wwPDB X-ray Structure Validation Summary Report (i)

Dec 5, 2016 – 02:42 PM EST

PDB ID	:	5L62
Title	:	Yeast 20S proteasome with human beta5c (1-138) and human beta6 (97-111; 118-133) in complex with epoxyketone inhibitor 16
Authors	:	Groll, M.; Huber, E.M.
Deposited on	:	2016-05-28
Resolution	:	2.80 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

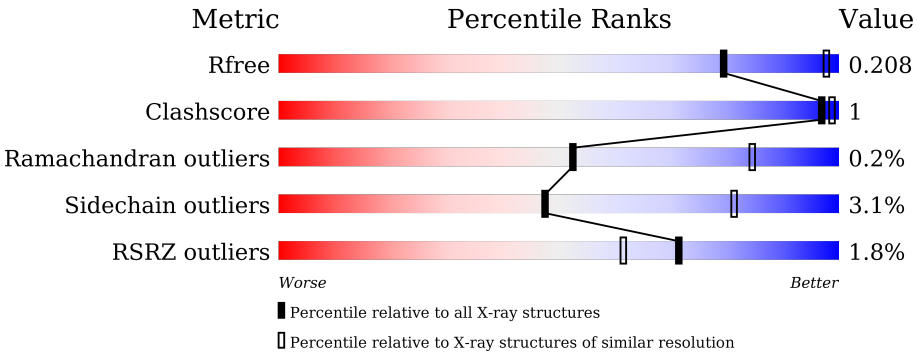
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	250	2% 98% ·
1	O	250	2% 98% ·
2	B	258	3% 90% · · 5%
2	P	258	3% 90% · · 5%
3	C	254	6% 87% 6% · 6%
3	Q	254	6% 87% 6% · 6%

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Mol	Chain	Length	Quality of chain
4	D	260	86% 10%
4	R	260	2% 87% 10%
5	E	234	3% 96%
5	S	234	% 96%
6	F	288	2% 82% 16%
6	T	288	% 82% 16%
7	G	252	2% 91% 5%
7	U	252	% 90% 5%
8	H	232	% 94%
8	V	232	2% 94%
9	I	205	94% 5%
9	W	205	% 94% 5%
10	J	198	% 90% 8%
10	X	198	2% 90% 8%
11	K	211	% 85% 12%
11	Y	211	86% 11%
12	L	222	% 94% 6%
12	Z	222	% 94% 6%
13	M	246	% 92% 5%
13	a	246	92% 5%
14	N	196	% 95%
14	b	196	% 97%

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
15	MG	A	301	-	-	-	X
15	MG	J	201	-	-	-	X
15	MG	Z	301	-	-	-	X
16	CL	N	202	-	-	-	X
17	MES	H	301	-	-	-	X
17	MES	K	304	-	-	-	X
17	MES	V	301	-	-	-	X
17	MES	Y	302	-	-	-	X

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 49807 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 subunit alpha type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
1	O	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

- Molecule 2 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			
2	P	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	240	Total	C	N	O	S	0	0	0
			1881	1176	329	372	4			
3	Q	240	Total	C	N	O	S	0	0	0
			1881	1176	329	372	4			

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	235	Total	C	N	O	S	0	0	0
			1813	1136	304	366	7			
4	R	235	Total	C	N	O	S	0	0	0
			1813	1136	304	366	7			

- Molecule 5 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	231	Total	C	N	O	S	0	0	0
			1773	1114	307	348	4			
5	S	231	Total	C	N	O	S	0	0	0
			1773	1114	307	348	4			

- Molecule 6 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	243	Total	C	N	O	S	0	0	0
			1892	1203	329	356	4			
6	T	243	Total	C	N	O	S	0	0	0
			1892	1203	329	356	4			

- Molecule 7 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	241	Total	C	N	O	S	0	0	0
			1907	1214	320	365	8			
7	U	241	Total	C	N	O	S	0	0	0
			1907	1214	320	365	8			

- Molecule 8 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	226	Total	C	N	O	S	0	0	0
			1719	1082	298	332	7			
8	V	226	Total	C	N	O	S	0	0	0
			1719	1082	298	332	7			

- Molecule 9 is a protein called Proteasome subunit beta type-3.

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 subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	195	Total	C	N	O	S	0	0	0
			1561	992	264	299	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	195	Total	C	N	O	S	0	0	0
			1561	992	264	299	6			

- Molecule 11 is a protein called Proteasome subunit beta type-5,Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	211	Total	C	N	O	S	0	0	0
			1632	1036	282	306	8			
11	Y	211	Total	C	N	O	S	0	0	0
			1632	1036	282	306	8			

- Molecule 12 is a protein called Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1764	1119	305	336	4			
12	Z	222	Total	C	N	O	S	0	1	0
			1776	1128	306	338	4			

- Molecule 13 is a protein called Proteasome subunit beta type-7.

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

- Molecule 14 is a protein called Proteasome subunit beta type-1.

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

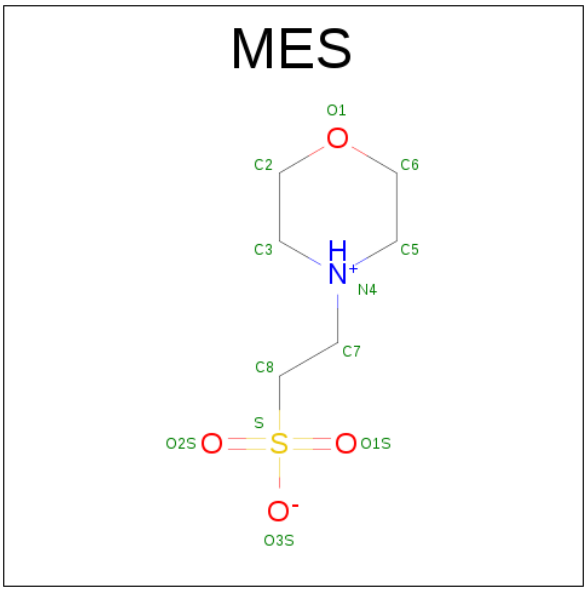
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	G	1	Total Mg 1 1	0	0
15	J	1	Total Mg 1 1	0	0
15	K	2	Total Mg 2 2	0	0
15	b	1	Total Mg 1 1	0	0
15	I	2	Total Mg 2 2	0	0
15	Z	1	Total Mg 1 1	0	0
15	A	1	Total Mg 1 1	0	0
15	N	1	Total Mg 1 1	0	0
15	X	1	Total Mg 1 1	0	0
15	L	1	Total Mg 1 1	0	0

- Molecule 16 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

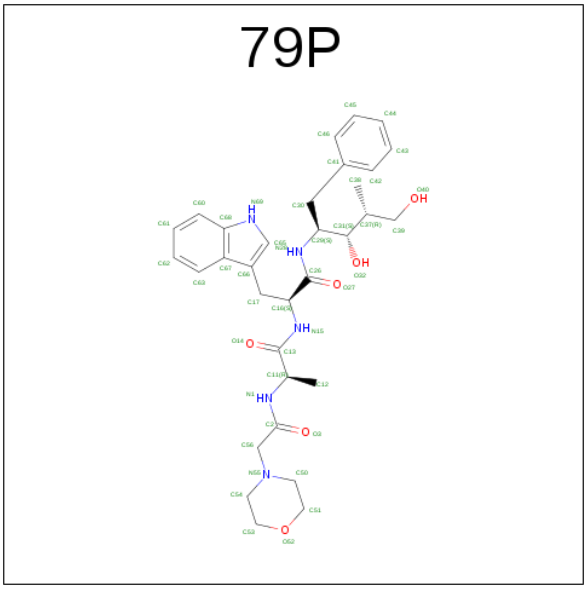
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total Cl 1 1	0	0
16	b	1	Total Cl 1 1	0	0
16	N	1	Total Cl 1 1	0	0
16	U	1	Total Cl 1 1	0	0

- Molecule 17 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
17	K	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
17	V	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
17	Y	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 18 is (2 {S})-3-(1 {H}-indol-3-yl)- {N}-[(2 {S},3 {S},4 {R})-4-methyl-3,5-bis(oxidanyl)-1-phenyl-pentan-2-yl]-2-[[(2 {R})-2-(2-morpholin-4-ylethanoylamino)propanoyl]amino]propanamide (three-letter code: 79P) (formula: $C_{32}H_{43}N_5O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	K	1	Total 43	C 32	N 5	O 6	0	0
18	Y	1	Total 43	C 32	N 5	O 6	0	0

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	12	Total 12	O 12	0	0
19	B	11	Total 11	O 11	0	0
19	C	4	Total 4	O 4	0	0
19	D	9	Total 9	O 9	0	0
19	E	5	Total 5	O 5	0	0
19	F	13	Total 13	O 13	0	0
19	G	10	Total 10	O 10	0	0
19	H	22	Total 22	O 22	0	0
19	I	11	Total 11	O 11	0	0
19	J	10	Total 10	O 10	0	0
19	K	5	Total 5	O 5	0	0
19	L	14	Total 14	O 14	0	0
19	M	16	Total 16	O 16	0	0
19	N	10	Total 10	O 10	0	0
19	O	9	Total 9	O 9	0	0
19	P	11	Total 11	O 11	0	0
19	Q	4	Total 4	O 4	0	0
19	R	4	Total 4	O 4	0	0

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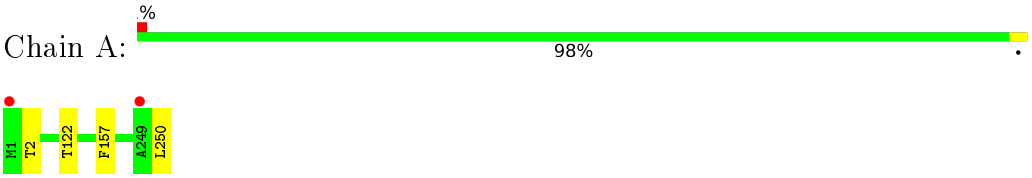
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	S	7	Total O 7 7	0	0
19	T	10	Total O 10 10	0	0
19	U	16	Total O 16 16	0	0
19	V	16	Total O 16 16	0	0
19	W	7	Total O 7 7	0	0
19	X	11	Total O 11 11	0	0
19	Y	9	Total O 9 9	0	0
19	Z	9	Total O 9 9	0	0
19	a	16	Total O 16 16	0	0
19	b	8	Total O 8 8	0	0

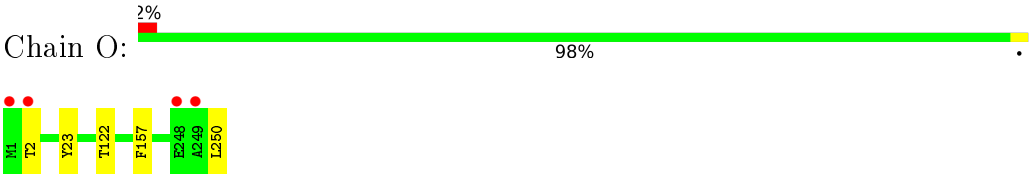
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

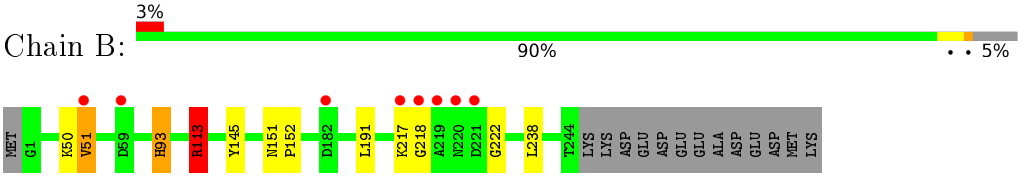
- Molecule 1: Proteasome subunit alpha type-2



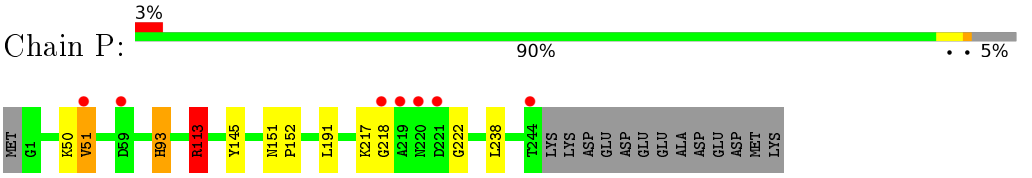
- Molecule 1: Proteasome subunit alpha type-2



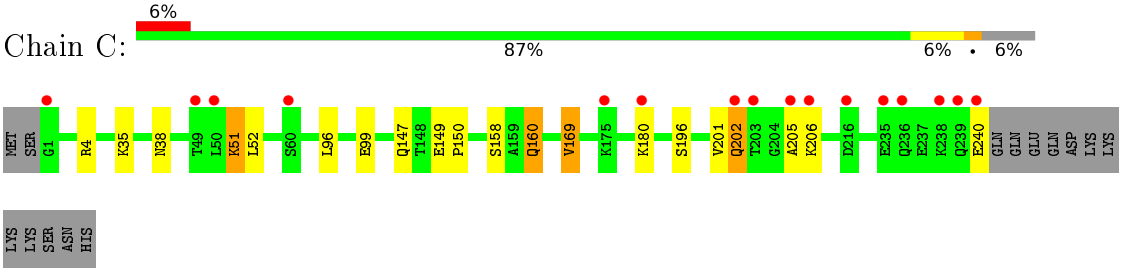
- Molecule 2: Proteasome subunit alpha type-3



- Molecule 2: Proteasome subunit alpha type-3

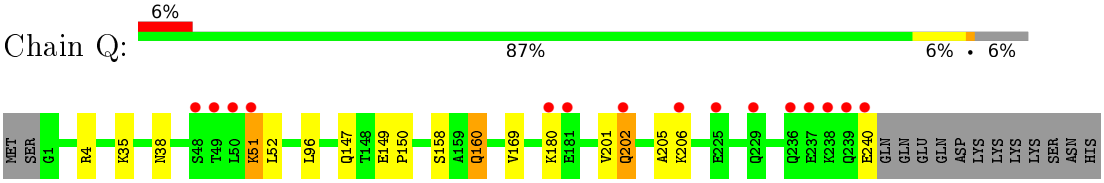


- Molecule 3: Proteasome subunit alpha type-4



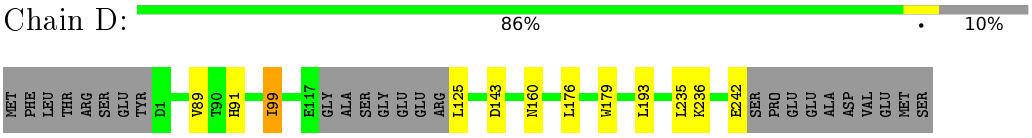
• Molecule 3: Proteasome subunit alpha type-4

Chain Q:



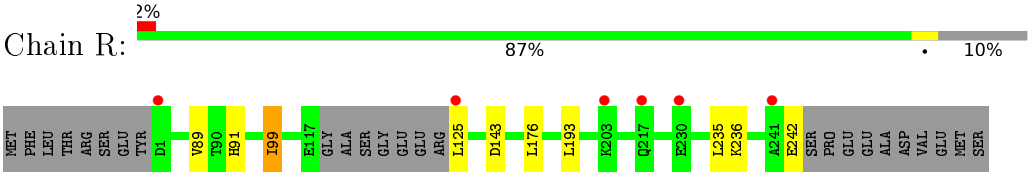
• Molecule 4: Proteasome subunit alpha type-5

Chain D:



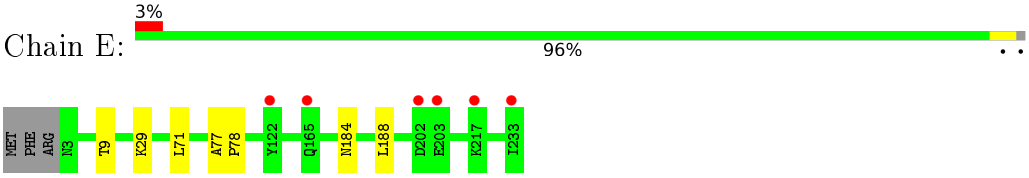
• Molecule 4: Proteasome subunit alpha type-5

Chain R:



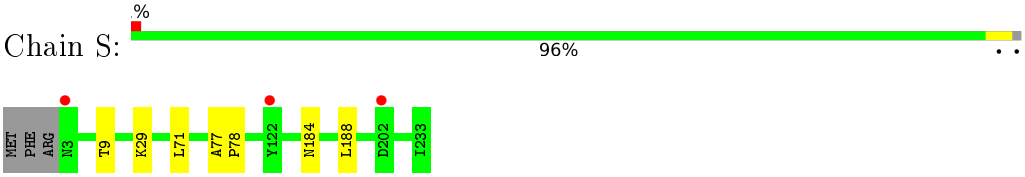
• Molecule 5: Proteasome subunit alpha type-6

Chain E:



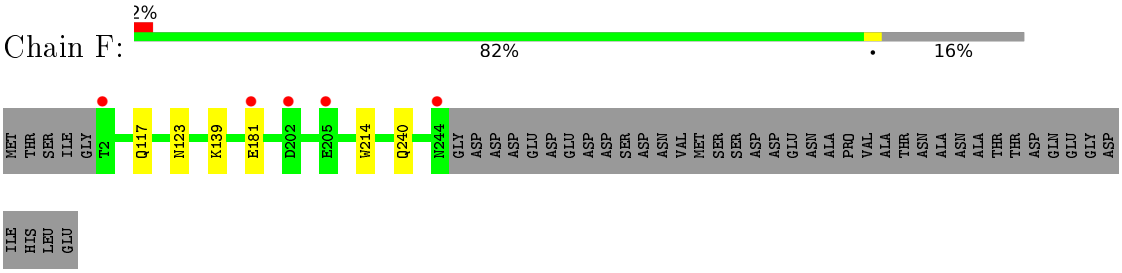
• Molecule 5: Proteasome subunit alpha type-6

Chain S:



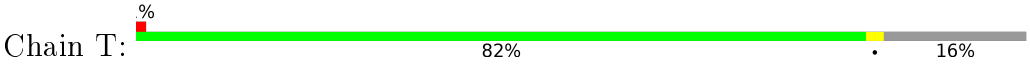
• Molecule 6: Probable proteasome subunit alpha type-7

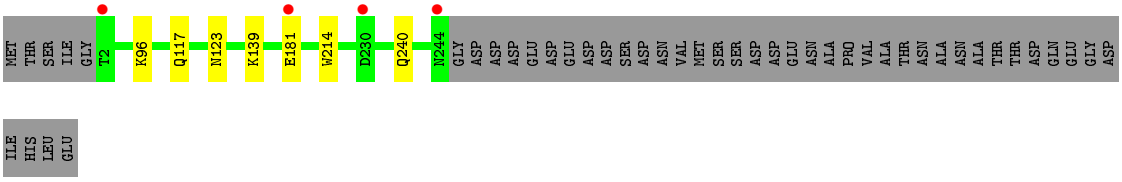
Chain F:



• Molecule 6: Probable proteasome subunit alpha type-7

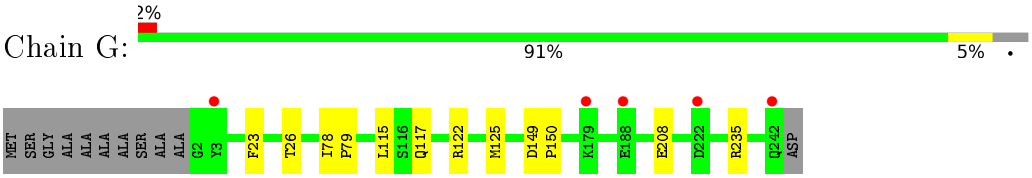
Chain T:





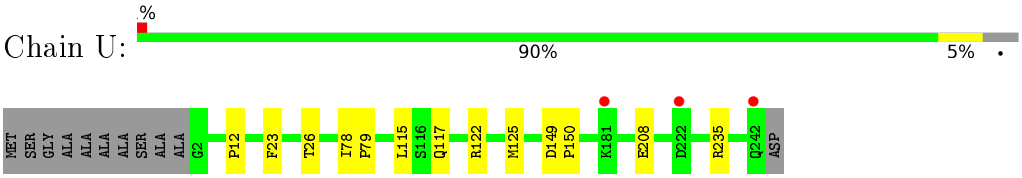
- Molecule 7: Proteasome subunit alpha type-1

Chain G:



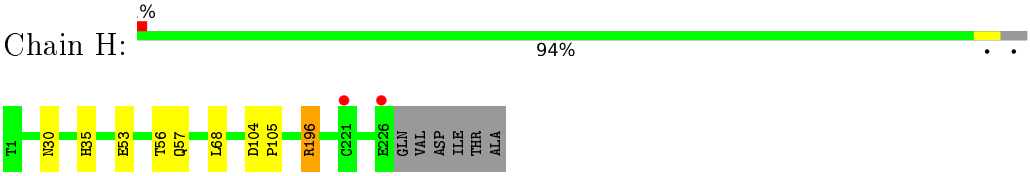
- Molecule 7: Proteasome subunit alpha type-1

Chain U:



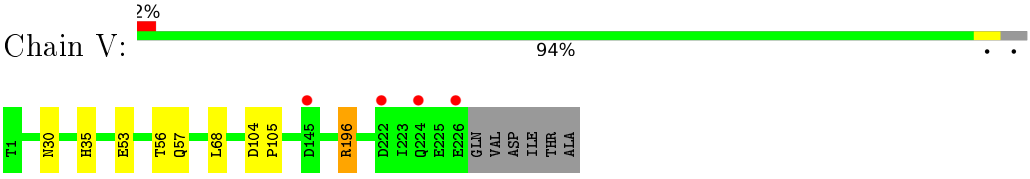
- Molecule 8: Proteasome subunit beta type-2

Chain H:



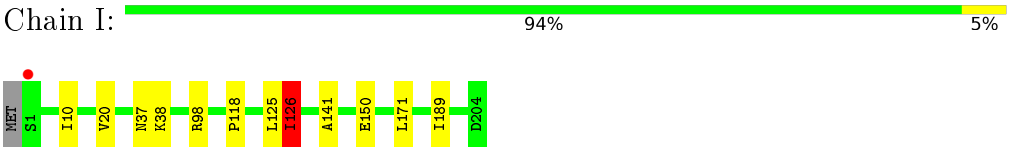
- Molecule 8: Proteasome subunit beta type-2

Chain V:



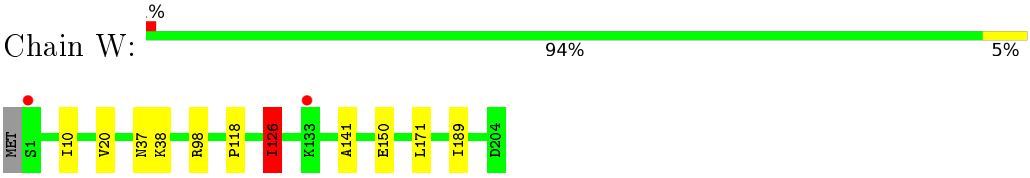
- Molecule 9: Proteasome subunit beta type-3

Chain I:



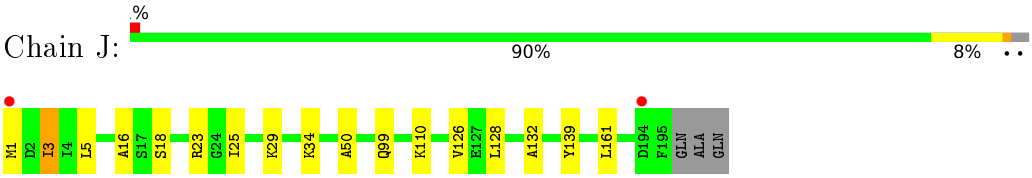
- Molecule 9: Proteasome subunit beta type-3

Chain W:



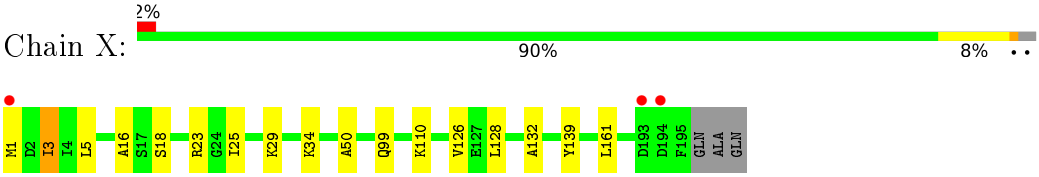
- Molecule 10: Proteasome subunit beta type-4

Chain J:



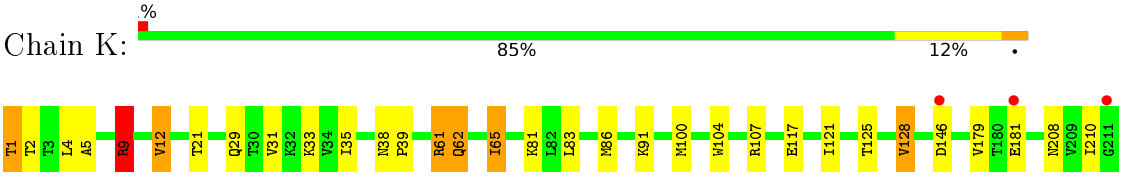
• Molecule 10: Proteasome subunit beta type-4

Chain X:



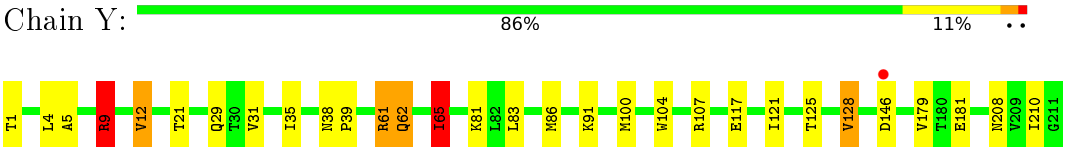
• Molecule 11: Proteasome subunit beta type-5,Proteasome subunit beta type-5

Chain K:



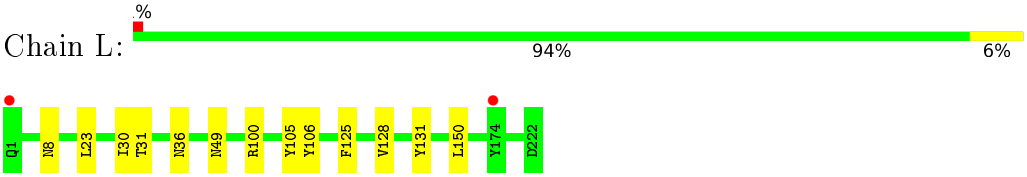
• Molecule 11: Proteasome subunit beta type-5,Proteasome subunit beta type-5

Chain Y:



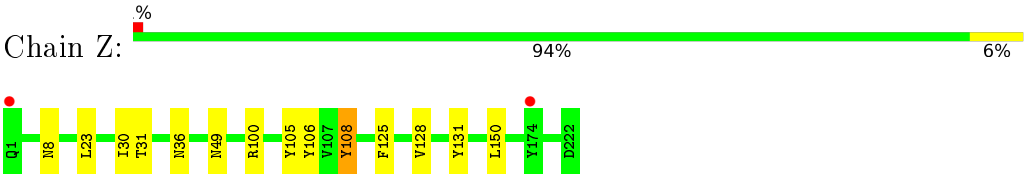
• Molecule 12: Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6

Chain L:



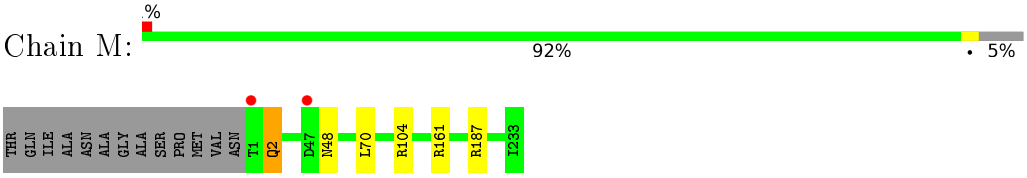
• Molecule 12: Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6

Chain Z:



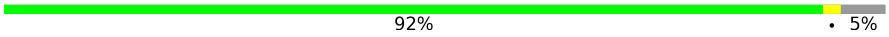
• Molecule 13: Proteasome subunit beta type-7

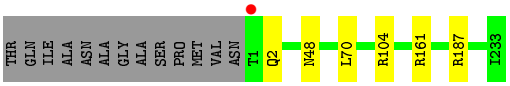
Chain M:



• Molecule 13: Proteasome subunit beta type-7

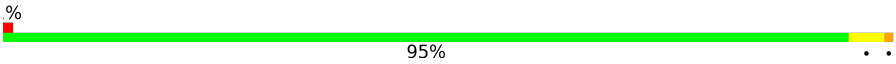
Chain a:

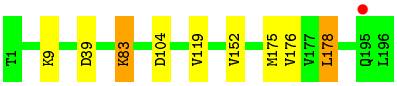




• Molecule 14: Proteasome subunit beta type-1

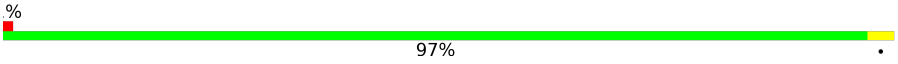
Chain N:

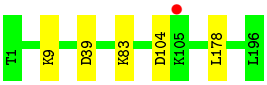




• Molecule 14: Proteasome subunit beta type-1

Chain b:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	135.91Å 300.50Å 145.54Å 90.00° 112.77° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.8 (15.00-2.80) 97.8 (15.00-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.86 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.181 , 0.204 0.186 , 0.208	Depositor DCC
R_{free} test set	12795 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	58.3	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 30.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	49807	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 79P, MES, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.27	0/1952	0.46	0/2642
1	O	0.27	0/1952	0.46	0/2642
2	B	0.29	0/1934	0.64	3/2618 (0.1%)
2	P	0.28	0/1934	0.57	1/2618 (0.0%)
3	C	0.27	0/1910	0.49	0/2586
3	Q	0.27	0/1910	0.49	0/2586
4	D	0.26	0/1837	0.46	0/2475
4	R	0.26	0/1837	0.46	0/2475
5	E	0.27	0/1800	0.46	0/2433
5	S	0.26	0/1800	0.46	0/2433
6	F	0.27	0/1932	0.44	0/2609
6	T	0.27	0/1932	0.44	0/2609
7	G	0.27	0/1945	0.46	0/2634
7	U	0.27	0/1945	0.46	0/2634
8	H	0.25	0/1750	0.47	0/2373
8	V	0.25	0/1750	0.48	0/2373
9	I	0.27	0/1611	0.63	2/2174 (0.1%)
9	W	0.27	0/1611	0.62	2/2174 (0.1%)
10	J	0.26	0/1589	0.48	0/2142
10	X	0.25	0/1589	0.48	0/2142
11	K	0.36	2/1668 (0.1%)	0.81	9/2253 (0.4%)
11	Y	0.36	1/1668 (0.1%)	0.86	9/2253 (0.4%)
12	L	0.30	0/1802	0.50	0/2430
12	Z	0.28	0/1815	0.49	0/2448
13	M	0.26	0/1855	0.50	0/2514
13	a	0.26	0/1855	0.50	0/2514
14	N	0.25	0/1541	0.48	0/2087
14	b	0.25	0/1541	0.47	0/2087
All	All	0.27	3/50265 (0.0%)	0.53	26/67958 (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
11	K	0	1
11	Y	0	1
12	Z	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	Y	9	ARG	CZ-NH2	-5.65	1.25	1.33
11	K	9	ARG	CZ-NH1	-5.41	1.26	1.33
11	K	107	ARG	CD-NE	-5.02	1.38	1.46

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	Y	9	ARG	NE-CZ-NH1	21.23	130.91	120.30
2	B	113	ARG	CG-CD-NE	18.52	150.68	111.80
9	I	126	ILE	CG1-CB-CG2	-16.17	75.82	111.40
11	K	107	ARG	NE-CZ-NH1	-15.04	112.78	120.30
9	W	126	ILE	CG1-CB-CG2	-14.40	79.71	111.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	K	9	ARG	Sidechain
11	Y	9	ARG	Sidechain
12	Z	108[B]	TYR	Mainchain

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	1915	0	1929	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	1915	0	1929	1	0
2	B	1904	0	1904	9	0
2	P	1904	0	1904	10	0
3	C	1881	0	1895	9	0
3	Q	1881	0	1895	7	0
4	D	1813	0	1797	3	0
4	R	1813	0	1797	2	0
5	E	1773	0	1775	1	0
5	S	1773	0	1775	1	0
6	F	1892	0	1883	0	0
6	T	1892	0	1883	1	0
7	G	1907	0	1901	3	0
7	U	1907	0	1901	4	0
8	H	1719	0	1719	5	0
8	V	1719	0	1719	5	0
9	I	1581	0	1574	11	0
9	W	1581	0	1574	7	0
10	J	1561	0	1569	9	0
10	X	1561	0	1569	9	0
11	K	1632	0	1590	17	0
11	Y	1632	0	1590	14	0
12	L	1764	0	1716	4	0
12	Z	1776	0	1724	5	0
13	M	1824	0	1832	1	0
13	a	1824	0	1832	0	0
14	N	1512	0	1481	3	0
14	b	1512	0	1481	0	0
15	A	1	0	0	0	0
15	G	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	K	2	0	0	0	0
15	L	1	0	0	0	0
15	N	1	0	0	0	0
15	X	1	0	0	0	0
15	Z	1	0	0	0	0
15	b	1	0	0	0	0
16	G	1	0	0	0	0
16	N	1	0	0	0	0
16	U	1	0	0	0	0
16	b	1	0	0	0	0
17	H	12	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	K	12	0	13	0	0
17	V	12	0	13	0	0
17	Y	12	0	13	0	0
18	K	43	0	0	1	0
18	Y	43	0	0	1	0
19	A	12	0	0	0	0
19	B	11	0	0	0	0
19	C	4	0	0	0	0
19	D	9	0	0	0	0
19	E	5	0	0	0	0
19	F	13	0	0	0	0
19	G	10	0	0	0	0
19	H	22	0	0	0	0
19	I	11	0	0	0	0
19	J	10	0	0	0	0
19	K	5	0	0	0	0
19	L	14	0	0	0	0
19	M	16	0	0	1	0
19	N	10	0	0	0	0
19	O	9	0	0	0	0
19	P	11	0	0	1	0
19	Q	4	0	0	0	0
19	R	4	0	0	0	0
19	S	7	0	0	0	0
19	T	10	0	0	1	0
19	U	16	0	0	0	0
19	V	16	0	0	0	0
19	W	7	0	0	0	0
19	X	11	0	0	0	0
19	Y	9	0	0	1	0
19	Z	9	0	0	0	0
19	a	16	0	0	0	0
19	b	8	0	0	0	0
All	All	49807	0	49190	125	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 1.

The worst 5 of 125 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)
2:B:93:HIS:NE2	2:B:113:ARG:CD	2.07	1.17
2:B:93:HIS:NE2	2:B:113:ARG:HD2	1.60	1.15
11:K:9:ARG:NH2	11:K:146:ASP:OD1	1.91	1.03
2:B:93:HIS:NE2	2:B:113:ARG:HD3	1.88	0.88
2:P:93:HIS:NE2	2:P:113:ARG:NE	2.26	0.83

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	248/250 (99%)	240 (97%)	7 (3%)	1 (0%)	39	74
1	O	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	39	74
2	B	242/258 (94%)	232 (96%)	7 (3%)	3 (1%)	16	47
2	P	242/258 (94%)	232 (96%)	7 (3%)	3 (1%)	16	47
3	C	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	24	58
3	Q	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	24	58
4	D	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
4	R	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
5	E	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
5	S	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
6	F	241/288 (84%)	239 (99%)	2 (1%)	0	100	100
6	T	241/288 (84%)	239 (99%)	2 (1%)	0	100	100
7	G	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
7	U	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
8	H	224/232 (97%)	221 (99%)	3 (1%)	0	100	100
8	V	224/232 (97%)	221 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
10	J	193/198 (98%)	190 (98%)	3 (2%)	0	100	100
10	X	193/198 (98%)	190 (98%)	3 (2%)	0	100	100
11	K	209/211 (99%)	201 (96%)	7 (3%)	1 (0%)	34	69
11	Y	209/211 (99%)	201 (96%)	7 (3%)	1 (0%)	34	69
12	L	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
12	Z	221/222 (100%)	216 (98%)	5 (2%)	0	100	100
13	M	231/246 (94%)	222 (96%)	9 (4%)	0	100	100
13	a	231/246 (94%)	222 (96%)	9 (4%)	0	100	100
14	N	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
14	b	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
All	All	6283/6612 (95%)	6122 (97%)	147 (2%)	14 (0%)	52	84

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN
2	P	51	VAL
3	Q	202	GLN
1	A	2	THR

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	209/209 (100%)	206 (99%)	3 (1%)	74	94
1	O	209/209 (100%)	206 (99%)	3 (1%)	74	94
2	B	203/216 (94%)	199 (98%)	4 (2%)	63	90
2	P	203/216 (94%)	199 (98%)	4 (2%)	63	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	212/226 (94%)	203 (96%)	9 (4%)	36	71
3	Q	212/226 (94%)	203 (96%)	9 (4%)	36	71
4	D	194/215 (90%)	186 (96%)	8 (4%)	37	72
4	R	194/215 (90%)	186 (96%)	8 (4%)	37	72
5	E	190/193 (98%)	185 (97%)	5 (3%)	54	86
5	S	190/193 (98%)	185 (97%)	5 (3%)	54	86
6	F	201/239 (84%)	195 (97%)	6 (3%)	48	82
6	T	201/239 (84%)	195 (97%)	6 (3%)	48	82
7	G	206/210 (98%)	200 (97%)	6 (3%)	50	83
7	U	206/210 (98%)	200 (97%)	6 (3%)	50	83
8	H	185/190 (97%)	182 (98%)	3 (2%)	70	93
8	V	185/190 (97%)	182 (98%)	3 (2%)	70	93
9	I	172/173 (99%)	169 (98%)	3 (2%)	68	92
9	W	172/173 (99%)	169 (98%)	3 (2%)	68	92
10	J	173/175 (99%)	169 (98%)	4 (2%)	58	88
10	X	173/175 (99%)	169 (98%)	4 (2%)	58	88
11	K	165/165 (100%)	150 (91%)	15 (9%)	12	33
11	Y	165/165 (100%)	149 (90%)	16 (10%)	10	29
12	L	186/186 (100%)	181 (97%)	5 (3%)	52	85
12	Z	187/186 (100%)	182 (97%)	5 (3%)	52	85
13	M	199/208 (96%)	193 (97%)	6 (3%)	48	82
13	a	199/208 (96%)	193 (97%)	6 (3%)	48	82
14	N	162/162 (100%)	157 (97%)	5 (3%)	47	81
14	b	162/162 (100%)	157 (97%)	5 (3%)	47	81
All	All	5315/5534 (96%)	5150 (97%)	165 (3%)	47	81

5 of 165 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	M	104	ARG
3	Q	147	GLN
12	Z	128	VAL
13	M	187	ARG
1	O	157	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 85 such sidechains are listed below:

Mol	Chain	Res	Type
12	L	49	ASN
3	Q	116	GLN
12	Z	3	ASN
12	L	70	ASN
2	P	20	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 22 ligands modelled in this entry, 16 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	MES	H	301	-	12,12,12	1.99	1 (8%)	15,16,16	2.14	3 (20%)
18	79P	K	301	11	45,46,46	1.85	8 (17%)	50,62,62	1.73	9 (18%)
17	MES	K	304	-	12,12,12	2.24	1 (8%)	15,16,16	1.53	2 (13%)
17	MES	V	301	-	12,12,12	2.12	1 (8%)	15,16,16	1.68	3 (20%)
18	79P	Y	301	11	45,46,46	1.86	8 (17%)	50,62,62	1.73	8 (16%)
17	MES	Y	302	-	12,12,12	2.15	1 (8%)	15,16,16	1.64	3 (20%)

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
17	MES	H	301	-	-	0/6/14/14	0/1/1/1
18	79P	K	301	11	-	0/41/50/50	0/4/4/4
17	MES	K	304	-	-	0/6/14/14	0/1/1/1
17	MES	V	301	-	-	0/6/14/14	0/1/1/1
18	79P	Y	301	11	-	0/41/50/50	0/4/4/4
17	MES	Y	302	-	-	0/6/14/14	0/1/1/1

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	304	MES	C8-S	-7.49	1.66	1.77
17	Y	302	MES	C8-S	-7.13	1.66	1.77
17	V	301	MES	C8-S	-6.95	1.67	1.77
17	H	301	MES	C8-S	-6.49	1.67	1.77
18	K	301	79P	C60-C68	-5.92	1.31	1.41

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	K	301	79P	C30-C29-N28	-7.05	102.37	110.17
18	Y	301	79P	C30-C29-N28	-6.78	102.68	110.17
18	Y	301	79P	C56-N55-C54	-3.49	106.02	111.14
18	K	301	79P	O32-C31-C29	-3.13	103.45	109.59
18	Y	301	79P	C17-C16-N15	-2.45	105.61	110.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	K	301	79P	1	0
18	Y	301	79P	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

6.1 Protein, DNA and RNA chains

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^{th} 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	250/250 (100%)	-0.46	2 (0%)	87	81	36, 52, 88, 127	0
1	O	250/250 (100%)	-0.46	4 (1%)	74	66	38, 55, 100, 138	0
2	B	244/258 (94%)	-0.37	8 (3%)	50	38	38, 58, 101, 154	0
2	P	244/258 (94%)	-0.38	7 (2%)	55	43	41, 58, 101, 153	0
3	C	240/254 (94%)	-0.18	16 (6%)	21	12	36, 65, 134, 169	0
3	Q	240/254 (94%)	-0.12	15 (6%)	23	14	42, 73, 152, 196	0
4	D	235/260 (90%)	-0.44	0	100	100	40, 60, 91, 127	0
4	R	235/260 (90%)	-0.34	6 (2%)	59	47	50, 68, 111, 138	0
5	E	231/234 (98%)	-0.36	6 (2%)	59	47	43, 64, 104, 146	0
5	S	231/234 (98%)	-0.34	3 (1%)	79	71	47, 69, 110, 147	0
6	F	243/288 (84%)	-0.50	5 (2%)	67	56	37, 57, 108, 134	0
6	T	243/288 (84%)	-0.43	4 (1%)	74	66	37, 63, 118, 152	0
7	G	241/252 (95%)	-0.50	5 (2%)	67	56	37, 55, 97, 153	0
7	U	241/252 (95%)	-0.50	3 (1%)	81	73	35, 54, 90, 130	0
8	H	226/232 (97%)	-0.51	2 (0%)	85	79	36, 52, 89, 142	0
8	V	226/232 (97%)	-0.50	4 (1%)	71	61	38, 52, 84, 153	0
9	I	204/205 (99%)	-0.69	1 (0%)	91	88	36, 50, 82, 103	0
9	W	204/205 (99%)	-0.66	2 (0%)	84	77	36, 51, 81, 106	0
10	J	195/198 (98%)	-0.51	2 (1%)	84	77	34, 56, 86, 128	0
10	X	195/198 (98%)	-0.49	3 (1%)	76	68	39, 58, 87, 133	0
11	K	211/211 (100%)	-0.44	3 (1%)	78	69	39, 59, 92, 122	0
11	Y	211/211 (100%)	-0.43	1 (0%)	91	88	40, 61, 93, 124	0
12	L	222/222 (100%)	-0.45	2 (0%)	85	79	44, 57, 100, 129	0
12	Z	222/222 (100%)	-0.46	2 (0%)	85	79	42, 59, 100, 132	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	M	233/246 (94%)	-0.60	2 (0%)	85	79	35, 54, 83, 99	0
13	a	233/246 (94%)	-0.57	1 (0%)	93	90	34, 55, 80, 99	0
14	N	196/196 (100%)	-0.63	1 (0%)	91	88	35, 49, 80, 104	0
14	b	196/196 (100%)	-0.64	1 (0%)	91	88	35, 49, 81, 107	0
All	All	6342/6612 (95%)	-0.46	111 (1%)	71	61	34, 58, 102, 196	0

The worst 5 of 111 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	W	1	SER	6.9
10	X	1	MET	6.7
10	J	1	MET	6.2
2	B	221	ASP	5.9
3	Q	206	LYS	5.6

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
17	MES	V	301	12/12	0.83	0.42	7.59	66,74,101,109	0
17	MES	H	301	12/12	0.90	0.36	7.02	69,75,92,95	0
16	CL	N	202	1/1	0.97	0.24	3.80	55,55,55,55	0
15	MG	Z	301	1/1	0.95	0.25	3.47	69,69,69,69	0
15	MG	J	201	1/1	0.97	0.16	3.01	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
17	MES	K	304	12/12	0.92	0.37	2.99	53,56,74,86	12
15	MG	A	301	1/1	0.94	0.20	2.77	52,52,52,52	0
17	MES	Y	302	12/12	0.91	0.31	2.63	55,57,72,77	12
16	CL	b	202	1/1	0.92	0.20	1.78	60,60,60,60	0
15	MG	X	201	1/1	0.87	0.15	1.78	47,47,47,47	0
18	79P	Y	301	43/43	0.92	0.21	1.30	52,59,86,90	0
18	79P	K	301	43/43	0.92	0.19	0.96	48,56,81,88	0
15	MG	b	201	1/1	0.97	0.13	0.39	44,44,44,44	0
15	MG	I	301	1/1	0.96	0.15	0.28	55,55,55,55	0
15	MG	N	201	1/1	0.94	0.12	-0.05	50,50,50,50	0
15	MG	K	302	1/1	0.99	0.08	-1.28	59,59,59,59	0
15	MG	G	301	1/1	0.98	0.05	-1.61	48,48,48,48	0
15	MG	I	302	1/1	0.98	0.07	-2.27	56,56,56,56	0
15	MG	L	301	1/1	0.97	0.06	-3.17	64,64,64,64	0
16	CL	U	301	1/1	1.00	0.19	-	44,44,44,44	0
15	MG	K	303	1/1	0.93	0.59	-	67,67,67,67	0
16	CL	G	302	1/1	0.99	0.12	-	44,44,44,44	0

6.5 Other polymers (i)

There are no such residues in this entry.