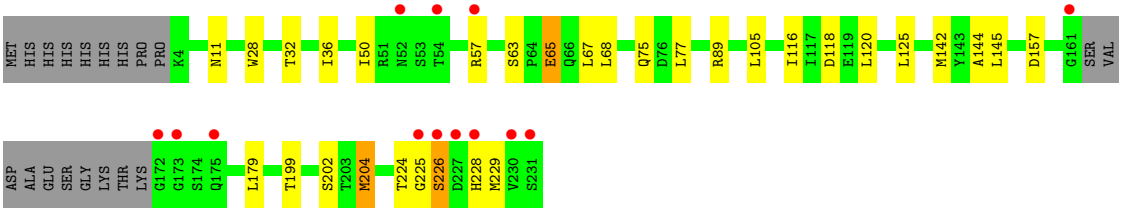
• Molecule 3: proteasome activator protein PA26

Chain Q:



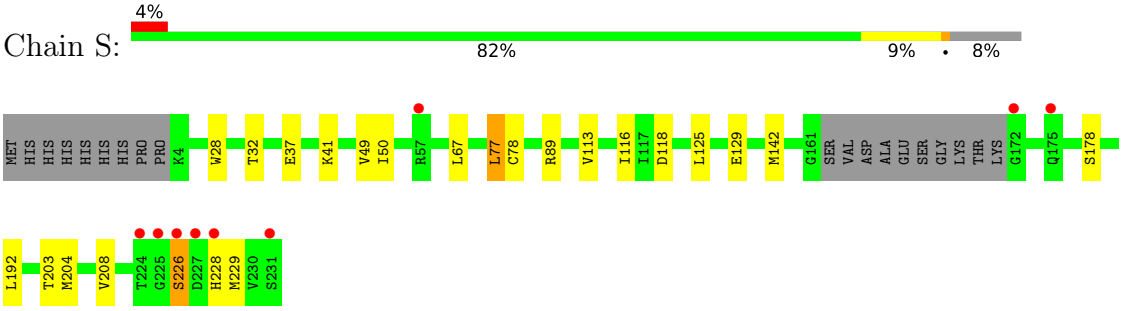
• Molecule 3: proteasome activator protein PA26

Chain R:



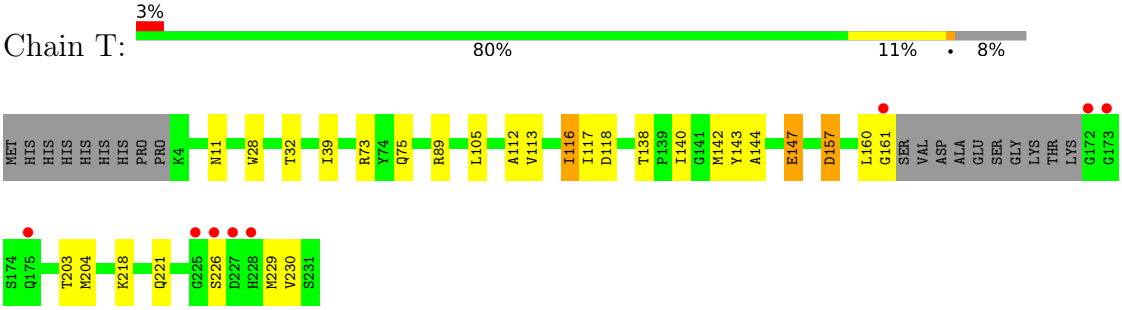
• Molecule 3: proteasome activator protein PA26

Chain S:



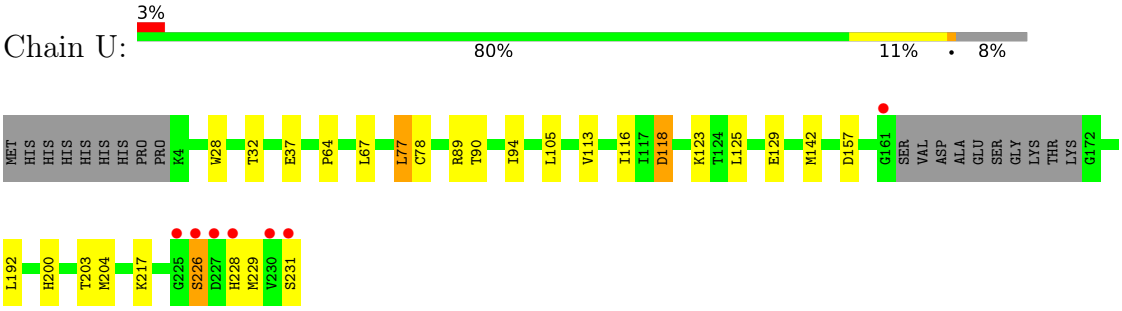
• Molecule 3: proteasome activator protein PA26

Chain T:



• Molecule 3: proteasome activator protein PA26

Chain U:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	254.87Å 127.51Å 181.18Å 90.00° 92.45° 90.00°	Depositor
Resolution (Å)	47.30 – 1.90 47.30 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.2 (47.30-1.90) 97.2 (47.30-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.72 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.182 , 0.216 0.182 , 0.213	Depositor DCC
R_{free} test set	1345 reflections (0.30%)	wwPDB-VP
Wilson B-factor (Å^2)	27.6	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 54.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.002 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	39593	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.57	0/1800	0.80	4/2425 (0.2%)
1	B	0.57	0/1800	0.75	2/2425 (0.1%)
1	C	0.57	0/1794	0.74	3/2417 (0.1%)
1	D	0.57	0/1800	0.75	3/2425 (0.1%)
1	E	0.59	0/1794	0.76	1/2417 (0.0%)
1	F	0.55	0/1794	0.74	4/2417 (0.2%)
1	G	0.57	0/1794	0.75	2/2417 (0.1%)
2	H	0.64	0/1633	0.83	4/2206 (0.2%)
2	I	0.61	0/1633	0.80	4/2206 (0.2%)
2	J	0.59	0/1633	0.83	6/2206 (0.3%)
2	K	0.59	0/1633	0.83	6/2206 (0.3%)
2	L	0.59	0/1633	0.82	3/2206 (0.1%)
2	M	0.65	0/1633	0.84	2/2206 (0.1%)
2	N	0.61	0/1633	0.84	7/2206 (0.3%)
3	O	0.51	0/1777	0.70	0/2398
3	P	0.50	0/1777	0.68	2/2398 (0.1%)
3	Q	0.50	0/1777	0.69	1/2398 (0.0%)
3	R	0.56	0/1777	0.69	1/2398 (0.0%)
3	S	0.62	0/1777	0.70	0/2398
3	T	0.61	0/1769	0.70	1/2388 (0.0%)
3	U	0.59	0/1777	0.71	2/2398 (0.1%)
All	All	0.58	0/36438	0.76	58/49161 (0.1%)

There are no bond length outliers.

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	71	ASP	CB-CG-OD2	8.91	126.32	118.30
1	D	71	ASP	CB-CG-OD2	8.29	125.76	118.30
1	G	71	ASP	CB-CG-OD2	8.27	125.74	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	71	ASP	CB-CG-OD2	8.18	125.66	118.30
2	N	149	ASP	CB-CG-OD2	7.37	124.93	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1777	0	1809	34	0
1	B	1777	0	1809	21	0
1	C	1771	0	1805	28	0
1	D	1777	0	1809	25	0
1	E	1771	0	1805	27	0
1	F	1771	0	1805	28	0
1	G	1771	0	1805	38	0
2	H	1613	0	1649	14	0
2	I	1613	0	1649	18	0
2	J	1613	0	1649	17	0
2	K	1613	0	1649	21	0
2	L	1613	0	1649	23	0
2	M	1613	0	1649	23	0
2	N	1613	0	1649	16	0
3	O	1754	0	1765	20	0
3	P	1754	0	1765	23	0
3	Q	1754	0	1765	30	0
3	R	1754	0	1765	34	0
3	S	1754	0	1765	39	0
3	T	1746	0	1757	30	0
3	U	1754	0	1765	33	0
4	A	5	0	0	0	0
4	B	10	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
4	F	10	0	0	0	0
4	G	5	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	10	0	0	1	0
4	I	5	0	0	0	0
4	J	10	0	0	0	0
4	K	10	0	0	0	0
4	L	10	0	0	0	0
4	M	10	0	0	1	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	153	0	0	5	0
6	B	145	0	0	4	0
6	C	128	0	0	8	0
6	D	130	0	0	1	0
6	E	153	0	0	6	0
6	F	122	0	0	3	0
6	G	133	0	0	9	0
6	H	165	0	0	5	0
6	I	165	0	0	7	0
6	J	159	0	0	5	0
6	K	177	0	0	4	0
6	L	153	0	0	4	0
6	M	180	0	0	8	0
6	N	179	0	0	6	0
6	O	178	0	0	4	0
6	P	162	0	0	3	0
6	Q	161	0	0	1	0
6	R	189	0	0	6	0
6	S	221	0	0	1	0
6	T	207	0	0	6	0
6	U	210	0	0	3	0
All	All	39593	0	36593	445	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 6.

The worst 5 of 445 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[B]:ARG:HH22	3:U:229:MET:CG	1.49	1.23
2:K:96[B]:MET:HE3	2:L:91:LYS:HZ1	1.02	1.10
1:E:28[B]:ARG:HH22	3:O:229:MET:HG3	0.98	1.09
1:F:28[B]:ARG:HH22	3:P:229:MET:HG2	1.10	1.09
2:L:202:ILE:HG22	2:L:203:LEU:H	1.05	1.08

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	226/233 (97%)	219 (97%)	5 (2%)	2 (1%)	17 7
1	B	226/233 (97%)	218 (96%)	7 (3%)	1 (0%)	34 24
1	C	225/233 (97%)	220 (98%)	4 (2%)	1 (0%)	34 24
1	D	226/233 (97%)	219 (97%)	6 (3%)	1 (0%)	34 24
1	E	225/233 (97%)	220 (98%)	5 (2%)	0	100 100
1	F	225/233 (97%)	216 (96%)	7 (3%)	2 (1%)	17 7
1	G	225/233 (97%)	217 (96%)	5 (2%)	3 (1%)	12 4
2	H	208/217 (96%)	204 (98%)	4 (2%)	0	100 100
2	I	208/217 (96%)	202 (97%)	6 (3%)	0	100 100
2	J	208/217 (96%)	204 (98%)	4 (2%)	0	100 100
2	K	208/217 (96%)	204 (98%)	4 (2%)	0	100 100
2	L	208/217 (96%)	201 (97%)	6 (3%)	1 (0%)	29 18
2	M	208/217 (96%)	204 (98%)	4 (2%)	0	100 100
2	N	208/217 (96%)	204 (98%)	4 (2%)	0	100 100
3	O	224/237 (94%)	220 (98%)	2 (1%)	2 (1%)	17 7
3	P	224/237 (94%)	218 (97%)	5 (2%)	1 (0%)	34 24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Q	224/237 (94%)	221 (99%)	3 (1%)	0	100	100
3	R	224/237 (94%)	220 (98%)	3 (1%)	1 (0%)	34	24
3	S	224/237 (94%)	217 (97%)	6 (3%)	1 (0%)	34	24
3	T	223/237 (94%)	219 (98%)	3 (1%)	1 (0%)	34	24
3	U	224/237 (94%)	219 (98%)	4 (2%)	1 (0%)	34	24
All	All	4601/4809 (96%)	4486 (98%)	97 (2%)	18 (0%)	34	24

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	SER
1	B	56	SER
1	D	56	SER
1	F	56	SER
1	G	56	SER

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	191/193 (99%)	185 (97%)	6 (3%)	40	32
1	B	191/193 (99%)	186 (97%)	5 (3%)	46	39
1	C	190/193 (98%)	183 (96%)	7 (4%)	34	25
1	D	191/193 (99%)	189 (99%)	2 (1%)	76	76
1	E	190/193 (98%)	186 (98%)	4 (2%)	53	48
1	F	190/193 (98%)	181 (95%)	9 (5%)	26	16
1	G	190/193 (98%)	185 (97%)	5 (3%)	46	39
2	H	177/183 (97%)	172 (97%)	5 (3%)	43	36
2	I	177/183 (97%)	174 (98%)	3 (2%)	60	57
2	J	177/183 (97%)	171 (97%)	6 (3%)	37	28
2	K	177/183 (97%)	170 (96%)	7 (4%)	31	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	177/183 (97%)	172 (97%)	5 (3%)	43	36
2	M	177/183 (97%)	172 (97%)	5 (3%)	43	36
2	N	177/183 (97%)	175 (99%)	2 (1%)	73	73
3	O	189/196 (96%)	184 (97%)	5 (3%)	46	39
3	P	189/196 (96%)	188 (100%)	1 (0%)	88	89
3	Q	189/196 (96%)	183 (97%)	6 (3%)	39	30
3	R	189/196 (96%)	184 (97%)	5 (3%)	46	39
3	S	189/196 (96%)	188 (100%)	1 (0%)	88	89
3	T	188/196 (96%)	180 (96%)	8 (4%)	29	19
3	U	189/196 (96%)	188 (100%)	1 (0%)	88	89
All	All	3894/4004 (97%)	3796 (98%)	98 (2%)	49	41

5 of 98 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	K	25	PHE
3	O	57	ARG
2	L	17	GLU
2	M	23	GLU
3	O	204[B]	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
2	M	73	ASN
3	U	79	HIS
3	O	79	HIS
3	T	79	HIS
2	N	164	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 monosaccharides 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	F	4006	-	4,4,4	0.18	0	6,6,6	0.12	0
4	SO4	I	4011	-	4,4,4	0.11	0	6,6,6	0.38	0
4	SO4	B	4016	-	4,4,4	0.14	0	6,6,6	0.42	0
4	SO4	F	4005	-	4,4,4	0.14	0	6,6,6	0.09	0
4	SO4	H	4015	-	4,4,4	0.20	0	6,6,6	0.39	0
5	GOL	K	5007	-	5,5,5	0.38	0	5,5,5	0.80	0
5	GOL	J	5006	-	5,5,5	0.53	0	5,5,5	0.58	0
4	SO4	G	4007	-	4,4,4	0.12	0	6,6,6	0.30	0
4	SO4	L	4019	-	4,4,4	0.09	0	6,6,6	0.19	0
5	GOL	L	5001	-	5,5,5	0.34	0	5,5,5	0.46	0
4	SO4	J	4017	-	4,4,4	0.16	0	6,6,6	0.13	0
4	SO4	C	4003	-	4,4,4	0.14	0	6,6,6	0.11	0
4	SO4	N	4021	-	4,4,4	0.15	0	6,6,6	0.19	0
4	SO4	D	4004	-	4,4,4	0.15	0	6,6,6	0.11	0
5	GOL	N	5003	-	5,5,5	0.34	0	5,5,5	0.67	0
4	SO4	M	4010	-	4,4,4	0.24	0	6,6,6	0.40	0
4	SO4	J	4012	-	4,4,4	0.10	0	6,6,6	0.41	0
5	GOL	H	5004	-	5,5,5	0.45	0	5,5,5	1.39	1 (20%)
5	GOL	I	5005	-	5,5,5	0.37	0	5,5,5	0.52	0
4	SO4	A	4001	-	4,4,4	0.14	0	6,6,6	0.07	0
4	SO4	N	4009	-	4,4,4	0.18	0	6,6,6	0.28	0
4	SO4	H	4008	-	4,4,4	0.27	0	6,6,6	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SO4	K	4018	-	4,4,4	0.15	0	6,6,6	0.46	0
4	SO4	M	4020	-	4,4,4	0.07	0	6,6,6	0.13	0
4	SO4	B	4002	-	4,4,4	0.16	0	6,6,6	0.18	0
4	SO4	L	4014	-	4,4,4	0.18	0	6,6,6	0.55	0
4	SO4	K	4013	-	4,4,4	0.12	0	6,6,6	0.68	0
5	GOL	M	5002	-	5,5,5	0.26	0	5,5,5	0.44	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	L	5001	-	-	2/4/4/4	-
5	GOL	M	5002	-	-	3/4/4/4	-
5	GOL	N	5003	-	-	1/4/4/4	-
5	GOL	H	5004	-	-	4/4/4/4	-
5	GOL	I	5005	-	-	1/4/4/4	-
5	GOL	K	5007	-	-	0/4/4/4	-
5	GOL	J	5006	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	5004	GOL	O2-C2-C1	2.26	119.06	109.12

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	5004	GOL	C1-C2-C3-O3
5	M	5002	GOL	O1-C1-C2-C3
5	H	5004	GOL	O1-C1-C2-C3
5	L	5001	GOL	O1-C1-C2-C3
5	H	5004	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	4015	SO4	1	0
4	G	4007	SO4	2	0
4	M	4020	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	221/233 (94%)	0.27	14 (6%)	20	22	18, 28, 61, 71	0
1	B	221/233 (94%)	0.46	19 (8%)	10	12	16, 29, 60, 71	0
1	C	221/233 (94%)	0.26	18 (8%)	12	13	17, 28, 63, 70	0
1	D	221/233 (94%)	0.53	19 (8%)	10	12	18, 31, 62, 73	0
1	E	221/233 (94%)	0.19	13 (5%)	22	25	18, 27, 55, 65	0
1	F	221/233 (94%)	0.42	21 (9%)	8	9	19, 31, 63, 75	0
1	G	221/233 (94%)	0.41	16 (7%)	15	17	18, 30, 58, 70	0
2	H	203/217 (93%)	-0.02	5 (2%)	57	60	18, 23, 38, 65	0
2	I	203/217 (93%)	0.12	5 (2%)	57	60	19, 24, 40, 61	0
2	J	203/217 (93%)	0.30	11 (5%)	25	29	20, 25, 41, 65	0
2	K	203/217 (93%)	0.07	9 (4%)	34	37	19, 25, 40, 62	0
2	L	203/217 (93%)	0.21	7 (3%)	45	48	19, 25, 40, 65	0
2	M	203/217 (93%)	-0.04	7 (3%)	45	48	17, 22, 37, 60	0
2	N	203/217 (93%)	0.34	5 (2%)	57	60	17, 24, 39, 65	0
3	O	218/237 (91%)	0.05	11 (5%)	28	32	22, 30, 47, 61	0
3	P	218/237 (91%)	0.07	8 (3%)	41	44	24, 32, 50, 67	0
3	Q	218/237 (91%)	0.12	12 (5%)	25	28	22, 32, 51, 79	0
3	R	218/237 (91%)	0.05	13 (5%)	21	24	17, 28, 49, 63	0
3	S	218/237 (91%)	-0.13	9 (4%)	37	40	17, 25, 42, 66	0
3	T	218/237 (91%)	-0.09	8 (3%)	41	44	16, 25, 44, 61	0
3	U	218/237 (91%)	-0.09	7 (3%)	47	50	18, 26, 41, 64	0
All	All	4494/4809 (93%)	0.17	237 (5%)	26	29	16, 27, 54, 79	0

The worst 5 of 237 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	203	LEU	14.0
2	L	203	LEU	13.6
2	I	203	LEU	11.8
2	N	202	ILE	11.2
2	K	202	ILE	10.3

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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	F	4005	5/5	0.83	0.19	106,106,106,106	0
4	SO4	D	4004	5/5	0.88	0.16	86,86,87,87	0
4	SO4	A	4001	5/5	0.90	0.21	105,106,106,106	0
4	SO4	B	4002	5/5	0.91	0.12	68,69,69,69	0
5	GOL	H	5004	6/6	0.92	0.12	33,37,38,38	0
4	SO4	F	4006	5/5	0.93	0.10	68,69,69,70	0
4	SO4	G	4007	5/5	0.93	0.13	70,71,72,72	0
4	SO4	C	4003	5/5	0.93	0.13	97,98,98,98	0
5	GOL	J	5006	6/6	0.94	0.16	35,37,39,43	0
5	GOL	N	5003	6/6	0.94	0.10	30,33,36,38	0
5	GOL	I	5005	6/6	0.95	0.11	31,34,35,40	0
5	GOL	K	5007	6/6	0.96	0.09	32,36,37,38	0
5	GOL	L	5001	6/6	0.96	0.12	35,36,37,39	0
5	GOL	M	5002	6/6	0.96	0.09	35,36,37,38	0
4	SO4	M	4010	5/5	0.96	0.12	43,46,47,49	0
4	SO4	I	4011	5/5	0.97	0.12	35,40,41,43	0
4	SO4	J	4017	5/5	0.97	0.10	50,51,52,52	0
4	SO4	K	4018	5/5	0.97	0.08	46,49,51,51	0
4	SO4	L	4019	5/5	0.97	0.10	51,54,54,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	B	4016	5/5	0.97	0.10	54,55,55,56	0
4	SO4	H	4015	5/5	0.97	0.10	45,47,48,49	0
4	SO4	J	4012	5/5	0.98	0.08	34,38,39,41	0
4	SO4	L	4014	5/5	0.98	0.08	36,40,40,40	0
4	SO4	H	4008	5/5	0.98	0.08	38,40,42,42	0
4	SO4	K	4013	5/5	0.98	0.12	36,39,41,42	0
4	SO4	M	4020	5/5	0.98	0.09	51,52,53,53	0
4	SO4	N	4009	5/5	0.98	0.07	38,39,42,42	0
4	SO4	N	4021	5/5	0.98	0.10	52,53,54,54	0

6.5 Other polymers (i)

There are no such residues in this entry.