Full wwPDB X-ray Structure Validation Report (i)

Dec 20, 2023 – 02:07 pm GMT

PDB ID	:	8BZL
Title	:	Human 20S Proteasome in complex with peptide activator peptide BLM42
Authors	:	Henneberg, F.; Chari, A.; Jankowska, E.; Witkowska, J.
Deposited on	:	2022-12-15
Resolution	:	2.14 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
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 (1)) were used in the production of this report:

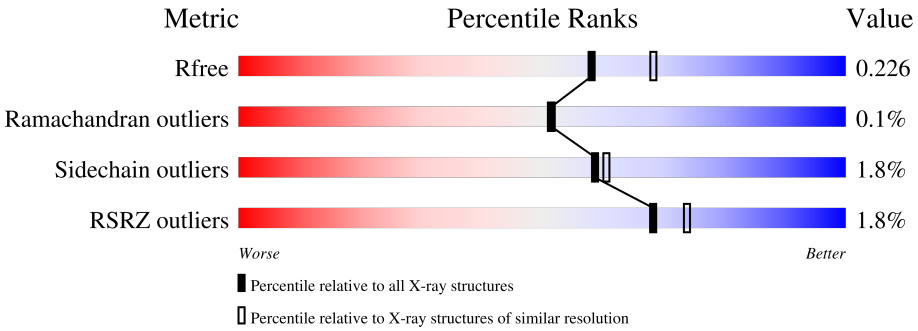
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.14 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	2523 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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	3	205	100%
1	I	205	99%
2	A	234	91% 6%
2	O	234	4% 91% 6%
3	B	261	2% 90% 9%
3	P	261	2% 89% 9%

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Mol	Chain	Length	Quality of chain
4	C	248	8% 88% 9%
4	Q	248	3% 88% 10%
5	D	241	7% 92% 7%
5	R	241	95% 5%
6	E	263	2% 86% 13%
6	S	263	2% 89% 10%
7	F	255	93% 6%
7	T	255	2% 91% 6%
8	G	246	97%
8	U	246	3% 91% 7%
9	H	277	78% 21%
9	V	277	78% 21%
10	J	201	95%
10	X	201	96%
11	K	263	75% 24%
11	Y	263	75% 24%
12	L	241	88% 12%
12	Z	241	88% 12%
13	M	264	80% 19%
13	a	264	81% 19%
14	N	239	82% 18%
14	b	239	% 82% 17%
15	c	14	7% 36% 64%
15	d	14	36% 64%
15	e	14	14% 21% 79%

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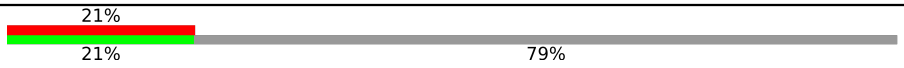
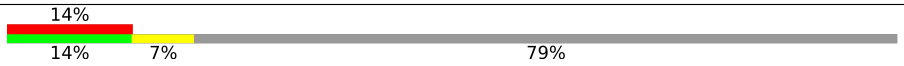
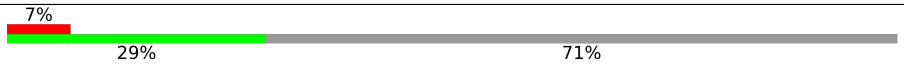
Mol	Chain	Length	Quality of chain
15	f	14	
15	g	14	
15	h	14	

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 50949 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 beta type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	3	204	Total	C	N	O	S	0	1	0
			1582	1007	264	292	19			
1	I	204	Total	C	N	O	S	13	7	0
			1639	1042	275	303	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	227	Total	C	N	O	S	0	2	0
			1773	1133	302	332	6			
2	O	221	Total	C	N	O	S	0	0	0
			1600	1021	274	299	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	238	Total	C	N	O	S	0	0	0
			1814	1146	312	346	10			
3	P	238	Total	C	N	O	S	0	2	0
			1785	1130	307	339	9			

- Molecule 4 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	225	Total	C	N	O	S	0	0	0
			1706	1074	306	321	5			
4	Q	222	Total	C	N	O	S	0	0	0
			1685	1060	300	320	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	225	Total	C	N	O	S	0	1	0
			1641	1031	274	325	11			
5	R	230	Total	C	N	O	S	0	0	0
			1745	1098	291	345	11			

- Molecule 6 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	228	Total	C	N	O	S	0	0	0
			1756	1105	314	326	11			
6	S	237	Total	C	N	O	S	0	3	0
			1855	1166	336	342	11			

- Molecule 7 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	F	240	Total	C	N	O	S	8	5	0
			1885	1198	320	354	13			
7	T	239	Total	C	N	O	S	0	1	0
			1844	1171	316	345	12			

- Molecule 8 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	243	Total	C	N	O	S	0	3	0
			1881	1194	318	356	13			
8	U	230	Total	C	N	O	S	0	0	0
			1747	1105	294	335	13			

- Molecule 9 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	220	Total	C	N	O	S	0	4	0
			1686	1062	291	320	13			
9	V	218	Total	C	N	O	S	5	2	0
			1625	1024	272	317	12			

- Molecule 10 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	196	Total	C	N	O	S	0	2	0
			1576	1011	267	288	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	196	Total	C	N	O	S	0	2	0
			1573	1009	269	285	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	200	Total	C	N	O	S	0	1	0
			1536	971	267	289	9			
11	Y	199	Total	C	N	O	S	0	3	0
			1560	986	275	289	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	213	Total	C	N	O	S	0	2	0
			1647	1044	280	312	11			
12	Z	213	Total	C	N	O	S	0	2	0
			1649	1046	282	310	11			

- Molecule 13 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	214	Total	C	N	O	S	0	0	0
			1669	1053	289	315	12			
13	a	215	Total	C	N	O	S	0	1	0
			1682	1062	290	318	12			

- Molecule 14 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	197	Total	C	N	O	S	0	1	0
			1473	924	249	287	13			
14	b	198	Total	C	N	O	S	0	2	0
			1489	935	252	288	14			

- Molecule 15 is a protein called ARG-SER-TYR-TYR-SER.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	c	5	Total	C	N	O	0	0	0
			41	27	5	9			
15	d	5	Total	C	N	O	0	0	0
			41	27	5	9			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
15	e	3	Total C N O 30 21 3 6	0	0	0
15	f	3	Total C N O 30 21 3 6	0	0	0
15	g	3	Total C N O 29 21 3 5	0	0	0
15	h	4	Total C N O 35 24 4 7	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	3	1	Total Cl 1 1	0	0
16	A	4	Total Cl 4 4	0	0
16	B	2	Total Cl 2 2	0	0
16	C	2	Total Cl 2 2	0	0
16	D	1	Total Cl 1 1	0	0
16	E	3	Total Cl 3 3	0	0
16	F	1	Total Cl 1 1	0	0
16	G	2	Total Cl 2 2	0	0
16	H	2	Total Cl 2 2	0	0
16	I	1	Total Cl 1 1	0	0
16	K	4	Total Cl 4 4	0	0
16	M	4	Total Cl 4 4	0	0
16	N	3	Total Cl 3 3	0	0
16	O	4	Total Cl 4 4	0	0
16	P	1	Total Cl 1 1	0	0

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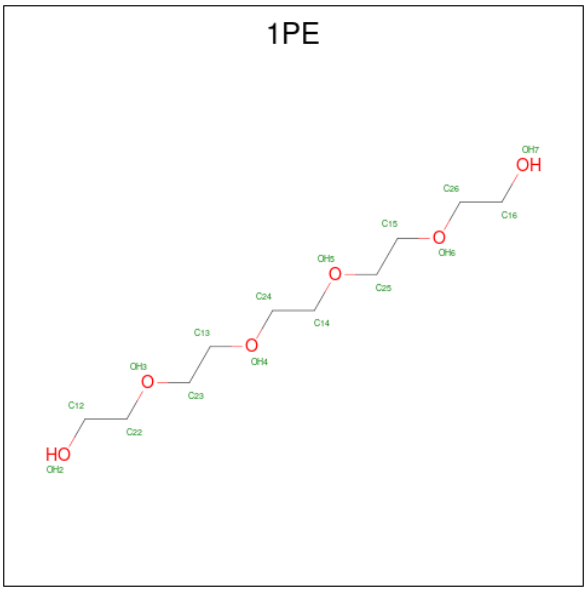
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	Q	2	Total Cl 2 2	0	0
16	R	1	Total Cl 1 1	0	0
16	S	2	Total Cl 2 2	0	0
16	U	1	Total Cl 1 1	0	0
16	V	2	Total Cl 2 2	0	0
16	Y	5	Total Cl 5 5	0	0
16	a	4	Total Cl 4 4	0	0
16	b	2	Total Cl 2 2	0	0

- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	3	1	Total Mg 1 1	0	0
17	H	2	Total Mg 2 2	0	0
17	I	1	Total Mg 1 1	0	0
17	J	1	Total Mg 1 1	0	0
17	K	1	Total Mg 1 1	0	0
17	V	2	Total Mg 2 2	0	0
17	X	1	Total Mg 1 1	0	0
17	Y	1	Total Mg 1 1	0	0

- Molecule 18 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	3	1	Total C O 16 10 6	0	0
18	G	1	Total C O 16 10 6	0	0
18	I	1	Total C O 16 10 6	0	0
18	I	1	Total C O 16 10 6	0	0
18	K	1	Total C O 16 10 6	0	0
18	M	1	Total C O 16 10 6	0	0
18	U	1	Total C O 16 10 6	0	0
18	Y	1	Total C O 16 10 6	0	0
18	a	1	Total C O 16 10 6	0	0

- Molecule 19 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	G	1	Total K 1 1	0	0
19	L	1	Total K 1 1	0	0
19	N	1	Total K 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	U	1	Total K 1 1	0	0
19	Z	1	Total K 1 1	0	0
19	b	1	Total K 1 1	0	0

- Molecule 20 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	3	98	Total O 98 98	0	0
20	A	98	Total O 98 98	0	0
20	B	111	Total O 111 111	0	0
20	C	59	Total O 59 59	0	0
20	D	56	Total O 56 56	0	0
20	E	116	Total O 116 116	0	0
20	F	188	Total O 188 188	0	0
20	G	166	Total O 166 166	0	0
20	H	160	Total O 160 160	0	0
20	I	159	Total O 159 159	0	0
20	J	144	Total O 144 144	0	0
20	K	117	Total O 117 117	0	0
20	L	111	Total O 111 111	0	0
20	M	178	Total O 178 178	0	0
20	N	161	Total O 161 161	0	0
20	O	50	Total O 50 50	0	0

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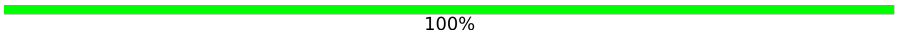
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	P	77	Total O 77 77	0	0
20	Q	51	Total O 51 51	0	0
20	R	111	Total O 111 111	0	0
20	S	103	Total O 103 103	0	0
20	T	104	Total O 104 104	0	0
20	U	82	Total O 82 82	0	0
20	V	110	Total O 110 110	0	0
20	X	131	Total O 131 131	0	0
20	Y	179	Total O 179 179	0	0
20	Z	172	Total O 172 172	0	0
20	a	195	Total O 195 195	0	0
20	b	123	Total O 123 123	0	0
20	c	1	Total O 1 1	0	0
20	d	1	Total O 1 1	0	0
20	e	3	Total O 3 3	0	0
20	f	3	Total O 3 3	0	0
20	g	5	Total O 5 5	0	0
20	h	3	Total O 3 3	0	0

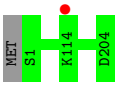
3 Residue-property plots (i)

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 subunit beta type-3

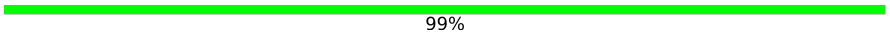
Chain 3:





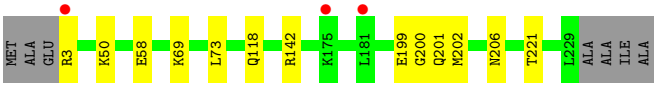
• Molecule 1: Proteasome subunit beta type-3

Chain I:



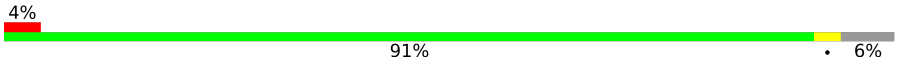
• Molecule 2: Proteasome subunit alpha type-2

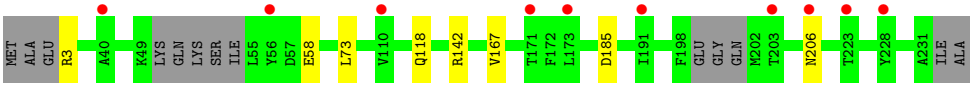
Chain A:



• Molecule 2: Proteasome subunit alpha type-2

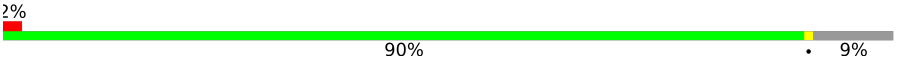
Chain O:

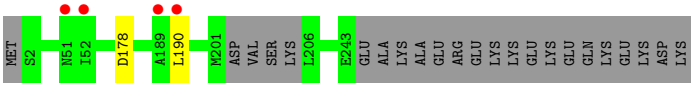




• Molecule 3: Proteasome subunit alpha type-4

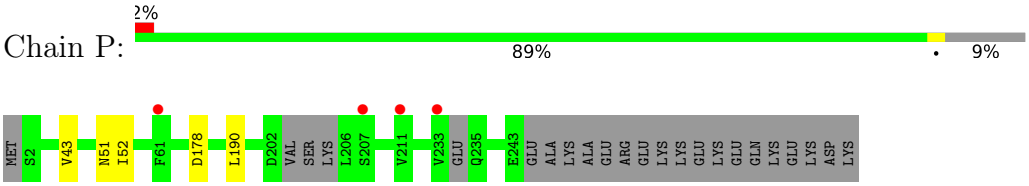
Chain B:





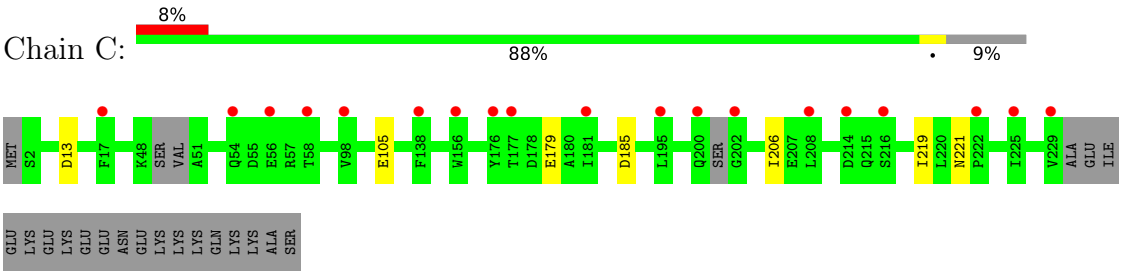
• Molecule 3: Proteasome subunit alpha type-4

Chain P:



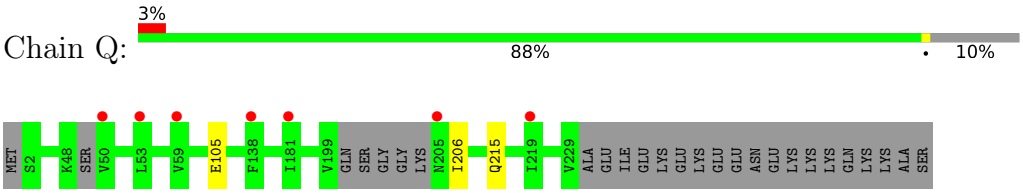
• Molecule 4: Proteasome subunit alpha type-7

Chain C:



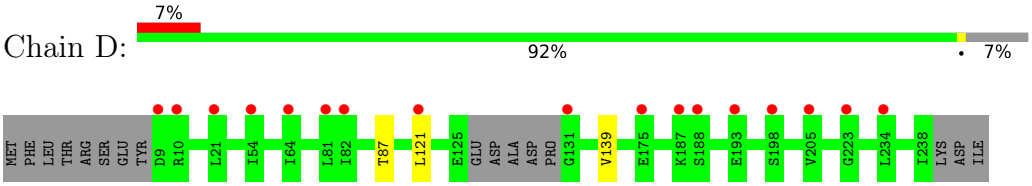
• Molecule 4: Proteasome subunit alpha type-7

Chain Q:



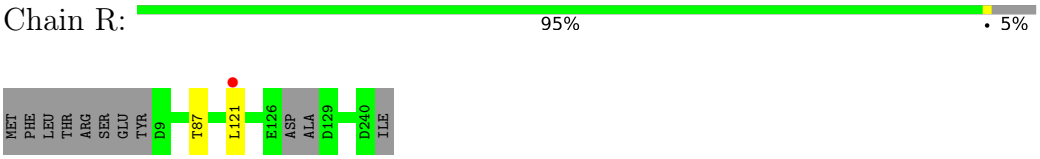
• Molecule 5: Proteasome subunit alpha type-5

Chain D:



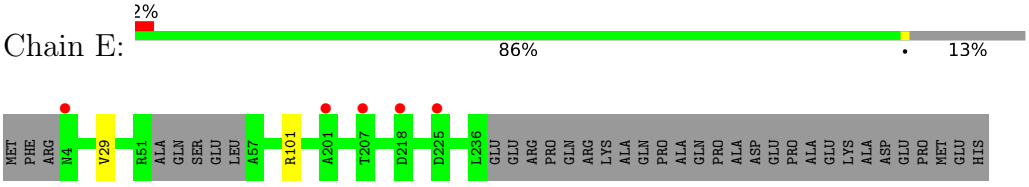
• Molecule 5: Proteasome subunit alpha type-5

Chain R:



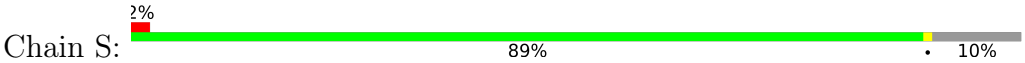
• Molecule 6: Proteasome subunit alpha type-1

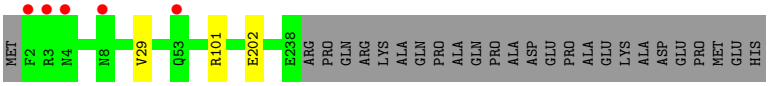
Chain E:



• Molecule 6: Proteasome subunit alpha type-1

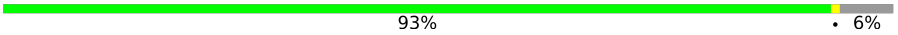
Chain S:

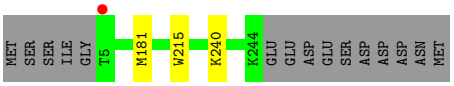




• Molecule 7: Proteasome subunit alpha type-3

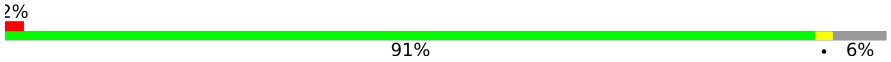
Chain F:

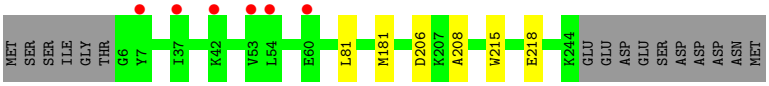




• Molecule 7: Proteasome subunit alpha type-3

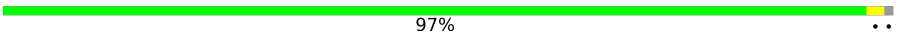
Chain T:





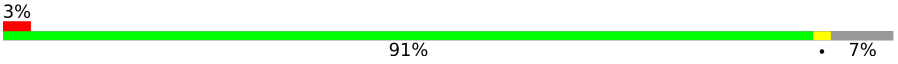
• Molecule 8: Proteasome subunit alpha type-6

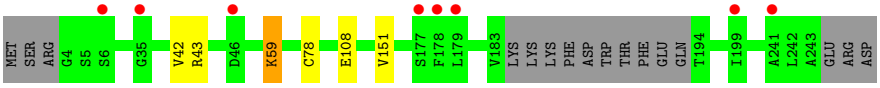
Chain G:



• Molecule 8: Proteasome subunit alpha type-6

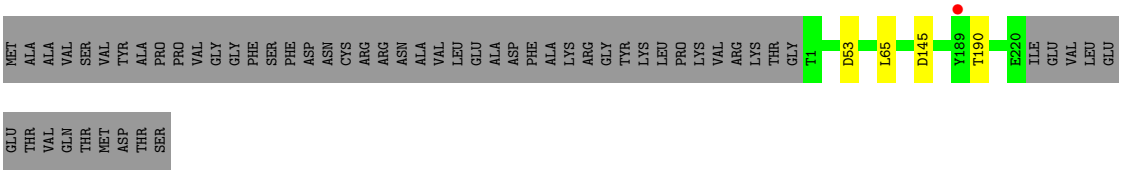
Chain U:





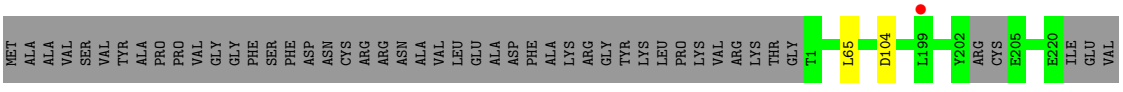
• Molecule 9: Proteasome subunit beta type-7

Chain H:



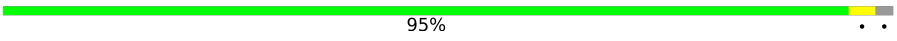
• Molecule 9: Proteasome subunit beta type-7

Chain V:



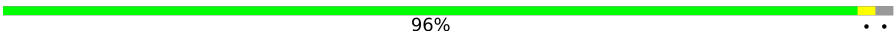
• Molecule 10: Proteasome subunit beta type-2

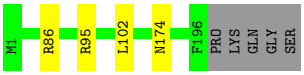
Chain J:



• Molecule 10: Proteasome subunit beta type-2

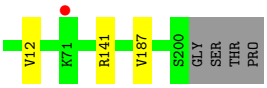
Chain X:





• Molecule 11: Proteasome subunit beta type-5

Chain K:

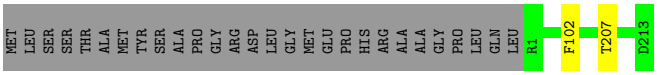


• Molecule 11: Proteasome subunit beta type-5

Chain Y:

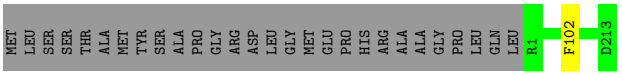
• Molecule 12: Proteasome subunit beta type-1

Chain L:



• Molecule 12: Proteasome subunit beta type-1

Chain Z:

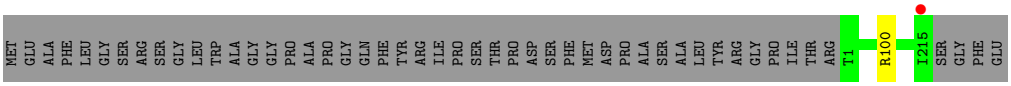


• Molecule 13: Proteasome subunit beta type-4

Chain M:

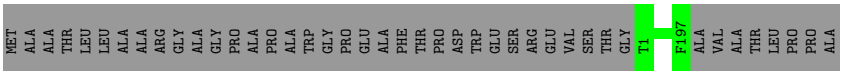
• Molecule 13: Proteasome subunit beta type-4

Chain a:



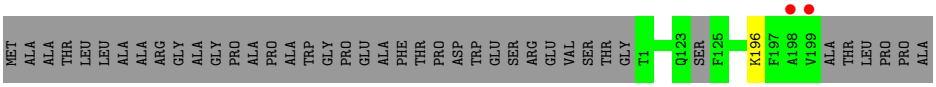
• Molecule 14: Proteasome subunit beta type-6

Chain N:



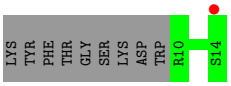
• Molecule 14: Proteasome subunit beta type-6

Chain b:



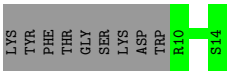
• Molecule 15: ARG-SER-TYR-TYR-SER

Chain c:



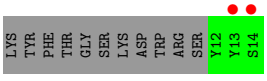
• Molecule 15: ARG-SER-TYR-TYR-SER

Chain d:



• Molecule 15: ARG-SER-TYR-TYR-SER

Chain e:



• Molecule 15: ARG-SER-TYR-TYR-SER

Chain f:

• Molecule 15: ARG-SER-TYR-TYR-SER

Chain g:

• Molecule 15: ARG-SER-TYR-TYR-SER

Chain h:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	113.92Å 203.26Å 316.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	107.12 – 2.14 107.18 – 2.14	Depositor EDS
% Data completeness (in resolution range)	81.6 (107.12-2.14) 81.6 (107.18-2.14)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.196 , 0.226 0.196 , 0.226	Depositor DCC
R_{free} test set	16355 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	39.2	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	50949	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% 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: CL, 6V1, 1PE, MG, K, YCM

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	3	0.25	0/1613	0.55	0/2177
1	I	0.26	0/1674	0.56	0/2255
2	A	0.26	0/1818	0.54	0/2467
2	O	0.27	0/1631	0.54	0/2224
3	B	0.26	0/1842	0.54	0/2494
3	P	0.26	0/1815	0.54	0/2461
4	C	0.25	0/1718	0.55	0/2327
4	Q	0.26	0/1698	0.55	0/2306
5	D	0.26	0/1665	0.52	0/2258
5	R	0.26	0/1771	0.53	0/2391
6	E	0.26	0/1772	0.55	0/2397
6	S	0.26	0/1883	0.55	0/2545
7	F	0.26	0/1932	0.54	0/2603
7	T	0.26	0/1882	0.55	0/2539
8	G	0.26	0/1893	0.55	0/2562
8	U	0.25	0/1749	0.54	0/2368
9	H	0.27	0/1719	0.55	0/2326
9	V	0.30	0/1657	0.54	0/2247
10	J	0.26	0/1612	0.55	0/2181
10	X	0.26	0/1612	0.55	0/2181
11	K	0.26	0/1567	0.56	0/2120
11	Y	0.27	0/1600	0.56	0/2160
12	L	0.27	0/1683	0.56	0/2270
12	Z	0.27	0/1682	0.57	0/2267
13	M	0.27	0/1702	0.58	0/2304
13	a	0.27	0/1718	0.58	0/2326
14	N	0.28	0/1502	0.52	0/2034
14	b	0.27	0/1517	0.52	0/2051
15	c	0.43	0/42	0.72	0/55
15	d	0.42	0/42	0.76	0/55
15	e	0.45	0/31	0.57	0/40
15	f	0.46	0/31	0.62	0/40

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
15	g	0.46	0/30	0.69	0/38
15	h	0.39	0/36	0.54	0/48
All	All	0.26	0/48139	0.55	0/65117

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3	203/205 (99%)	197 (97%)	6 (3%)	0	100	100
1	I	208/205 (102%)	200 (96%)	8 (4%)	0	100	100
2	A	227/234 (97%)	216 (95%)	7 (3%)	4 (2%)	8	2
2	O	215/234 (92%)	210 (98%)	5 (2%)	0	100	100
3	B	234/261 (90%)	229 (98%)	5 (2%)	0	100	100
3	P	233/261 (89%)	227 (97%)	4 (2%)	2 (1%)	17	10
4	C	218/248 (88%)	208 (95%)	9 (4%)	1 (0%)	29	22
4	Q	215/248 (87%)	210 (98%)	5 (2%)	0	100	100
5	D	222/241 (92%)	219 (99%)	3 (1%)	0	100	100
5	R	226/241 (94%)	222 (98%)	4 (2%)	0	100	100
6	E	223/263 (85%)	218 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	S	237/263 (90%)	232 (98%)	5 (2%)	0	100	100
7	F	243/255 (95%)	240 (99%)	3 (1%)	0	100	100
7	T	238/255 (93%)	235 (99%)	2 (1%)	1 (0%)	34	29
8	G	242/246 (98%)	239 (99%)	3 (1%)	0	100	100
8	U	224/246 (91%)	220 (98%)	3 (1%)	1 (0%)	34	29
9	H	222/277 (80%)	218 (98%)	4 (2%)	0	100	100
9	V	216/277 (78%)	212 (98%)	4 (2%)	0	100	100
10	J	196/201 (98%)	192 (98%)	4 (2%)	0	100	100
10	X	196/201 (98%)	192 (98%)	4 (2%)	0	100	100
11	K	199/263 (76%)	196 (98%)	3 (2%)	0	100	100
11	Y	200/263 (76%)	197 (98%)	3 (2%)	0	100	100
12	L	213/241 (88%)	211 (99%)	2 (1%)	0	100	100
12	Z	213/241 (88%)	211 (99%)	2 (1%)	0	100	100
13	M	212/264 (80%)	207 (98%)	5 (2%)	0	100	100
13	a	214/264 (81%)	210 (98%)	4 (2%)	0	100	100
14	N	196/239 (82%)	195 (100%)	1 (0%)	0	100	100
14	b	196/239 (82%)	193 (98%)	3 (2%)	0	100	100
15	c	3/14 (21%)	3 (100%)	0	0	100	100
15	d	3/14 (21%)	3 (100%)	0	0	100	100
15	e	1/14 (7%)	1 (100%)	0	0	100	100
15	f	1/14 (7%)	1 (100%)	0	0	100	100
15	g	1/14 (7%)	1 (100%)	0	0	100	100
15	h	2/14 (14%)	2 (100%)	0	0	100	100
All	All	6092/6960 (88%)	5967 (98%)	116 (2%)	9 (0%)	51	51

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	P	52	ILE
2	A	199	GLU
2	A	50	LYS
3	P	51	ASN
7	T	208	ALA
8	U	59	LYS

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Mol	Chain	Res	Type
4	C	13	ASP
2	A	201	GLN
2	A	200	GLY

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	3	170/174 (98%)	170 (100%)	0	100	100
1	I	179/174 (103%)	178 (99%)	1 (1%)	86	89
2	A	185/191 (97%)	176 (95%)	9 (5%)	25	20
2	O	153/191 (80%)	145 (95%)	8 (5%)	23	18
3	B	185/221 (84%)	183 (99%)	2 (1%)	73	76
3	P	177/221 (80%)	174 (98%)	3 (2%)	60	63
4	C	170/210 (81%)	164 (96%)	6 (4%)	36	33
4	Q	168/210 (80%)	165 (98%)	3 (2%)	59	60
5	D	168/203 (83%)	165 (98%)	3 (2%)	59	60
5	R	190/203 (94%)	188 (99%)	2 (1%)	73	76
6	E	183/223 (82%)	181 (99%)	2 (1%)	73	76
6	S	196/223 (88%)	193 (98%)	3 (2%)	65	68
7	F	197/212 (93%)	194 (98%)	3 (2%)	65	68
7	T	189/212 (89%)	184 (97%)	5 (3%)	46	45
8	G	197/208 (95%)	193 (98%)	4 (2%)	55	57
8	U	181/208 (87%)	175 (97%)	6 (3%)	38	35
9	H	184/228 (81%)	180 (98%)	4 (2%)	52	53
9	V	174/228 (76%)	171 (98%)	3 (2%)	60	63
10	J	167/171 (98%)	161 (96%)	6 (4%)	35	32
10	X	167/171 (98%)	163 (98%)	4 (2%)	49	49
11	K	151/202 (75%)	148 (98%)	3 (2%)	55	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	Y	156/202 (77%)	153 (98%)	3 (2%)	57 59
12	L	177/199 (89%)	175 (99%)	2 (1%)	73 76
12	Z	176/199 (88%)	175 (99%)	1 (1%)	86 89
13	M	176/215 (82%)	173 (98%)	3 (2%)	60 63
13	a	178/215 (83%)	177 (99%)	1 (1%)	86 89
14	N	152/181 (84%)	152 (100%)	0	100 100
14	b	153/181 (84%)	152 (99%)	1 (1%)	84 87
15	c	3/13 (23%)	3 (100%)	0	100 100
15	d	3/13 (23%)	3 (100%)	0	100 100
15	e	2/13 (15%)	2 (100%)	0	100 100
15	f	2/13 (15%)	2 (100%)	0	100 100
15	g	2/13 (15%)	1 (50%)	1 (50%)	0 0
15	h	3/13 (23%)	3 (100%)	0	100 100
All	All	4914/5754 (85%)	4822 (98%)	92 (2%)	59 59

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	3	ARG
2	A	58	GLU
2	A	69	LYS
2	A	73	LEU
2	A	118	GLN
2	A	142	ARG
2	A	202	MET
2	A	206	ASN
2	A	221	THR
3	B	178	ASP
3	B	190	LEU
4	C	105	GLU
4	C	179	GLU
4	C	185	ASP
4	C	206	ILE
4	C	219	ILE
4	C	221	ASN
5	D	87	THR
5	D	121	LEU

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Mol	Chain	Res	Type
5	D	139	VAL
6	E	29	VAL
6	E	101	ARG
7	F	181	MET
7	F	215	TRP
7	F	240	LYS
8	G	42	VAL
8	G	43	ARG
8	G	78	CYS
8	G	183	VAL
9	H	53	ASP
9	H	65	LEU
9	H	145	ASP
9	H	190	THR
1	I	115	THR
10	J	1	MET
10	J	27	GLN
10	J	86	ARG
10	J	102	LEU
10	J	153	ARG
10	J	174	ASN
11	K	12	VAL
11	K	141	ARG
11	K	187	VAL
12	L	102	PHE
12	L	207	THR
13	M	92	LEU
13	M	100	ARG
13	M	155	GLU
2	O	3	ARG
2	O	58	GLU
2	O	73	LEU
2	O	118	GLN
2	O	142	ARG
2	O	167	VAL
2	O	185	ASP
2	O	206	ASN
3	P	43	VAL
3	P	178	ASP
3	P	190	LEU
4	Q	105	GLU
4	Q	206	ILE

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Mol	Chain	Res	Type
4	Q	215	GLN
5	R	87	THR
5	R	121	LEU
6	S	29	VAL
6	S	101	ARG
6	S	202	GLU
7	T	81	LEU
7	T	181	MET
7	T	206	ASP
7	T	215	TRP
7	T	218	GLU
8	U	42	VAL
8	U	43	ARG
8	U	59	LYS
8	U	78	CYS
8	U	108	GLU
8	U	151	VAL
9	V	65	LEU
9	V	104[A]	ASP
9	V	104[B]	ASP
10	X	86	ARG
10	X	95	ARG
10	X	102	LEU
10	X	174	ASN
11	Y	141[A]	ARG
11	Y	141[B]	ARG
11	Y	197	GLU
12	Z	102	PHE
13	a	100	ARG
14	b	196	LYS
15	g	12	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	118	GLN
2	A	206	ASN
3	B	40	ASN
3	B	146	GLN
3	B	155	ASN
4	C	18	GLN
4	C	221	ASN

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Mol	Chain	Res	Type
5	D	227	HIS
6	E	65	HIS
6	E	68	ASN
6	E	86	ASN
7	F	147	GLN
8	G	12	HIS
9	H	91	GLN
9	H	153	ASN
1	I	161	HIS
10	J	24	ASN
10	J	132	HIS
10	J	174	ASN
11	K	162	GLN
11	K	196	HIS
12	L	108	ASN
12	L	157	ASN
13	M	47	ASN
13	M	162	GLN
13	M	208	ASN
14	N	193	GLN
2	O	118	GLN
3	P	40	ASN
3	P	146	GLN
4	Q	18	GLN
4	Q	94	HIS
5	R	227	HIS
6	S	20	HIS
6	S	86	ASN
8	U	128	ASN
9	V	91	GLN
10	X	174	ASN
11	Y	162	GLN
12	Z	79	ASN
12	Z	108	ASN
13	a	47	ASN
13	a	89	HIS
13	a	162	GLN
13	a	208	ASN
14	b	193	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

8 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
8	6V1	U	161	8	12,15,16	0.54	0	9,20,22	0.95	0
8	6V1	G	161	8	12,15,16	0.63	0	9,20,22	1.07	0
8	YCM	U	137	8	7,9,10	0.54	0	4,10,12	0.46	0
6	6V1	E	148	6	12,15,16	0.63	0	9,20,22	0.79	0
4	YCM	C	63	4	7,9,10	0.49	0	4,10,12	0.52	0
6	6V1	S	148	6	12,15,16	0.66	0	9,20,22	0.89	0
8	YCM	G	137	8	7,9,10	0.56	0	4,10,12	0.46	0
4	YCM	Q	63	4	7,9,10	0.46	0	4,10,12	0.59	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
8	6V1	U	161	8	-	2/6/25/27	0/1/1/1
8	6V1	G	161	8	-	0/6/25/27	0/1/1/1
8	YCM	U	137	8	-	4/6/8/10	-
6	6V1	E	148	6	-	1/6/25/27	0/1/1/1
4	YCM	C	63	4	-	2/6/8/10	-
6	6V1	S	148	6	-	1/6/25/27	0/1/1/1
8	YCM	G	137	8	-	4/6/8/10	-
4	YCM	Q	63	4	-	5/6/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	G	137	YCM	C-CA-CB-SG
8	G	137	YCM	CE-CD-SG-CB
8	G	137	YCM	SG-CD-CE-NZ2
4	Q	63	YCM	N-CA-CB-SG
4	Q	63	YCM	C-CA-CB-SG
4	Q	63	YCM	CE-CD-SG-CB
4	Q	63	YCM	SG-CD-CE-OZ1
4	Q	63	YCM	SG-CD-CE-NZ2
8	U	137	YCM	C-CA-CB-SG
8	U	137	YCM	CE-CD-SG-CB
8	U	137	YCM	SG-CD-CE-NZ2
8	U	161	6V1	C-CA-CB-SG
4	C	63	YCM	CE-CD-SG-CB
8	U	161	6V1	N-CA-CB-SG
4	C	63	YCM	SG-CD-CE-NZ2
8	G	137	YCM	N-CA-CB-SG
8	U	137	YCM	N-CA-CB-SG
6	E	148	6V1	CA-CB-SG-C1
6	S	148	6V1	CA-CB-SG-C1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 79 ligands modelled in this entry, 70 are monoatomic - leaving 9 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	$\#\|Z\|>2$
18	1PE	I	304	-	15,15,15	0.16	0	14,14,14	0.13	0
18	1PE	Y	307	-	15,15,15	0.19	0	14,14,14	0.11	0
18	1PE	U	303	-	15,15,15	0.19	0	14,14,14	0.11	0
18	1PE	a	305	-	15,15,15	0.19	0	14,14,14	0.10	0
18	1PE	M	305	-	15,15,15	0.19	0	14,14,14	0.10	0
18	1PE	G	304	-	15,15,15	0.16	0	14,14,14	0.12	0
18	1PE	3	303	-	15,15,15	0.19	0	14,14,14	0.11	0
18	1PE	K	306	-	15,15,15	0.17	0	14,14,14	0.14	0
18	1PE	I	303	-	15,15,15	0.22	0	14,14,14	0.11	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
18	1PE	I	304	-	-	6/13/13/13	-
18	1PE	Y	307	-	-	9/13/13/13	-
18	1PE	U	303	-	-	3/13/13/13	-
18	1PE	a	305	-	-	4/13/13/13	-
18	1PE	M	305	-	-	7/13/13/13	-
18	1PE	G	304	-	-	6/13/13/13	-
18	1PE	3	303	-	-	9/13/13/13	-
18	1PE	K	306	-	-	8/13/13/13	-
18	1PE	I	303	-	-	7/13/13/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	G	304	1PE	OH2-C12-C22-OH3
18	I	304	1PE	OH5-C14-C24-OH4
18	I	304	1PE	OH6-C15-C25-OH5
18	3	303	1PE	OH6-C15-C25-OH5
18	Y	307	1PE	OH5-C14-C24-OH4
18	I	303	1PE	OH7-C16-C26-OH6
18	3	303	1PE	OH5-C14-C24-OH4

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Mol	Chain	Res	Type	Atoms
18	G	304	1PE	OH7-C16-C26-OH6
18	a	305	1PE	OH7-C16-C26-OH6
18	Y	307	1PE	OH4-C13-C23-OH3
18	I	304	1PE	OH7-C16-C26-OH6
18	K	306	1PE	OH2-C12-C22-OH3
18	K	306	1PE	OH7-C16-C26-OH6
18	M	305	1PE	OH2-C12-C22-OH3
18	a	305	1PE	OH2-C12-C22-OH3
18	I	303	1PE	OH6-C15-C25-OH5
18	I	304	1PE	OH4-C13-C23-OH3
18	M	305	1PE	OH7-C16-C26-OH6
18	U	303	1PE	OH7-C16-C26-OH6
18	K	306	1PE	OH5-C14-C24-OH4
18	M	305	1PE	C13-C23-OH3-C22
18	M	305	1PE	C23-C13-OH4-C24
18	I	303	1PE	C14-C24-OH4-C13
18	U	303	1PE	C12-C22-OH3-C23
18	K	306	1PE	C25-C15-OH6-C26
18	a	305	1PE	C13-C23-OH3-C22
18	3	303	1PE	C12-C22-OH3-C23
18	I	303	1PE	C12-C22-OH3-C23
18	I	303	1PE	C25-C15-OH6-C26
18	Y	307	1PE	C24-C14-OH5-C25
18	G	304	1PE	C13-C23-OH3-C22
18	Y	307	1PE	C16-C26-OH6-C15
18	3	303	1PE	OH2-C12-C22-OH3
18	I	304	1PE	C15-C25-OH5-C14
18	Y	307	1PE	C12-C22-OH3-C23
18	3	303	1PE	C23-C13-OH4-C24
18	U	303	1PE	C25-C15-OH6-C26
18	3	303	1PE	OH4-C13-C23-OH3
18	3	303	1PE	C24-C14-OH5-C25
18	K	306	1PE	C14-C24-OH4-C13
18	G	304	1PE	C14-C24-OH4-C13
18	K	306	1PE	C13-C23-OH3-C22
18	K	306	1PE	OH4-C13-C23-OH3
18	I	304	1PE	C13-C23-OH3-C22
18	Y	307	1PE	C13-C23-OH3-C22
18	3	303	1PE	C14-C24-OH4-C13
18	Y	307	1PE	C25-C15-OH6-C26
18	M	305	1PE	C24-C14-OH5-C25
18	K	306	1PE	C12-C22-OH3-C23

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Mol	Chain	Res	Type	Atoms
18	Y	307	1PE	C15-C25-OH5-C14
18	M	305	1PE	C25-C15-OH6-C26
18	a	305	1PE	OH5-C14-C24-OH4
18	I	303	1PE	C13-C23-OH3-C22
18	3	303	1PE	C15-C25-OH5-C14
18	Y	307	1PE	OH6-C15-C25-OH5
18	G	304	1PE	OH5-C14-C24-OH4
18	M	305	1PE	OH6-C15-C25-OH5
18	G	304	1PE	C25-C15-OH6-C26
18	I	303	1PE	OH5-C14-C24-OH4

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	3	204/205 (99%)	-0.07	1 (0%) 91 93	32, 47, 66, 83	0
1	I	204/205 (99%)	-0.14	0 100 100	22, 31, 50, 69	0
2	A	227/234 (97%)	0.06	3 (1%) 77 81	27, 45, 84, 100	0
2	O	221/234 (94%)	0.26	10 (4%) 33 40	42, 62, 98, 107	0
3	B	238/261 (91%)	0.15	4 (1%) 70 75	30, 53, 88, 114	0
3	P	238/261 (91%)	0.16	4 (1%) 70 75	35, 56, 98, 127	0
4	C	224/248 (90%)	0.57	19 (8%) 10 14	37, 63, 103, 120	0
4	Q	221/248 (89%)	0.25	7 (3%) 47 55	34, 58, 104, 115	0
5	D	225/241 (93%)	0.51	17 (7%) 13 17	39, 66, 90, 98	0
5	R	230/241 (95%)	0.15	1 (0%) 92 94	25, 50, 74, 98	0
6	E	227/263 (86%)	0.14	5 (2%) 62 68	28, 45, 83, 102	0
6	S	236/263 (89%)	0.09	5 (2%) 63 69	32, 47, 80, 105	0
7	F	240/255 (94%)	0.01	1 (0%) 92 94	24, 34, 61, 81	0
7	T	239/255 (93%)	0.19	6 (2%) 57 64	36, 52, 79, 97	0
8	G	241/246 (97%)	0.00	1 (0%) 92 94	22, 37, 72, 98	0
8	U	228/246 (92%)	0.31	8 (3%) 44 51	41, 62, 92, 107	0
9	H	220/277 (79%)	0.11	1 (0%) 91 93	21, 30, 77, 106	0
9	V	218/277 (78%)	0.04	1 (0%) 91 93	34, 47, 78, 107	0
10	J	196/201 (97%)	-0.09	1 (0%) 91 93	24, 37, 54, 72	0
10	X	196/201 (97%)	-0.07	0 100 100	29, 40, 55, 73	0
11	K	200/263 (76%)	-0.06	1 (0%) 91 93	31, 43, 65, 75	0
11	Y	199/263 (75%)	-0.09	0 100 100	23, 32, 52, 66	0
12	L	213/241 (88%)	0.04	0 100 100	29, 47, 74, 87	0
12	Z	213/241 (88%)	-0.00	0 100 100	20, 33, 58, 79	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	214/264 (81%)	0.02	0 100 100	22, 36, 64, 86	0
13	a	215/264 (81%)	0.00	1 (0%) 91 93	21, 33, 61, 86	0
14	N	197/239 (82%)	-0.09	0 100 100	20, 29, 49, 63	0
14	b	198/239 (82%)	-0.10	2 (1%) 82 86	26, 37, 59, 81	0
15	c	5/14 (35%)	0.97	1 (20%) 1 1	54, 55, 56, 56	3 (60%)
15	d	5/14 (35%)	1.07	0 100 100	59, 61, 61, 63	2 (40%)
15	e	3/14 (21%)	2.05	2 (66%) 0 0	82, 82, 91, 98	0
15	f	3/14 (21%)	3.49	3 (100%) 0 0	90, 90, 92, 94	0
15	g	3/14 (21%)	3.07	2 (66%) 0 0	59, 59, 60, 66	2 (66%)
15	h	4/14 (28%)	1.34	1 (25%) 0 0	59, 63, 65, 69	3 (75%)
All	All	6145/6960 (88%)	0.10	108 (1%) 68 74	20, 45, 85, 127	10 (0%)

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	f	12	TYR	4.6
4	C	176	TYR	4.3
4	C	138	PHE	4.2
6	E	201	ALA	4.0
4	C	200	GLN	4.0
15	g	13	TYR	3.8
4	Q	138	PHE	3.7
4	Q	59	VAL	3.6
15	g	12	TYR	3.6
7	F	5	THR	3.6
5	R	121	LEU	3.4
15	f	13	TYR	3.4
2	O	171	THR	3.3
4	Q	181	ILE	3.3
6	S	4	ASN	3.3
4	Q	50	VAL	3.3
5	D	188	SER	3.2
2	O	191	ILE	3.2
4	C	225	ILE	3.2
5	D	223	GLY	3.1
3	P	233	VAL	3.1
3	B	51	ASN	3.1
4	Q	53	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
5	D	234	LEU	3.0
4	C	222	PRO	3.0
5	D	82	ILE	3.0
5	D	198	SER	3.0
8	U	199	ILE	3.0
2	O	228	TYR	3.0
4	Q	219	ILE	2.9
8	U	179	LEU	2.9
4	C	156	TRP	2.9
10	J	1	MET	2.8
14	b	199	VAL	2.8
6	E	225	ASP	2.7
15	e	14	SER	2.7
5	D	131	GLY	2.7
4	C	202	GLY	2.7
5	D	64	ILE	2.7
2	O	173	LEU	2.7
7	T	53	VAL	2.6
4	C	195	LEU	2.6
4	C	229	VAL	2.6
4	C	98	VAL	2.6
6	S	3	ARG	2.6
2	O	223	THR	2.6
8	U	6	SER	2.5
2	A	3	ARG	2.5
5	D	9	ASP	2.5
6	S	2	PHE	2.5
2	A	175	LYS	2.5
3	B	189	ALA	2.5
15	f	14	SER	2.5
8	U	35	GLY	2.5
4	C	56	GLU	2.5
7	T	60	GLU	2.5
7	T	42	LYS	2.5
4	C	54	GLN	2.4
3	B	190	LEU	2.4
3	P	61	PHE	2.4
9	V	199	LEU	2.4
14	b	198	ALA	2.4
2	O	206	ASN	2.3
5	D	121	LEU	2.3
5	D	205	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	O	40	ALA	2.3
11	K	71	LYS	2.3
6	E	218	ASP	2.3
5	D	81	LEU	2.3
3	P	207	SER	2.3
5	D	10	ARG	2.3
4	C	214	ASP	2.3
7	T	37	ILE	2.3
15	h	13	TYR	2.2
8	U	241	ALA	2.2
4	C	58	THR	2.2
5	D	193	GLU	2.2
3	P	211	VAL	2.2
8	G	187[A]	PHE	2.2
15	c	14	SER	2.2
15	e	13	TYR	2.2
8	U	177	SER	2.2
5	D	187	LYS	2.2
7	T	7	TYR	2.2
9	H	189	TYR	2.2
4	C	181	ILE	2.1
5	D	54	ILE	2.1
7	T	54	LEU	2.1
2	O	110	VAL	2.1
4	C	17	PHE	2.1
6	E	4	ASN	2.1
8	U	178	PHE	2.1
4	C	216	SER	2.1
6	E	207	THR	2.1
6	S	53	GLN	2.1
4	Q	205	ASN	2.1
2	A	181	LEU	2.1
2	O	56	TYR	2.1
2	O	203	THR	2.1
5	D	21	LEU	2.1
4	C	177	THR	2.1
1	3	114	LYS	2.1
8	U	46	ASP	2.0
5	D	175[A]	GLU	2.0
6	S	8	ASN	2.0
3	B	52	ILE	2.0
13	a	215	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
4	C	208	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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^{th} 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	YCM	Q	63	10/11	0.83	0.15	57,61,68,69	0
6	6V1	S	148	15/16	0.87	0.19	42,71,80,81	0
8	YCM	U	137	10/11	0.88	0.19	53,60,71,71	0
6	6V1	E	148	15/16	0.89	0.17	40,65,73,75	0
8	6V1	U	161	15/16	0.89	0.20	59,77,83,84	0
4	YCM	C	63	10/11	0.93	0.14	57,59,65,67	0
8	YCM	G	137	10/11	0.93	0.14	35,42,56,59	0
8	6V1	G	161	15/16	0.94	0.13	32,48,54,56	0

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, 95^{th} 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
17	MG	H	303	1/1	0.73	0.10	42,42,42,42	0
18	1PE	K	306	16/16	0.77	0.21	62,69,79,79	0
18	1PE	a	305	16/16	0.78	0.23	73,82,88,89	0
18	1PE	I	304	16/16	0.79	0.27	65,79,92,92	0
19	K	L	301	1/1	0.79	0.16	73,73,73,73	0
18	1PE	M	305	16/16	0.81	0.17	83,87,93,94	0
18	1PE	Y	307	16/16	0.81	0.21	63,77,82,83	0
16	CL	M	302	1/1	0.81	0.13	76,76,76,76	0
18	1PE	I	303	16/16	0.81	0.17	59,69,74,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
17	MG	X	301	1/1	0.84	0.04	51,51,51,51	0
18	1PE	3	303	16/16	0.84	0.12	70,74,78,80	0
16	CL	E	303	1/1	0.84	0.19	91,91,91,91	0
17	MG	K	305	1/1	0.85	0.06	44,44,44,44	0
16	CL	K	303	1/1	0.85	0.17	83,83,83,83	0
16	CL	S	302	1/1	0.86	0.15	78,78,78,78	0
16	CL	O	303	1/1	0.87	0.10	83,83,83,83	0
19	K	b	303	1/1	0.87	0.10	59,59,59,59	0
16	CL	C	302	1/1	0.88	0.22	85,85,85,85	0
16	CL	Y	303	1/1	0.89	0.12	65,65,65,65	0
18	1PE	U	303	16/16	0.89	0.15	53,56,70,71	0
16	CL	D	301	1/1	0.90	0.13	88,88,88,88	0
16	CL	C	301	1/1	0.90	0.12	73,73,73,73	0
16	CL	O	304	1/1	0.91	0.11	91,91,91,91	0
16	CL	O	301	1/1	0.91	0.09	71,71,71,71	0
16	CL	K	302	1/1	0.92	0.09	75,75,75,75	0
16	CL	V	302	1/1	0.92	0.08	87,87,87,87	0
17	MG	V	303	1/1	0.93	0.09	48,48,48,48	0
16	CL	I	301	1/1	0.93	0.10	49,49,49,49	0
16	CL	A	304	1/1	0.93	0.10	76,76,76,76	0
17	MG	J	301	1/1	0.94	0.05	44,44,44,44	0
16	CL	B	302	1/1	0.94	0.07	62,62,62,62	0
16	CL	V	301	1/1	0.94	0.06	73,73,73,73	0
16	CL	3	301	1/1	0.94	0.10	67,67,67,67	0
16	CL	Q	302	1/1	0.94	0.08	67,67,67,67	0
16	CL	a	301	1/1	0.94	0.09	63,63,63,63	0
16	CL	R	301	1/1	0.94	0.06	66,66,66,66	0
18	1PE	G	304	16/16	0.95	0.13	41,46,55,56	0
16	CL	S	301	1/1	0.95	0.51	85,85,85,85	0
16	CL	F	301	1/1	0.95	0.10	73,73,73,73	0
16	CL	G	302	1/1	0.95	0.10	92,92,92,92	0
16	CL	H	301	1/1	0.95	0.11	66,66,66,66	0
16	CL	E	302	1/1	0.96	0.06	54,54,54,54	0
16	CL	Y	305	1/1	0.96	0.14	63,63,63,63	0
16	CL	A	302	1/1	0.96	0.09	70,70,70,70	0
16	CL	a	302	1/1	0.96	0.14	63,63,63,63	0
19	K	U	302	1/1	0.96	0.07	50,50,50,50	0
16	CL	P	301	1/1	0.96	0.11	55,55,55,55	0
16	CL	U	301	1/1	0.97	0.11	59,59,59,59	0
16	CL	a	304	1/1	0.97	0.08	58,58,58,58	0
16	CL	N	301	1/1	0.97	0.09	50,50,50,50	0
16	CL	K	301	1/1	0.97	0.07	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
16	CL	Y	301	1/1	0.97	0.10	41,41,41,41	0
16	CL	O	302	1/1	0.97	0.08	66,66,66,66	0
17	MG	V	304	1/1	0.97	0.09	51,51,51,51	0
16	CL	Y	304	1/1	0.97	0.08	63,63,63,63	0
19	K	N	304	1/1	0.97	0.08	47,47,47,47	0
16	CL	K	304	1/1	0.97	0.08	74,74,74,74	0
19	K	Z	301	1/1	0.97	0.12	51,51,51,51	0
16	CL	B	301	1/1	0.97	0.07	42,42,42,42	0
16	CL	H	302	1/1	0.98	0.17	58,58,58,58	0
16	CL	E	301	1/1	0.98	0.11	71,71,71,71	0
16	CL	b	301	1/1	0.98	0.05	49,49,49,49	0
16	CL	b	302	1/1	0.98	0.10	57,57,57,57	0
17	MG	3	302	1/1	0.98	0.05	38,38,38,38	0
16	CL	M	301	1/1	0.98	0.14	69,69,69,69	0
17	MG	H	304	1/1	0.98	0.06	33,33,33,33	0
16	CL	A	301	1/1	0.98	0.06	56,56,56,56	0
16	CL	M	304	1/1	0.98	0.08	61,61,61,61	0
16	CL	Q	301	1/1	0.98	0.07	79,79,79,79	0
16	CL	A	303	1/1	0.98	0.08	63,63,63,63	0
16	CL	N	302	1/1	0.98	0.07	48,48,48,48	0
16	CL	N	303	1/1	0.98	0.07	40,40,40,40	0
19	K	G	303	1/1	0.99	0.08	40,40,40,40	0
17	MG	I	302	1/1	0.99	0.08	33,33,33,33	0
16	CL	M	303	1/1	0.99	0.07	40,40,40,40	0
16	CL	a	303	1/1	0.99	0.09	43,43,43,43	0
16	CL	Y	302	1/1	0.99	0.07	66,66,66,66	0
16	CL	G	301	1/1	0.99	0.13	46,46,46,46	0
17	MG	Y	306	1/1	1.00	0.06	29,29,29,29	0

6.5 Other polymers (i)

There are no such residues in this entry.