



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 10:02 PM UTC

PDB ID : 5LF6 / pdb_00005lf6
Title : Human 20S proteasome complex with Z-LLY-ketoaldehyde at 2.1 Angstrom
Authors : Schrader, J.; Henneberg, F.; Mata, R.; Tittmann, K.; Schneider, T.R.; Stark, H.; Bourenkov, G.; Chari, A.
Deposited on : 2016-06-30
Resolution : 2.07 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

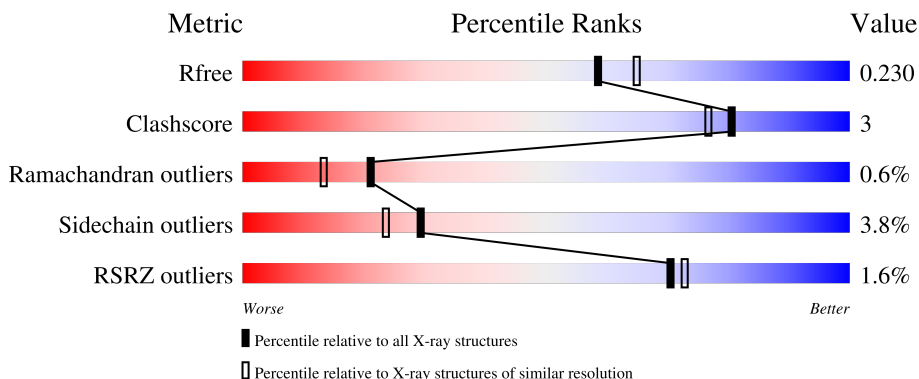
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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}	180053	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	234	 2% 88% 9% ..
1	O	234	 2% 90% 7% ..
2	B	261	 % 85% 9% 5%
2	P	261	 3% 83% 11% . 5%
3	C	248	 3% 85% 7% . .

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Mol	Chain	Length	Quality of chain
3	Q	248	3% 83% 12% ..
4	D	241	% 90% 6% .
4	R	241	2% 90% 6% .
5	E	263	3% 82% 6% . 11%
5	S	263	4% 81% 8% . 10%
6	F	255	% 83% 10% . 6%
6	T	255	2% 83% 10% . 6%
7	G	246	2% 91% 7% ..
7	U	246	2% 86% 9% ..
8	H	234	86% 6% . 6%
8	V	234	3% 86% 6% . 6%
9	I	205	92% 7%
9	W	205	94% 5%
10	J	201	83% 13% ..
10	X	201	87% 9% ..
11	c	4	100%
11	d	4	100%
12	K	204	88% 9% ..
12	Y	204	% 84% 11% ..
13	L	213	93% 6%
13	Z	213	95% 5%
14	M	219	92% 6% .
14	a	219	% 91% 7% ..
15	N	205	% 92% 5% ..
15	b	205	% 94% ..

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 51953 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
			Total	C	N	O	S			
1	A	230	Total	C	N	O	S	0	3	0
			1788	1145	301	336	6			
1	O	230	Total	C	N	O	S	0	0	0
			1741	1111	293	331	6			

- Molecule 2 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	248	Total	C	N	O	S	0	2	0
			1926	1220	332	363	11			
2	P	248	Total	C	N	O	S	0	2	0
			1909	1206	325	367	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	237	Total	C	N	O	S	0	2	0
			1798	1121	320	352	5			
3	Q	239	Total	C	N	O	S	0	0	0
			1820	1136	320	359	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	233	Total	C	N	O	S	0	1	0
			1762	1105	290	356	11			
4	R	233	Total	C	N	O	S	0	1	0
			1753	1103	293	346	11			

- Molecule 5 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	234	Total 1813	C 1138	N 324	O 340	S 11	0	1	0
5	S	238	Total 1866	C 1169	N 339	O 347	S 11	0	3	0

- Molecule 6 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	239	Total 1888	C 1198	N 325	O 353	S 12	0	4	0
6	T	240	Total 1856	C 1178	N 315	O 351	S 12	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	244	Total 1894	C 1202	N 319	O 360	S 13	0	2	0
7	U	238	Total 1797	C 1135	N 302	O 346	S 14	0	1	0

- Molecule 8 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	220	Total 1664	C 1047	N 284	O 320	S 13	0	2	0
8	V	220	Total 1622	C 1023	N 269	O 318	S 12	0	2	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	I	204	Total 1613	C 1028	N 270	O 295	S 20	0	3	0
9	W	204	Total 1599	C 1018	N 267	O 295	S 19	0	2	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	J	196	Total 1581	C 1015	N 270	O 286	S 10	0	3	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	X	196	1567	1006	266	285	10	0	2	0

- Molecule 11 is a protein called Z-LLY-ketoaldehyde peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
11	c	4	40	30	3	7	0	0	0
11	d	4	40	30	3	7	0	0	0

- Molecule 12 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	K	200	1550	978	269	293	10	0	1	0
12	Y	201	1580	996	280	294	10	0	3	0

- Molecule 13 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	L	213	1636	1038	277	310	11	0	2	0
13	Z	213	1642	1041	280	310	11	0	1	0

- Molecule 14 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	M	216	1692	1067	291	322	12	0	1	0
14	a	216	1688	1064	291	321	12	0	2	0

- Molecule 15 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	N	202	1516	950	258	295	13	0	1	0
15	b	203	1524	956	259	296	13	0	1	0

- Molecule 16 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

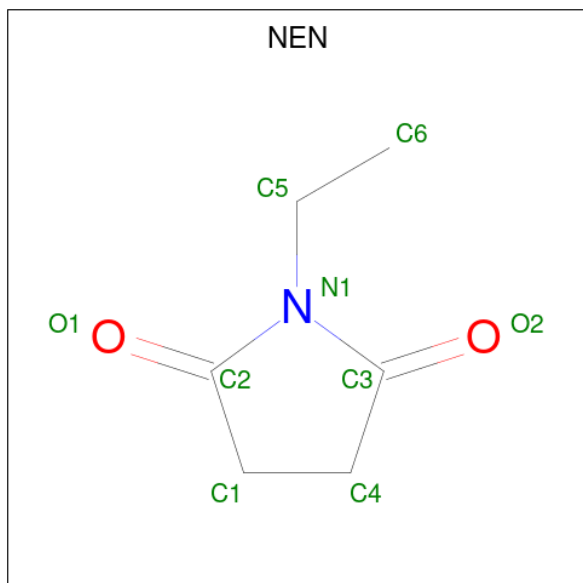
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	4	Total 4	Cl 4	0	0
16	B	2	Total 2	Cl 2	0	0
16	C	2	Total 2	Cl 2	0	0
16	D	2	Total 2	Cl 2	0	0
16	E	3	Total 3	Cl 3	0	0
16	F	1	Total 1	Cl 1	0	0
16	G	2	Total 2	Cl 2	0	0
16	H	2	Total 2	Cl 2	0	0
16	I	1	Total 1	Cl 1	0	0
16	K	3	Total 3	Cl 3	0	0
16	M	3	Total 3	Cl 3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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	a	3	Total Cl 3 3	0	0
16	b	3	Total Cl 3 3	0	0

- Molecule 17 is 1-ETHYL-PYRROLIDINE-2,5-DIONE (CCD ID: NEN) (formula: C₆H₉NO₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	E	1	Total C N O 9 6 1 2	0	0
17	G	1	Total C N O 9 6 1 2	0	0
17	G	1	Total C N O 9 6 1 2	0	0
17	J	1	Total C N O 9 6 1 2	0	0
17	S	1	Total C N O 9 6 1 2	0	0
17	U	1	Total C N O 9 6 1 2	0	0
17	U	1	Total C N O 9 6 1 2	0	0
17	X	1	Total C N O 9 6 1 2	0	0

- Molecule 18 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	G	1	Total K 1 1	0	0
18	L	1	Total K 1 1	0	0
18	N	1	Total K 1 1	0	0
18	U	1	Total K 1 1	0	0
18	Z	1	Total K 1 1	0	0
18	b	1	Total K 1 1	0	0

- Molecule 19 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 20 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	D	86	Total O 86 86	0	0
21	E	137	Total O 137 137	0	0
21	F	179	Total O 179 179	0	0
21	G	190	Total O 190 190	0	0
21	H	150	Total O 150 150	0	0
21	I	157	Total O 157 157	0	0
21	J	133	Total O 133 133	0	0
21	c	3	Total O 3 3	0	0
21	K	92	Total O 92 92	0	0
21	L	121	Total O 121 121	0	0
21	M	145	Total O 145 145	0	0
21	N	156	Total O 156 156	0	0
21	O	89	Total O 89 89	0	0
21	P	109	Total O 109 109	0	0
21	Q	71	Total O 71 71	0	0
21	R	119	Total O 119 119	0	0
21	S	124	Total O 124 124	0	0
21	T	91	Total O 91 91	0	0
21	U	103	Total O 103 103	0	0
21	V	109	Total O 109 109	0	0
21	W	108	Total O 108 108	0	0

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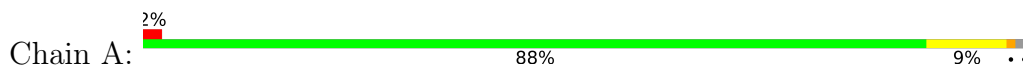
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	X	124	Total O 124 124	0	0
21	d	2	Total O 2 2	0	0
21	Y	141	Total O 141 141	0	0
21	Z	167	Total O 167 167	0	0
21	a	172	Total O 172 172	0	0
21	b	121	Total O 121 121	0	0

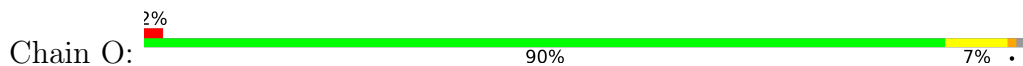
3 Residue-property plots [i](#)

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.

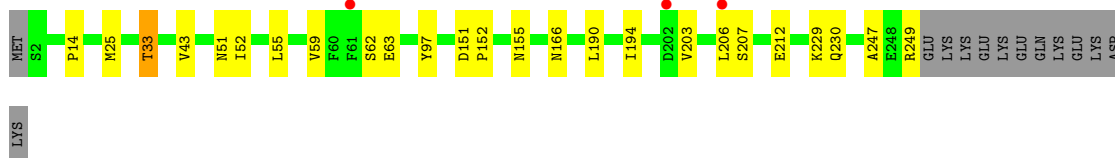
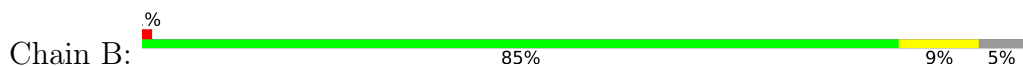
- Molecule 1: Proteasome subunit alpha type-2



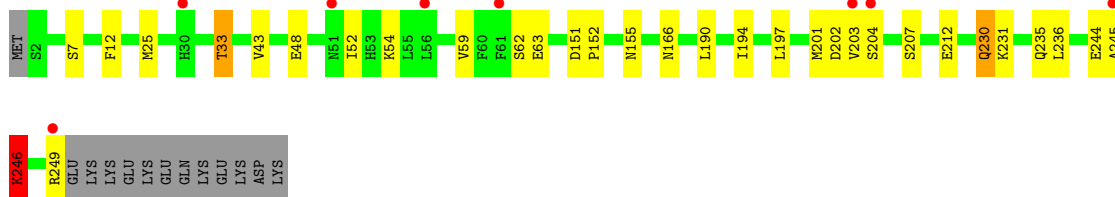
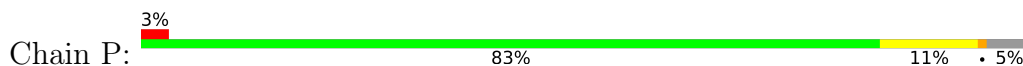
- Molecule 1: Proteasome subunit alpha type-2



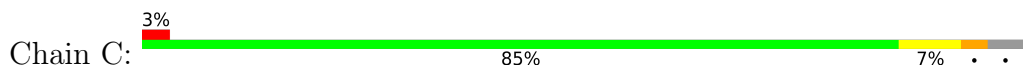
- Molecule 2: Proteasome subunit alpha type-4

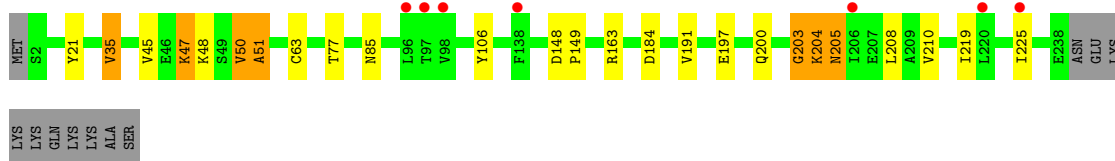


- Molecule 2: Proteasome subunit alpha type-4

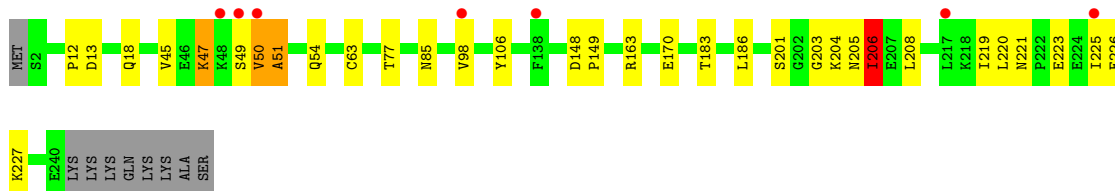
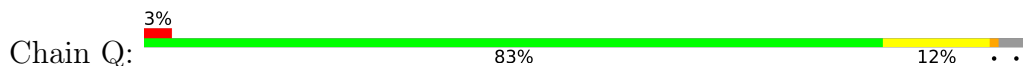


- Molecule 3: Proteasome subunit alpha type-7

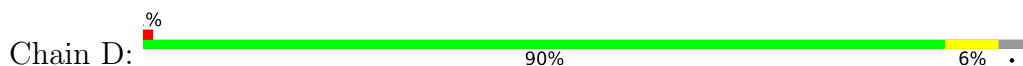




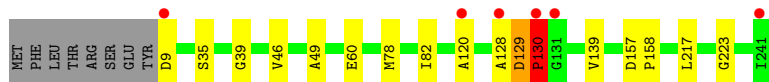
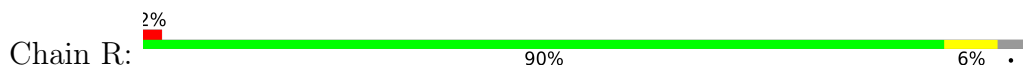
• Molecule 3: Proteasome subunit alpha type-7



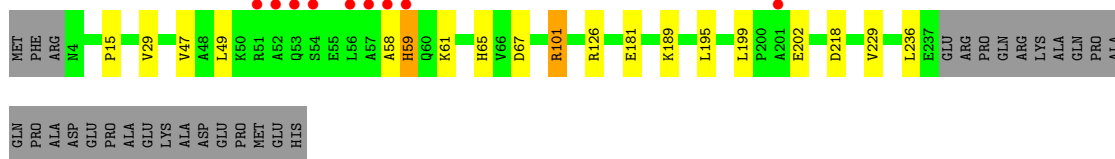
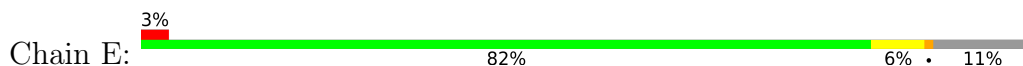
• Molecule 4: Proteasome subunit alpha type-5



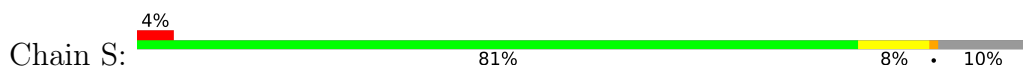
• Molecule 4: Proteasome subunit alpha type-5

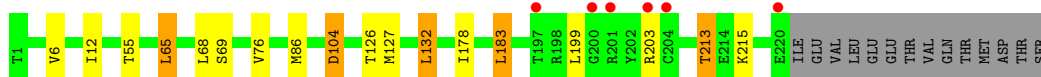


• Molecule 5: Proteasome subunit alpha type-1



• Molecule 5: Proteasome subunit alpha type-1

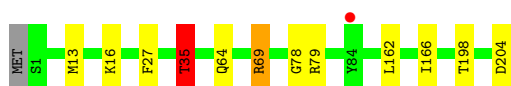




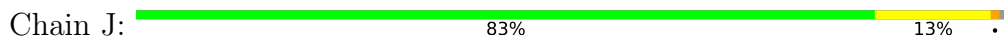
- Molecule 9: Proteasome subunit beta type-3



- Molecule 9: Proteasome subunit beta type-3



- Molecule 10: Proteasome subunit beta type-2



- Molecule 10: Proteasome subunit beta type-2



- Molecule 11: Z-LLY-ketoaldehyde peptide



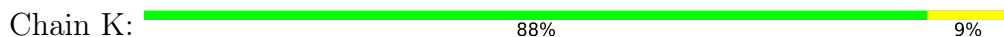
There are no outlier residues recorded for this chain.

- Molecule 11: Z-LLY-ketoaldehyde peptide

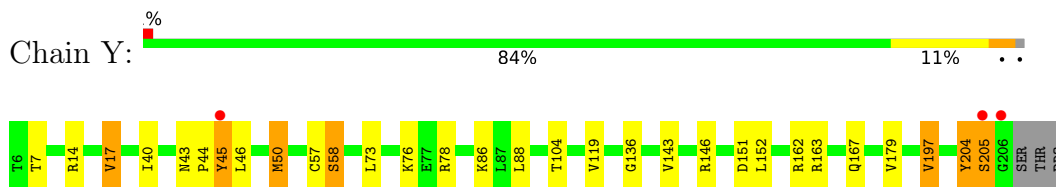


There are no outlier residues recorded for this chain.

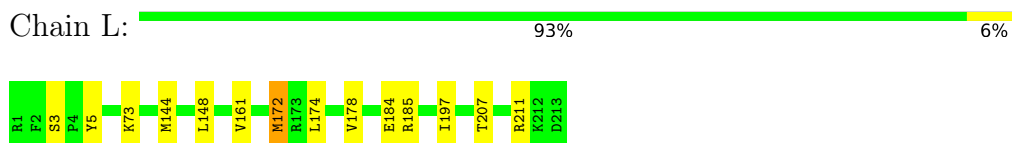
- Molecule 12: Proteasome subunit beta type-5



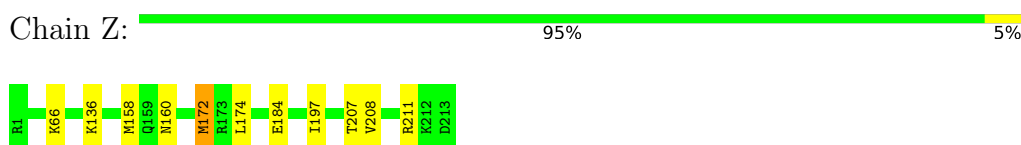
- Molecule 12: Proteasome subunit beta type-5



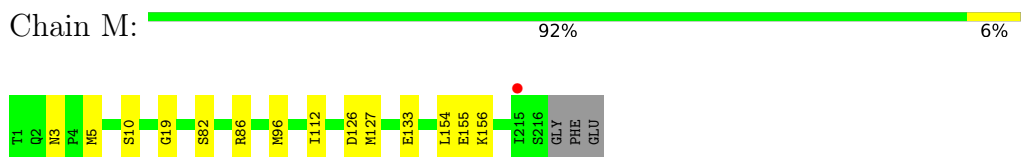
- Molecule 13: Proteasome subunit beta type-1



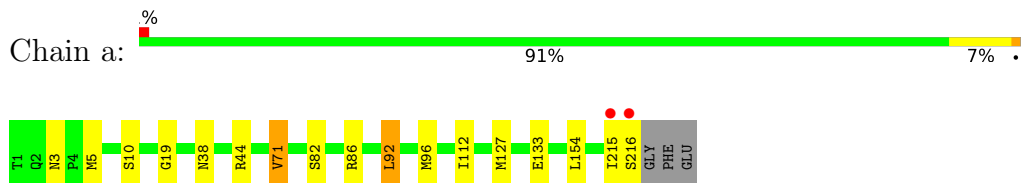
- Molecule 13: Proteasome subunit beta type-1



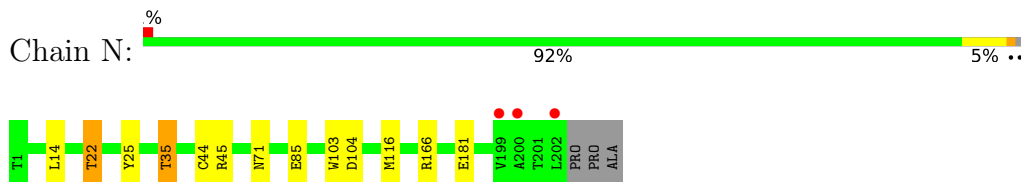
- Molecule 14: Proteasome subunit beta type-4



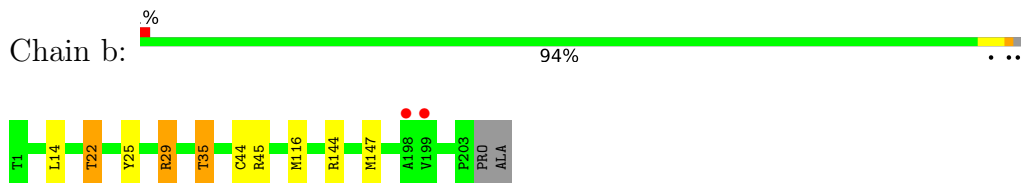
- Molecule 14: Proteasome subunit beta type-4



- Molecule 15: Proteasome subunit beta type-6



- Molecule 15: Proteasome subunit beta type-6



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.87Å 203.48Å 315.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	171.02 – 2.07 171.02 – 2.07	Depositor EDS
% Data completeness (in resolution range)	96.4 (171.02-2.07) 96.4 (171.02-2.07)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 2.07Å)	Xtrriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.186 , 0.227 0.193 , 0.230	Depositor DCC
R_{free} test set	21152 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	43.8	Xtrriage
Anisotropy	0.245	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	51953	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: YCM, PHQ, CL, 1PE, NEN, MG, 6VF, K

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	0.93	0/1833	0.95	0/2489
1	O	0.82	0/1778	0.94	0/2419
2	B	1.00	1/1962 (0.1%)	1.02	5/2649 (0.2%)
2	P	0.84	0/1945	0.98	1/2631 (0.0%)
3	C	0.98	0/1818	1.09	3/2469 (0.1%)
3	Q	0.96	2/1834 (0.1%)	1.09	8/2490 (0.3%)
4	D	0.91	0/1789	0.99	1/2424 (0.0%)
4	R	1.06	1/1780 (0.1%)	1.04	2/2408 (0.1%)
5	E	1.02	1/1849 (0.1%)	1.03	1/2505 (0.0%)
5	S	1.01	1/1908 (0.1%)	1.05	3/2583 (0.1%)
6	F	1.12	1/1935 (0.1%)	1.08	4/2605 (0.2%)
6	T	1.02	1/1894 (0.1%)	1.10	6/2556 (0.2%)
7	G	1.07	3/1923 (0.2%)	1.04	4/2601 (0.2%)
7	U	0.92	1/1818 (0.1%)	0.98	1/2463 (0.0%)
8	H	1.13	0/1697	1.01	1/2299 (0.0%)
8	V	0.93	0/1655	0.96	0/2251
9	I	1.07	2/1648 (0.1%)	1.12	8/2219 (0.4%)
9	W	0.84	0/1630	1.01	7/2197 (0.3%)
10	J	1.14	2/1620 (0.1%)	1.02	0/2191
10	X	0.99	0/1606	0.98	0/2174
11	c	0.72	0/15	1.44	0/19
11	d	1.17	0/15	1.24	0/19
12	K	0.99	0/1584	1.02	0/2141
12	Y	1.11	1/1620 (0.1%)	1.10	4/2185 (0.2%)
13	L	0.93	1/1672 (0.1%)	0.98	1/2257 (0.0%)
13	Z	1.11	0/1675	1.03	1/2257 (0.0%)
14	M	1.06	1/1728 (0.1%)	1.01	2/2339 (0.1%)
14	a	1.12	1/1724 (0.1%)	1.05	3/2336 (0.1%)
15	N	1.18	2/1545 (0.1%)	1.10	2/2091 (0.1%)
15	b	1.11	0/1554	1.10	2/2104 (0.1%)
All	All	1.02	22/49054 (0.0%)	1.03	70/66371 (0.1%)

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
2	P	0	4
3	Q	0	2
4	D	0	2
4	R	0	2
6	T	0	1
9	I	0	1
9	W	0	1
10	J	0	2
10	X	0	1
14	a	0	1
All	All	0	17

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	M	3	ASN	C-O	-7.96	1.18	1.25
9	I	34	VAL	N-CA	6.83	1.53	1.45
5	S	3	ARG	N-CA	6.50	1.54	1.46
9	I	98	ARG	C-O	-6.12	1.16	1.24
3	Q	206	ILE	CA-C	5.83	1.60	1.52

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	190	VAL	CB-CA-C	-10.16	98.73	112.04
6	T	190	VAL	CB-CA-C	-8.85	100.45	112.04
9	I	16[A]	LYS	CA-C-N	8.65	134.80	122.08
9	I	16[A]	LYS	C-N-CA	8.65	134.80	122.08
9	I	16[B]	LYS	CA-C-N	8.65	134.80	122.08

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	175[A]	GLU	Peptide
4	D	175[B]	GLU	Peptide
9	I	78	GLY	Peptide
10	J	1[A]	MET	Peptide

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Mol	Chain	Res	Type	Group
10	J	1[B]	MET	Peptide

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	1788	0	1761	9	0
1	O	1741	0	1683	6	0
2	B	1926	0	1924	7	0
2	P	1909	0	1874	10	0
3	C	1798	0	1718	16	0
3	Q	1820	0	1749	8	0
4	D	1762	0	1709	3	0
4	R	1753	0	1726	6	0
5	E	1813	0	1783	9	0
5	S	1866	0	1822	23	0
6	F	1888	0	1882	14	0
6	T	1856	0	1816	9	0
7	G	1894	0	1890	6	0
7	U	1797	0	1756	14	0
8	H	1664	0	1681	11	0
8	V	1622	0	1595	8	0
9	I	1613	0	1646	8	0
9	W	1599	0	1621	8	0
10	J	1581	0	1585	20	0
10	X	1567	0	1565	16	0
11	c	40	0	28	0	0
11	d	40	0	28	0	0
12	K	1550	0	1503	8	0
12	Y	1580	0	1554	20	0
13	L	1636	0	1625	6	0
13	Z	1642	0	1635	6	0
14	M	1692	0	1670	7	0
14	a	1688	0	1658	9	0
15	N	1516	0	1487	9	0
15	b	1524	0	1496	8	0
16	A	4	0	0	0	0
16	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	C	2	0	0	0	0
16	D	2	0	0	0	0
16	E	3	0	0	0	0
16	F	1	0	0	0	0
16	G	2	0	0	1	0
16	H	2	0	0	0	0
16	I	1	0	0	0	0
16	K	3	0	0	0	0
16	M	3	0	0	0	0
16	N	4	0	0	0	0
16	O	4	0	0	0	0
16	P	1	0	0	0	0
16	Q	2	0	0	0	0
16	R	2	0	0	0	0
16	S	3	0	0	0	0
16	U	1	0	0	0	0
16	V	2	0	0	0	0
16	W	1	0	0	0	0
16	Y	4	0	0	0	0
16	a	3	0	0	2	0
16	b	3	0	0	1	0
17	E	9	0	8	0	0
17	G	18	0	16	1	0
17	J	9	0	8	1	0
17	S	9	0	8	0	0
17	U	18	0	16	0	0
17	X	9	0	8	1	0
18	G	1	0	0	0	0
18	L	1	0	0	0	0
18	N	1	0	0	0	0
18	U	1	0	0	0	0
18	Z	1	0	0	0	0
18	b	1	0	0	0	0
19	H	2	0	0	0	0
19	I	1	0	0	0	0
19	J	1	0	0	0	0
19	K	1	0	0	0	0
19	V	2	0	0	0	0
19	W	1	0	0	0	0
19	X	1	0	0	0	0
19	Y	1	0	0	0	0
20	I	32	0	44	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	L	16	0	22	0	0
20	M	16	0	22	0	0
20	N	16	0	22	0	0
20	W	16	0	22	0	0
20	Z	16	0	22	0	0
20	a	16	0	22	0	0
20	b	16	0	22	0	0
21	A	108	0	0	0	0
21	B	119	0	0	0	0
21	C	75	0	0	0	0
21	D	86	0	0	0	0
21	E	137	0	0	2	0
21	F	179	0	0	6	0
21	G	190	0	0	0	0
21	H	150	0	0	2	0
21	I	157	0	0	1	0
21	J	133	0	0	3	0
21	K	92	0	0	0	0
21	L	121	0	0	0	0
21	M	145	0	0	0	0
21	N	156	0	0	1	0
21	O	89	0	0	1	0
21	P	109	0	0	0	0
21	Q	71	0	0	1	0
21	R	119	0	0	0	0
21	S	124	0	0	5	0
21	T	91	0	0	1	0
21	U	103	0	0	0	0
21	V	109	0	0	0	0
21	W	108	0	0	1	0
21	X	124	0	0	1	0
21	Y	141	0	0	0	0
21	Z	167	0	0	2	0
21	a	172	0	0	1	0
21	b	121	0	0	0	0
21	c	3	0	0	0	0
21	d	2	0	0	0	0
All	All	51953	0	47732	252	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 3.

The worst 5 of 252 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)
12:Y:50:MET:HE1	12:Y:58:SER:HA	1.46	0.97
5:S:152[B]:ASN:ND2	21:S:401:HOH:O	2.07	0.87
5:S:65[A]:HIS:CE1	21:S:402:HOH:O	2.29	0.84
13:L:144:MET:HE1	13:L:185:ARG:HB2	1.66	0.78
1:A:108:GLN:HE21	1:A:112:ARG:HH12	1.32	0.74

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	231/234 (99%)	218 (94%)	9 (4%)	4 (2%)	7 2
1	O	228/234 (97%)	214 (94%)	9 (4%)	5 (2%)	5 1
2	B	248/261 (95%)	234 (94%)	13 (5%)	1 (0%)	30 23
2	P	248/261 (95%)	234 (94%)	12 (5%)	2 (1%)	16 8
3	C	236/248 (95%)	217 (92%)	14 (6%)	5 (2%)	5 1
3	Q	236/248 (95%)	217 (92%)	12 (5%)	7 (3%)	3 0
4	D	232/241 (96%)	223 (96%)	6 (3%)	3 (1%)	9 3
4	R	232/241 (96%)	221 (95%)	8 (3%)	3 (1%)	9 3
5	E	233/263 (89%)	227 (97%)	4 (2%)	2 (1%)	14 7
5	S	239/263 (91%)	232 (97%)	6 (2%)	1 (0%)	30 23
6	F	241/255 (94%)	238 (99%)	3 (1%)	0	100 100
6	T	239/255 (94%)	230 (96%)	6 (2%)	3 (1%)	9 3
7	G	243/246 (99%)	237 (98%)	6 (2%)	0	100 100
7	U	234/246 (95%)	229 (98%)	3 (1%)	2 (1%)	14 7
8	H	220/234 (94%)	217 (99%)	3 (1%)	0	100 100
8	V	220/234 (94%)	216 (98%)	3 (1%)	1 (0%)	24 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	205/205 (100%)	200 (98%)	5 (2%)	0	100	100
9	W	204/205 (100%)	198 (97%)	6 (3%)	0	100	100
10	J	196/201 (98%)	192 (98%)	4 (2%)	0	100	100
10	X	196/201 (98%)	193 (98%)	3 (2%)	0	100	100
11	c	1/4 (25%)	1 (100%)	0	0	100	100
11	d	1/4 (25%)	1 (100%)	0	0	100	100
12	K	199/204 (98%)	196 (98%)	3 (2%)	0	100	100
12	Y	202/204 (99%)	198 (98%)	3 (2%)	1 (0%)	24	17
13	L	213/213 (100%)	211 (99%)	2 (1%)	0	100	100
13	Z	212/213 (100%)	210 (99%)	2 (1%)	0	100	100
14	M	215/219 (98%)	208 (97%)	7 (3%)	0	100	100
14	a	216/219 (99%)	207 (96%)	9 (4%)	0	100	100
15	N	201/205 (98%)	200 (100%)	1 (0%)	0	100	100
15	b	202/205 (98%)	201 (100%)	1 (0%)	0	100	100
All	All	6223/6466 (96%)	6020 (97%)	163 (3%)	40 (1%)	21	13

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	LYS
1	A	53	SER
4	D	176	GLY
5	E	59	HIS
1	O	52	LYS

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	185/191 (97%)	174 (94%)	11 (6%)	18	10
1	O	176/191 (92%)	167 (95%)	9 (5%)	21	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	200/221 (90%)	190 (95%)	10 (5%)	22	14
2	P	197/221 (89%)	182 (92%)	15 (8%)	12	6
3	C	179/210 (85%)	171 (96%)	8 (4%)	24	18
3	Q	184/210 (88%)	172 (94%)	12 (6%)	15	8
4	D	189/203 (93%)	183 (97%)	6 (3%)	34	29
4	R	187/203 (92%)	183 (98%)	4 (2%)	47	45
5	E	193/224 (86%)	185 (96%)	8 (4%)	27	21
5	S	198/224 (88%)	193 (98%)	5 (2%)	42	38
6	F	199/212 (94%)	190 (96%)	9 (4%)	24	18
6	T	192/212 (91%)	183 (95%)	9 (5%)	23	16
7	G	204/209 (98%)	197 (97%)	7 (3%)	32	27
7	U	188/209 (90%)	182 (97%)	6 (3%)	34	29
8	H	181/195 (93%)	172 (95%)	9 (5%)	22	14
8	V	172/195 (88%)	161 (94%)	11 (6%)	16	9
9	I	176/174 (101%)	173 (98%)	3 (2%)	53	53
9	W	173/174 (99%)	171 (99%)	2 (1%)	63	65
10	J	167/171 (98%)	161 (96%)	6 (4%)	31	25
10	X	166/171 (97%)	162 (98%)	4 (2%)	43	40
11	c	2/2 (100%)	2 (100%)	0	100	100
11	d	2/2 (100%)	2 (100%)	0	100	100
12	K	155/159 (98%)	145 (94%)	10 (6%)	15	8
12	Y	159/159 (100%)	152 (96%)	7 (4%)	25	19
13	L	175/178 (98%)	170 (97%)	5 (3%)	37	33
13	Z	175/178 (98%)	172 (98%)	3 (2%)	53	53
14	M	180/181 (99%)	176 (98%)	4 (2%)	45	43
14	a	178/181 (98%)	173 (97%)	5 (3%)	38	34
15	N	157/159 (99%)	155 (99%)	2 (1%)	61	62
15	b	158/159 (99%)	155 (98%)	3 (2%)	50	49
All	All	5047/5378 (94%)	4854 (96%)	193 (4%)	29	23

5 of 193 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	P	204	SER
6	T	17	ASP
2	P	236	LEU
3	Q	223	GLU
6	T	223	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
7	U	100	ASN
13	Z	79	ASN
8	V	116	HIS
10	X	63	ASN
14	a	162	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](#)

4 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
7	YCM	U	137	7	7,9,10	0.96	0	5,10,12	1.36	1 (20%)
3	YCM	C	63	3	7,9,10	1.04	1 (14%)	5,10,12	1.06	0
3	YCM	Q	63	3	7,9,10	1.30	1 (14%)	5,10,12	3.38	4 (80%)
7	YCM	G	137	7	7,9,10	1.73	2 (28%)	5,10,12	2.05	1 (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
7	YCM	U	137	7	-	2/6/8/10	-
3	YCM	C	63	3	-	0/6/8/10	-
3	YCM	Q	63	3	-	3/6/8/10	-
7	YCM	G	137	7	-	3/6/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	137	YCM	CE-NZ2	2.88	1.42	1.32
3	Q	63	YCM	CD-SG	-2.60	1.75	1.81
7	G	137	YCM	CD-SG	2.23	1.87	1.81
3	C	63	YCM	CD-SG	-2.04	1.76	1.81

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	63	YCM	CE-CD-SG	-4.88	98.41	113.81
7	G	137	YCM	CE-CD-SG	3.87	126.04	113.81
3	Q	63	YCM	CA-CB-SG	-3.54	100.45	113.51
3	Q	63	YCM	CB-SG-CD	3.33	133.92	104.24
3	Q	63	YCM	CB-CA-C	-2.69	103.48	110.80

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	137	YCM	CE-CD-SG-CB
7	G	137	YCM	SG-CD-CE-NZ2
3	Q	63	YCM	CE-CD-SG-CB
3	Q	63	YCM	SG-CD-CE-OZ1
7	G	137	YCM	SG-CD-CE-OZ1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [\(i\)](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 88 ligands modelled in this entry, 71 are monoatomic - leaving 17 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	NEN	G	304	7	9,9,9	1.57	2 (22%)	12,12,12	3.17	9 (75%)
17	NEN	S	304	5	9,9,9	1.25	2 (22%)	12,12,12	2.86	6 (50%)
20	1PE	I	303	-	15,15,15	0.58	0	14,14,14	1.09	2 (14%)
17	NEN	J	302	10	9,9,9	0.94	1 (11%)	12,12,12	4.34	7 (58%)
20	1PE	M	304	-	15,15,15	0.53	0	14,14,14	0.38	0
20	1PE	b	304	-	15,15,15	0.68	0	14,14,14	0.78	0
20	1PE	L	301	-	15,15,15	0.59	0	14,14,14	0.72	0
17	NEN	X	302	10	9,9,9	1.43	1 (11%)	12,12,12	4.69	9 (75%)
20	1PE	W	303	-	15,15,15	0.52	0	14,14,14	0.42	0
20	1PE	Z	301	-	15,15,15	0.55	0	14,14,14	0.40	0
20	1PE	a	304	-	15,15,15	0.53	0	14,14,14	0.41	0
17	NEN	E	304	5	9,9,9	1.27	1 (11%)	12,12,12	3.04	7 (58%)
20	1PE	N	305	-	15,15,15	0.57	0	14,14,14	0.57	0
20	1PE	I	304	-	15,15,15	0.51	0	14,14,14	0.52	0
17	NEN	U	304	7	9,9,9	1.44	2 (22%)	12,12,12	2.92	5 (41%)
17	NEN	G	305	7	9,9,9	1.89	2 (22%)	12,12,12	3.02	4 (33%)
17	NEN	U	303	7	9,9,9	1.38	2 (22%)	12,12,12	4.41	7 (58%)

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	NEN	G	304	7	-	2/2/15/15	0/1/1/1
17	NEN	S	304	5	-	0/2/15/15	0/1/1/1
20	1PE	I	303	-	-	8/13/13/13	-
17	NEN	J	302	10	-	2/2/15/15	0/1/1/1
20	1PE	M	304	-	-	7/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	1PE	b	304	-	-	8/13/13/13	-
20	1PE	L	301	-	-	6/13/13/13	-
17	NEN	X	302	10	-	2/2/15/15	0/1/1/1
20	1PE	W	303	-	-	6/13/13/13	-
20	1PE	Z	301	-	-	5/13/13/13	-
20	1PE	a	304	-	-	5/13/13/13	-
17	NEN	E	304	5	-	2/2/15/15	0/1/1/1
20	1PE	N	305	-	-	6/13/13/13	-
20	1PE	I	304	-	-	7/13/13/13	-
17	NEN	U	304	7	-	0/2/15/15	0/1/1/1
17	NEN	G	305	7	-	0/2/15/15	0/1/1/1
17	NEN	U	303	7	-	2/2/15/15	0/1/1/1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	G	305	NEN	C3-N1	-4.45	1.31	1.38
17	G	304	NEN	C3-N1	-3.81	1.32	1.38
17	X	302	NEN	C3-N1	-3.70	1.33	1.38
17	G	305	NEN	C2-N1	-3.36	1.33	1.38
17	U	304	NEN	C3-N1	-3.35	1.33	1.38

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	U	303	NEN	C3-N1-C2	-10.71	108.26	112.94
17	X	302	NEN	C3-N1-C2	-8.19	109.36	112.94
17	E	304	NEN	C3-N1-C2	-7.55	109.64	112.94
17	J	302	NEN	C5-N1-C2	7.51	131.40	122.52
17	X	302	NEN	O1-C2-N1	7.41	131.88	123.94

There are no chirality outliers.

5 of 68 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	E	304	NEN	C6-C5-N1-C2
17	E	304	NEN	C6-C5-N1-C3
17	J	302	NEN	C6-C5-N1-C2
17	J	302	NEN	C6-C5-N1-C3

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Mol	Chain	Res	Type	Atoms
17	X	302	NEN	C6-C5-N1-C2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	G	304	NEN	1	0
17	J	302	NEN	1	0
17	X	302	NEN	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	230/234 (98%)	-0.03	4 (1%) 69 71	27, 52, 90, 106	3 (1%)
1	O	230/234 (98%)	0.33	5 (2%) 62 64	43, 70, 110, 140	0
2	B	248/261 (95%)	0.05	3 (1%) 76 78	23, 56, 99, 133	2 (0%)
2	P	248/261 (95%)	0.27	8 (3%) 50 50	34, 66, 117, 153	2 (0%)
3	C	236/248 (95%)	0.36	7 (2%) 52 53	31, 67, 112, 136	2 (0%)
3	Q	238/248 (95%)	0.41	7 (2%) 53 55	36, 68, 128, 154	0
4	D	233/241 (96%)	0.21	2 (0%) 81 83	34, 66, 99, 141	1 (0%)
4	R	233/241 (96%)	-0.07	6 (2%) 57 59	22, 47, 75, 115	1 (0%)
5	E	234/263 (88%)	0.01	9 (3%) 44 44	27, 47, 98, 121	1 (0%)
5	S	238/263 (90%)	-0.01	10 (4%) 40 41	22, 50, 89, 110	3 (1%)
6	F	239/255 (93%)	-0.30	3 (1%) 75 77	23, 39, 64, 80	4 (1%)
6	T	240/255 (94%)	0.14	5 (2%) 63 66	30, 55, 92, 134	1 (0%)
7	G	243/246 (98%)	-0.20	4 (1%) 70 73	23, 43, 80, 113	2 (0%)
7	U	237/246 (96%)	0.20	4 (1%) 69 71	32, 64, 98, 116	1 (0%)
8	H	220/234 (94%)	-0.25	1 (0%) 87 89	21, 39, 70, 117	2 (0%)
8	V	220/234 (94%)	0.05	6 (2%) 56 58	27, 54, 85, 123	2 (0%)
9	I	204/205 (99%)	-0.40	0 100 100	23, 39, 60, 73	3 (1%)
9	W	204/205 (99%)	0.02	1 (0%) 87 89	32, 55, 80, 92	2 (0%)
10	J	196/201 (97%)	-0.30	1 (0%) 87 89	18, 43, 61, 85	3 (1%)
10	X	196/201 (97%)	-0.17	0 100 100	20, 47, 62, 86	2 (1%)
11	c	2/4 (50%)	-0.27	0 100 100	40, 40, 40, 43	0
11	d	2/4 (50%)	-0.68	0 100 100	32, 32, 32, 36	0
12	K	200/204 (98%)	-0.08	1 (0%) 87 89	28, 51, 78, 95	1 (0%)
12	Y	201/204 (98%)	-0.34	3 (1%) 72 74	23, 40, 61, 78	3 (1%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	L	213/213 (100%)	-0.04	0 100 100	27, 54, 77, 91	2 (0%)
13	Z	213/213 (100%)	-0.33	0 100 100	29, 40, 64, 78	1 (0%)
14	M	216/219 (98%)	-0.27	1 (0%) 87 89	30, 43, 68, 103	1 (0%)
14	a	216/219 (98%)	-0.33	2 (0%) 81 83	26, 41, 64, 97	2 (0%)
15	N	202/205 (98%)	-0.37	3 (1%) 72 74	23, 37, 59, 94	1 (0%)
15	b	203/205 (99%)	-0.21	2 (0%) 79 82	32, 42, 71, 99	1 (0%)
All	All	6235/6466 (96%)	-0.05	98 (1%) 70 73	18, 50, 93, 154	49 (0%)

The worst 5 of 98 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	T	5	THR	5.0
15	N	202	LEU	4.7
12	K	44	TYR	4.3
12	Y	45	TYR	4.2
12	Y	206	GLY	4.0

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, 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
7	YCM	G	137	10/11	0.88	0.13	37,44,55,55	0
7	YCM	U	137	10/11	0.90	0.12	55,65,80,83	0
3	YCM	C	63	10/11	0.93	0.10	63,66,76,78	0
3	YCM	Q	63	10/11	0.95	0.08	57,61,67,67	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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
17	NEN	U	304	9/9	0.82	0.16	115,118,121,123	0
17	NEN	E	304	9/9	0.83	0.16	64,68,73,74	0
16	CL	Q	301	1/1	0.83	0.11	98,98,98,98	0
17	NEN	S	304	9/9	0.84	0.17	71,76,78,81	0
16	CL	D	301	1/1	0.84	0.21	83,83,83,83	0
20	1PE	I	304	16/16	0.84	0.15	69,85,101,102	0
16	CL	S	301	1/1	0.85	0.23	76,76,76,76	0
16	CL	D	302	1/1	0.86	0.20	77,77,77,77	0
16	CL	O	304	1/1	0.87	0.19	80,80,80,80	0
17	NEN	X	302	9/9	0.87	0.13	58,60,63,71	0
17	NEN	U	303	9/9	0.87	0.14	86,89,92,92	0
20	1PE	M	304	16/16	0.87	0.17	69,80,114,115	0
20	1PE	W	303	16/16	0.87	0.13	68,73,84,87	0
17	NEN	J	302	9/9	0.88	0.12	57,62,65,66	0
20	1PE	I	303	16/16	0.88	0.13	59,68,77,84	0
16	CL	E	303	1/1	0.88	0.16	75,75,75,75	0
16	CL	Y	305	1/1	0.88	0.28	73,73,73,73	0
16	CL	O	303	1/1	0.88	0.10	103,103,103,103	0
16	CL	S	302	1/1	0.89	0.14	76,76,76,76	0
16	CL	K	304	1/1	0.89	0.22	79,79,79,79	0
20	1PE	Z	301	16/16	0.89	0.12	59,72,80,84	0
20	1PE	b	304	16/16	0.89	0.14	50,58,92,98	0
20	1PE	L	301	16/16	0.90	0.12	65,79,84,90	0
17	NEN	G	305	9/9	0.90	0.12	65,68,70,75	0
16	CL	V	303	1/1	0.90	0.16	73,73,73,73	0
16	CL	K	303	1/1	0.90	0.17	73,73,73,73	0
20	1PE	a	304	16/16	0.90	0.15	62,70,101,101	0
16	CL	Q	302	1/1	0.90	0.19	77,77,77,77	0
16	CL	K	302	1/1	0.91	0.14	92,92,92,92	0
20	1PE	N	305	16/16	0.91	0.11	44,57,68,68	0
16	CL	C	302	1/1	0.91	0.21	79,79,79,79	0
16	CL	C	301	1/1	0.91	0.12	74,74,74,74	0
16	CL	O	302	1/1	0.91	0.14	71,71,71,71	0
16	CL	a	303	1/1	0.91	0.11	69,69,69,69	0
16	CL	H	303	1/1	0.92	0.20	63,63,63,63	0
16	CL	I	302	1/1	0.92	0.11	57,57,57,57	0
16	CL	M	303	1/1	0.92	0.11	61,61,61,61	0
16	CL	N	301	1/1	0.92	0.11	55,55,55,55	0
16	CL	G	302	1/1	0.92	0.09	76,76,76,76	0
16	CL	N	302	1/1	0.93	0.14	66,66,66,66	0
17	NEN	G	304	9/9	0.93	0.09	59,60,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
16	CL	R	301	1/1	0.93	0.11	63,63,63,63	0
16	CL	N	303	1/1	0.93	0.22	70,70,70,70	0
16	CL	B	302	1/1	0.93	0.15	69,69,69,69	0
16	CL	E	302	1/1	0.93	0.14	61,61,61,61	0
16	CL	A	302	1/1	0.93	0.09	76,76,76,76	0
16	CL	F	301	1/1	0.93	0.12	60,60,60,60	0
18	K	b	305	1/1	0.93	0.14	49,49,49,49	0
16	CL	A	304	1/1	0.94	0.13	63,63,63,63	0
16	CL	V	304	1/1	0.94	0.15	66,66,66,66	0
16	CL	Y	303	1/1	0.94	0.12	90,90,90,90	0
18	K	U	302	1/1	0.94	0.11	46,46,46,46	0
16	CL	A	301	1/1	0.94	0.12	64,64,64,64	0
16	CL	a	301	1/1	0.94	0.15	69,69,69,69	0
16	CL	H	304	1/1	0.94	0.12	57,57,57,57	0
16	CL	b	301	1/1	0.94	0.18	66,66,66,66	0
16	CL	b	302	1/1	0.94	0.17	68,68,68,68	0
16	CL	N	304	1/1	0.94	0.17	50,50,50,50	0
16	CL	R	302	1/1	0.94	0.21	62,62,62,62	0
16	CL	M	301	1/1	0.94	0.29	67,67,67,67	0
16	CL	E	301	1/1	0.94	0.14	69,69,69,69	0
16	CL	S	303	1/1	0.94	0.15	60,60,60,60	0
16	CL	Y	302	1/1	0.95	0.22	71,71,71,71	0
16	CL	O	301	1/1	0.95	0.12	63,63,63,63	0
16	CL	b	303	1/1	0.95	0.14	64,64,64,64	0
16	CL	B	301	1/1	0.95	0.10	46,46,46,46	0
16	CL	P	301	1/1	0.95	0.09	65,65,65,65	0
16	CL	a	302	1/1	0.95	0.09	48,48,48,48	0
19	MG	I	301	1/1	0.95	0.09	34,34,34,34	0
16	CL	W	302	1/1	0.95	0.07	61,61,61,61	0
16	CL	Y	304	1/1	0.96	0.09	66,66,66,66	0
16	CL	G	301	1/1	0.96	0.24	52,52,52,52	0
18	K	G	303	1/1	0.96	0.10	38,38,38,38	0
18	K	N	306	1/1	0.96	0.11	44,44,44,44	0
16	CL	A	303	1/1	0.97	0.08	58,58,58,58	0
19	MG	W	301	1/1	0.97	0.08	43,43,43,43	0
19	MG	Y	301	1/1	0.97	0.10	29,29,29,29	0
16	CL	M	302	1/1	0.97	0.10	44,44,44,44	0
19	MG	V	302	1/1	0.98	0.05	58,58,58,58	0
18	K	Z	302	1/1	0.98	0.09	44,44,44,44	0
16	CL	U	301	1/1	0.98	0.13	67,67,67,67	0
19	MG	H	302	1/1	0.98	0.11	34,34,34,34	0
18	K	L	302	1/1	0.98	0.09	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
19	MG	K	301	1/1	0.98	0.11	40,40,40,40	0
19	MG	H	301	1/1	0.99	0.04	48,48,48,48	0
19	MG	X	301	1/1	0.99	0.02	54,54,54,54	0
19	MG	V	301	1/1	0.99	0.09	43,43,43,43	0
19	MG	J	301	1/1	0.99	0.04	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.