wwPDB X-ray Structure Validation Summary Report (i)

Jan 4, 2024 – 09:16 pm GMT

PDB ID	:	5LE5
Title	:	Native human 20S proteasome at 1.8 Angstrom
Authors	:	Schrader, J.; Henneberg, F.; Mata, R.; Tittmann, K.; Schneider, T.R.; Stark, H.; Bourenkov, G.; Chari, A.
Deposited on	:	2016-06-29
Resolution	:	1.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
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:

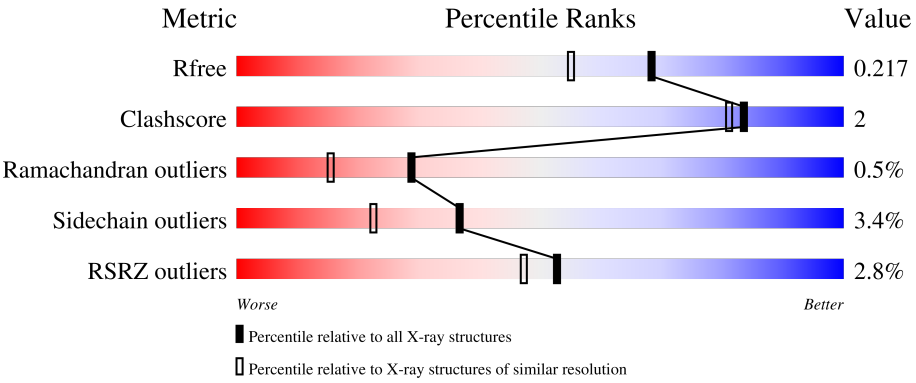
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	234	2% 89% 8%
1	O	234	7% 87% 9%
2	B	261	3% 88% 6% 5%
2	P	261	7% 84% 8% 5%
3	C	248	8% 80% 15%

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Mol	Chain	Length	Quality of chain
3	Q	248	6% 81% 12% 6%
4	D	241	5% 89% 7%
4	R	241	2% 89% 6%
5	E	263	5% 81% 8% 11%
5	S	263	3% 83% 7% 10%
6	F	255	84% 8% 6%
6	T	255	4% 83% 9% 6%
7	G	246	90% 7%
7	U	246	6% 86% 8%
8	H	234	2% 87% 7% 6%
8	V	234	3% 85% 8% 6%
9	I	205	95%
9	W	205	96%
10	J	201	85% 11%
10	X	201	87% 9%
11	K	204	91% 6%
11	Y	204	89% 7%
12	L	213	92% 8%
12	Z	213	94% 5%
13	M	219	92% 7%
13	a	219	94%
14	N	205	93% 5%
14	b	205	97%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	6V1	U	47	X	-	-	-

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 52161 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	2	0
			1799	1151	307	335	6			
1	O	230	Total	C	N	O	S	0	0	0
			1779	1136	301	336	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	248	Total	C	N	O	S	0	1	0
			1942	1226	332	373	11			
2	P	247	Total	C	N	O	S	0	2	0
			1919	1211	326	371	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	237	Total	C	N	O	S	0	0	0
			1836	1152	328	351	5			
3	Q	234	Total	C	N	O	S	0	0	0
			1821	1143	319	354	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	233	Total	C	N	O	S	0	2	0
			1783	1118	294	360	11			
4	R	233	Total	C	N	O	S	0	1	0
			1773	1115	295	352	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	234	Total	C	N	O	S	0	0	0
			1833	1150	328	344	11			
5	S	238	Total	C	N	O	S	0	3	0
			1880	1179	339	351	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	239	Total	C	N	O	S	0	4	0
			1890	1200	323	355	12			
6	T	240	Total	C	N	O	S	0	1	0
			1867	1186	320	349	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	244	Total	C	N	O	S	0	2	0
			1928	1223	322	370	13			
7	U	235	Total	C	N	O	S	0	0	0
			1820	1151	306	350	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	220	Total	C	N	O	S	0	2	0
			1672	1053	286	320	13			
8	V	220	Total	C	N	O	S	0	2	0
			1655	1042	278	322	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	204	Total	C	N	O	S	0	6	0
			1633	1039	274	301	19			
9	W	204	Total	C	N	O	S	0	2	0
			1604	1021	269	295	19			

- 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
			1585	1017	268	290	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	196	Total	C	N	O	S	0	2	0
			1590	1019	270	291	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	201	Total	C	N	O	S	0	0	0
			1543	974	267	293	9			
11	Y	199	Total	C	N	O	S	0	3	0
			1564	988	275	291	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
			1656	1048	283	314	11			
12	Z	213	Total	C	N	O	S	0	1	0
			1644	1043	281	309	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	216	Total	C	N	O	S	0	0	0
			1687	1064	291	320	12			
13	a	216	Total	C	N	O	S	0	1	0
			1688	1065	291	320	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	202	Total	C	N	O	S	0	1	0
			1515	951	258	293	13			
14	b	203	Total	C	N	O	S	0	1	0
			1526	958	259	296	13			

- Molecule 15 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	4	Total	Cl	0	0
			4	4		
15	B	2	Total	Cl	0	0
			2	2		

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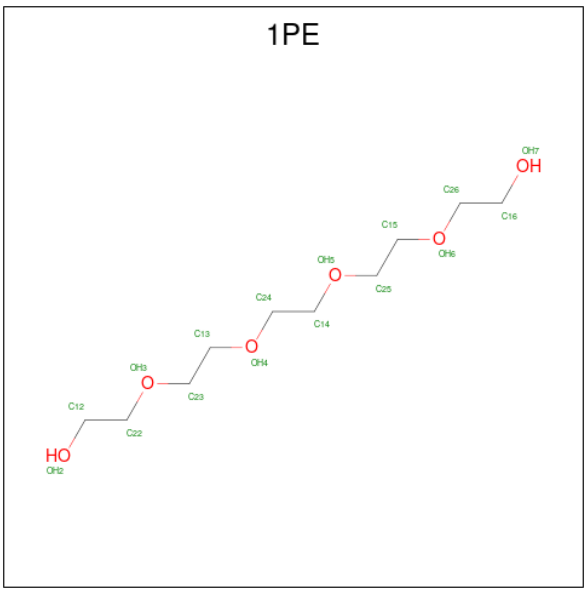
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	C	2	Total Cl 2 2	0	0
15	D	2	Total Cl 2 2	0	0
15	E	3	Total Cl 3 3	0	0
15	F	1	Total Cl 1 1	0	0
15	G	2	Total Cl 2 2	0	0
15	H	2	Total Cl 2 2	0	0
15	I	1	Total Cl 1 1	0	0
15	K	4	Total Cl 4 4	0	0
15	M	4	Total Cl 4 4	0	0
15	N	3	Total Cl 3 3	0	0
15	O	4	Total Cl 4 4	0	0
15	P	1	Total Cl 1 1	0	0
15	Q	2	Total Cl 2 2	0	0
15	R	2	Total Cl 2 2	0	0
15	S	3	Total Cl 3 3	0	0
15	U	1	Total Cl 1 1	0	0
15	V	2	Total Cl 2 2	0	0
15	W	1	Total Cl 1 1	0	0
15	Y	5	Total Cl 5 5	0	0
15	a	3	Total Cl 3 3	0	0
15	b	3	Total Cl 3 3	0	0

- Molecule 16 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total C O 16 10 6	0	0
16	I	1	Total C O 16 10 6	0	0
16	I	1	Total C O 16 10 6	0	0
16	L	1	Total C O 16 10 6	0	0
16	W	1	Total C O 16 10 6	0	0
16	Z	1	Total C O 16 10 6	0	0
16	a	1	Total C O 16 10 6	0	0
16	b	1	Total C O 16 10 6	0	0
16	b	1	Total C O 16 10 6	0	0

- Molecule 17 is POTASSIUM ION (three-letter code: K) (formula: K).

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

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

- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 19 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	112	Total O 112 112	0	0
19	B	123	Total O 123 123	0	0
19	C	75	Total O 75 75	0	0
19	D	83	Total O 83 83	0	0
19	E	134	Total O 134 134	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	F	189	Total O 189 189	0	0
19	G	190	Total O 190 190	0	0
19	H	151	Total O 151 151	0	0
19	I	149	Total O 149 149	0	0
19	J	127	Total O 127 127	0	0
19	K	108	Total O 108 108	0	0
19	L	115	Total O 115 115	0	0
19	M	155	Total O 155 155	0	0
19	N	164	Total O 164 164	0	0
19	O	85	Total O 85 85	0	0
19	P	111	Total O 111 111	0	0
19	Q	66	Total O 66 66	0	0
19	R	126	Total O 126 126	0	0
19	S	115	Total O 115 115	0	0
19	T	85	Total O 85 85	0	0
19	U	100	Total O 100 100	0	0
19	V	108	Total O 108 108	0	0
19	W	117	Total O 117 117	0	0
19	X	120	Total O 120 120	0	0
19	Y	145	Total O 145 145	0	0
19	Z	168	Total O 168 168	0	0

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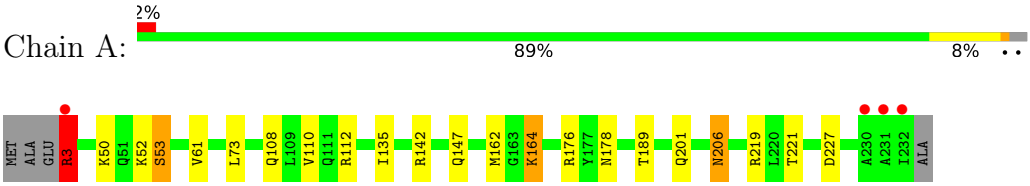
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	a	164	Total O 164 164	0	0
19	b	127	Total O 127 127	0	0

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.

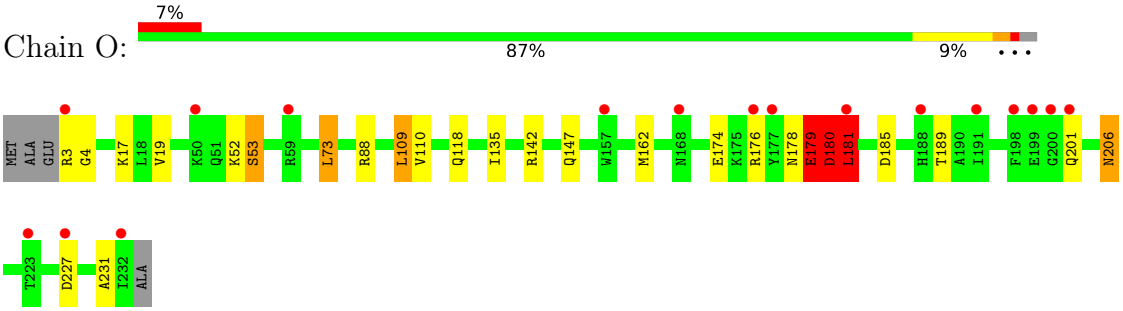
• Molecule 1: Proteasome subunit alpha type-2

Chain A:



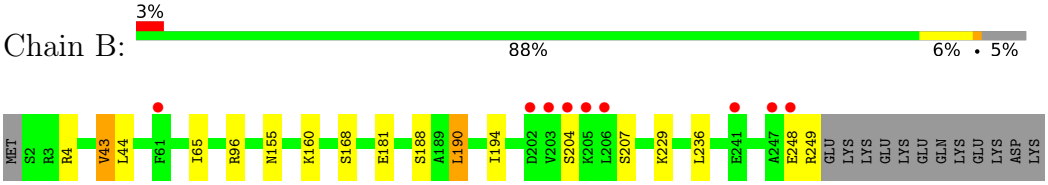
• Molecule 1: Proteasome subunit alpha type-2

Chain O:



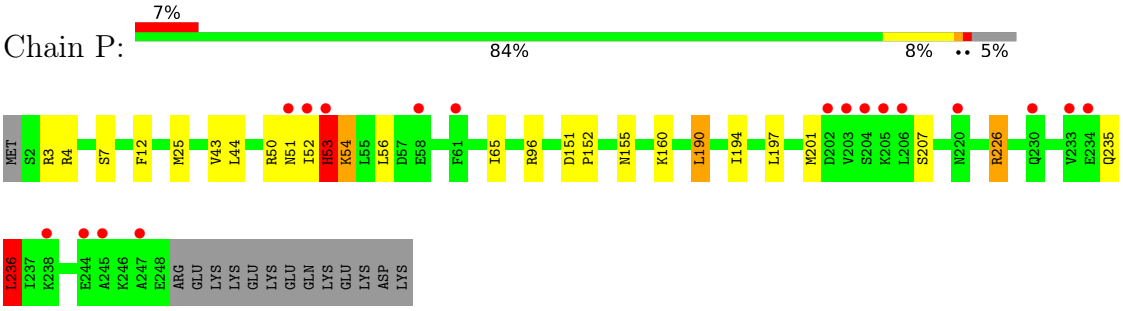
• Molecule 2: Proteasome subunit alpha type-4

Chain B:

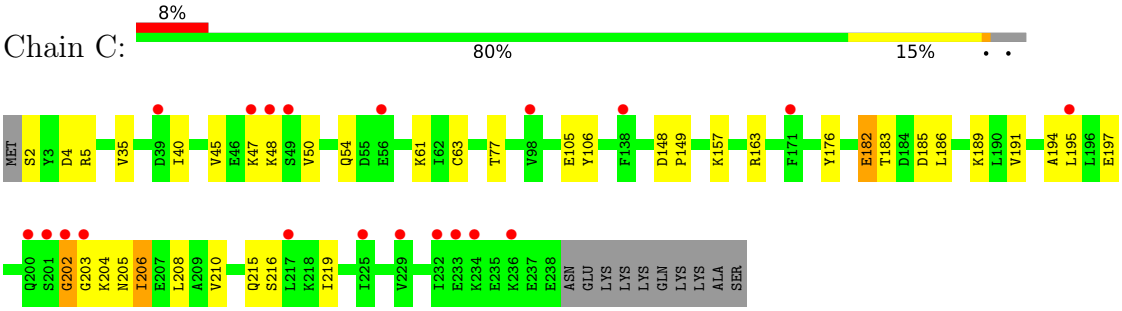


• Molecule 2: Proteasome subunit alpha type-4

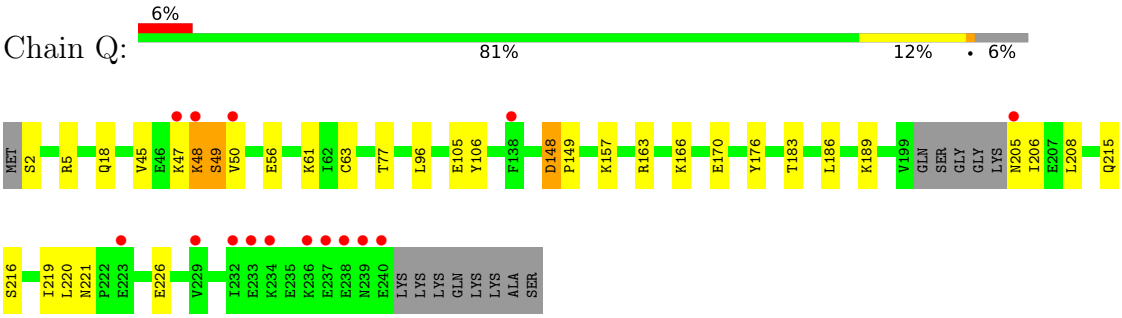
Chain P:



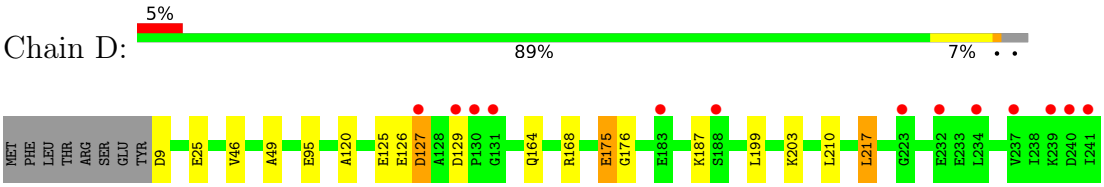
• Molecule 3: Proteasome subunit alpha type-7



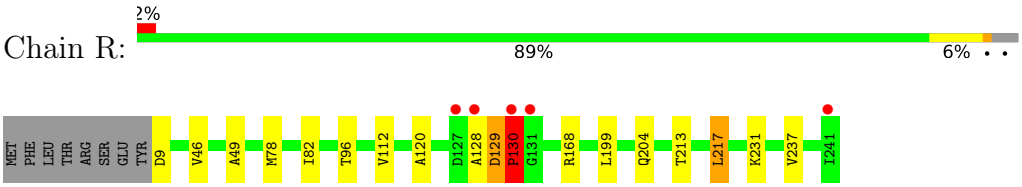
• Molecule 3: Proteasome subunit alpha type-7



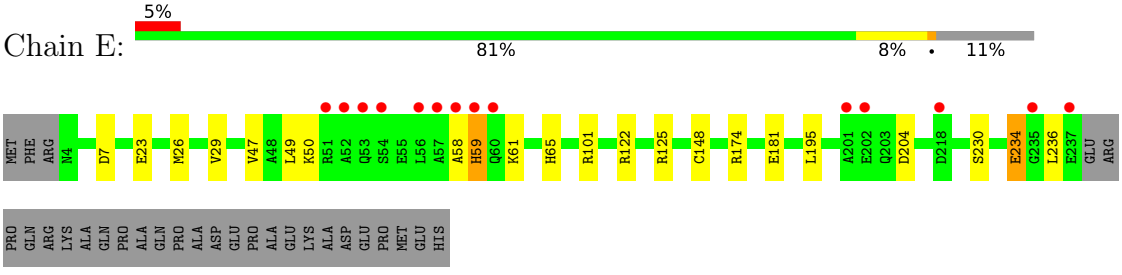
• Molecule 4: Proteasome subunit alpha type-5



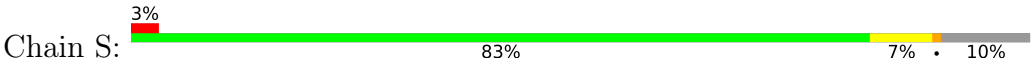
• Molecule 4: Proteasome subunit alpha type-5

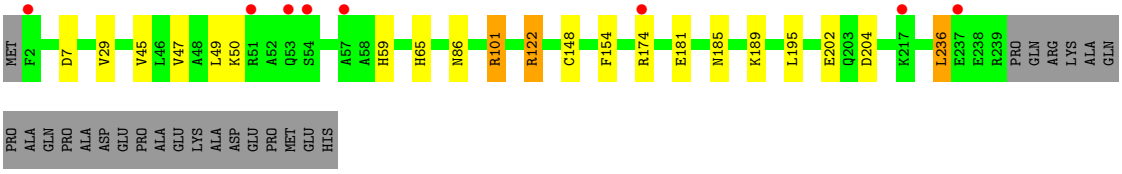


• Molecule 5: Proteasome subunit alpha type-1

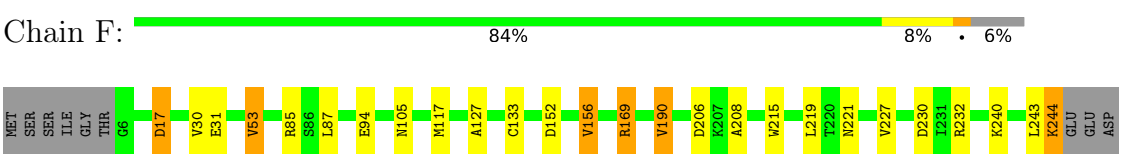


• Molecule 5: Proteasome subunit alpha type-1

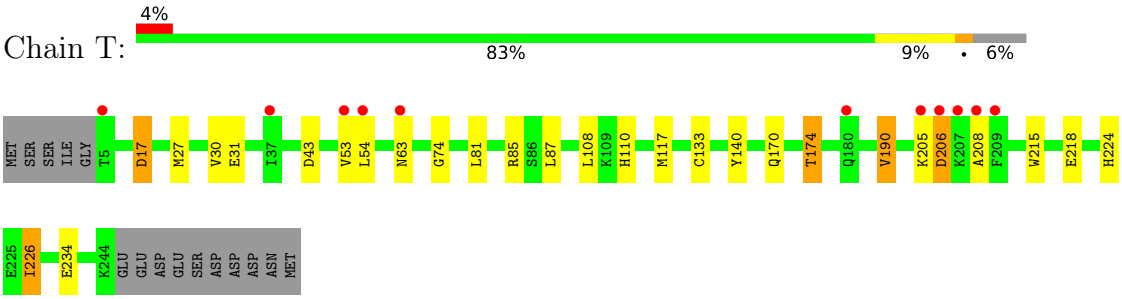




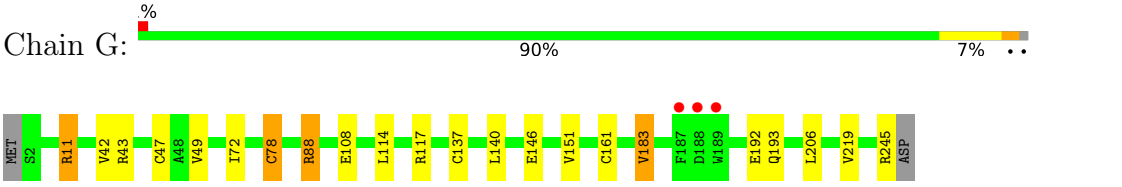
• Molecule 6: Proteasome subunit alpha type-3



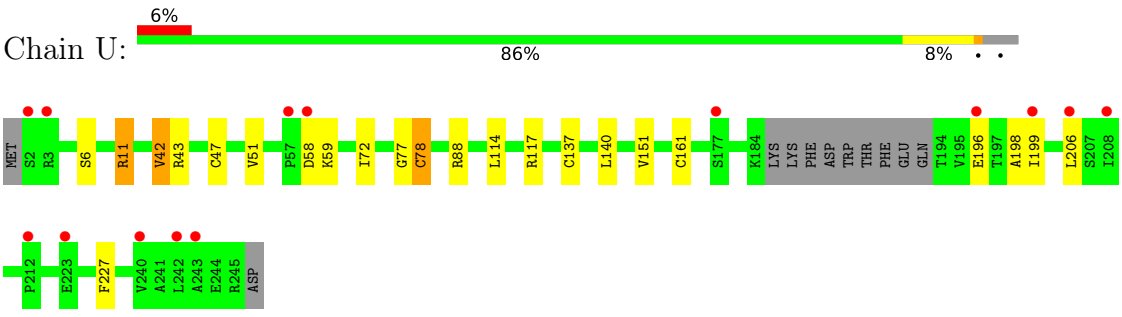
• Molecule 6: Proteasome subunit alpha type-3



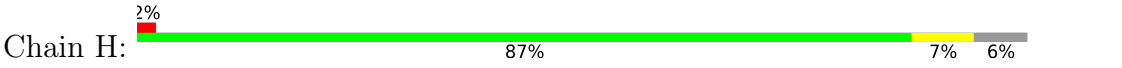
• Molecule 7: Proteasome subunit alpha type-6

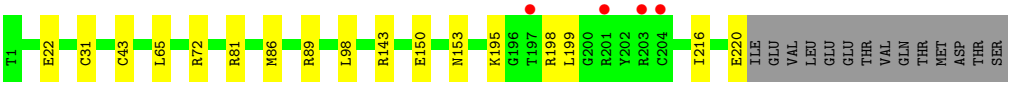


• Molecule 7: Proteasome subunit alpha type-6

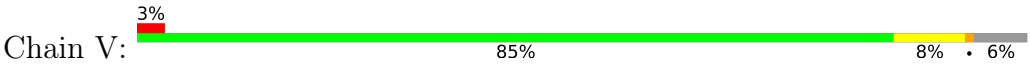


• Molecule 8: Proteasome subunit beta type-7

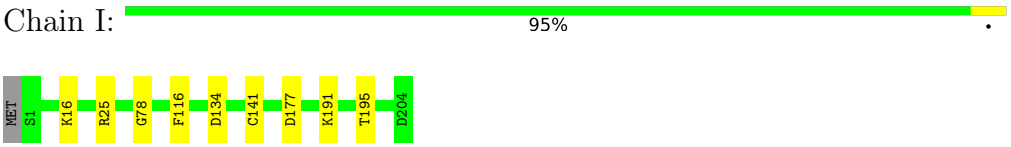




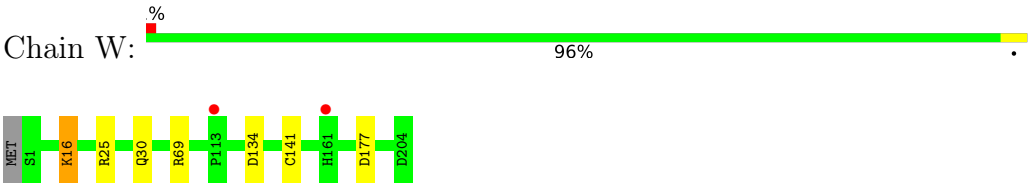
• Molecule 8: Proteasome subunit beta type-7



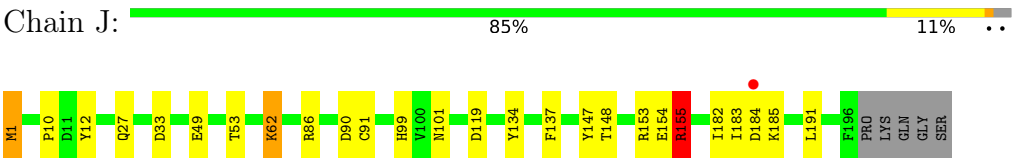
• Molecule 9: Proteasome subunit beta type-3



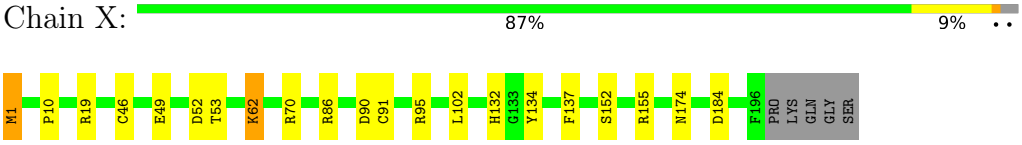
• Molecule 9: Proteasome subunit beta type-3



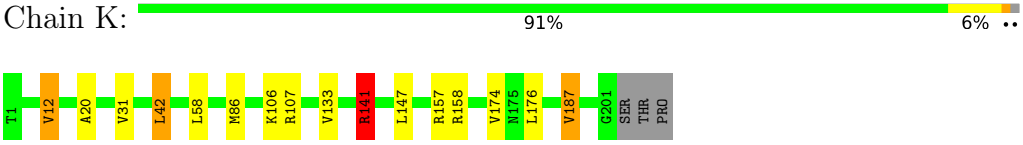
• Molecule 10: Proteasome subunit beta type-2



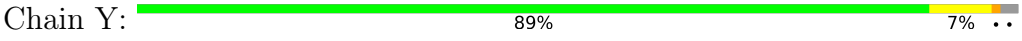
• Molecule 10: Proteasome subunit beta type-2



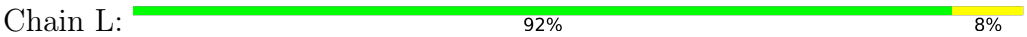
• Molecule 11: Proteasome subunit beta type-5



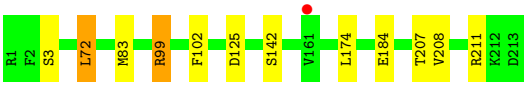
• Molecule 11: Proteasome subunit beta type-5



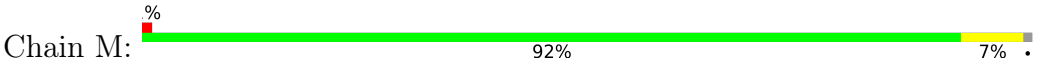
• Molecule 12: Proteasome subunit beta type-1



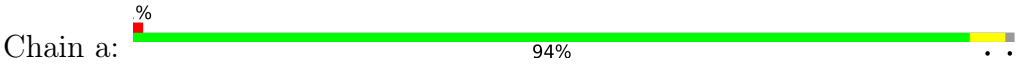
• Molecule 12: Proteasome subunit beta type-1



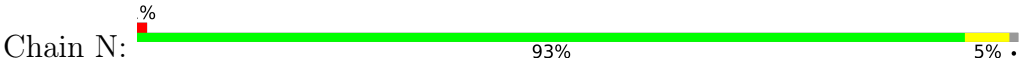
• Molecule 13: Proteasome subunit beta type-4

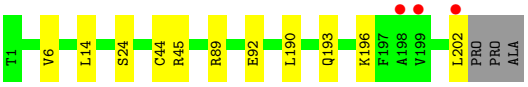


• Molecule 13: Proteasome subunit beta type-4



• Molecule 14: Proteasome subunit beta type-6





• Molecule 14: Proteasome subunit beta type-6

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	113.44Å 202.77Å 316.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	170.66 – 1.80 106.77 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (170.66-1.80) 99.9 (106.77-1.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.11 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.182 , 0.212 0.190 , 0.217	Depositor DCC
R_{free} test set	33208 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	34.1	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 42.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	52161	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: YCM, K, MG, CL, 6V1, 1PE

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	0.73	1/1844 (0.1%)	0.82	1/2500 (0.0%)
1	O	0.64	0/1818	0.86	5/2467 (0.2%)
2	B	0.81	2/1975 (0.1%)	0.94	4/2665 (0.2%)
2	P	0.75	0/1955	0.90	6/2642 (0.2%)
3	C	1.16	3/1851 (0.2%)	0.91	3/2502 (0.1%)
3	Q	0.79	1/1835 (0.1%)	0.89	2/2485 (0.1%)
4	D	0.76	1/1810 (0.1%)	0.91	4/2448 (0.2%)
4	R	0.81	0/1800	0.94	4/2431 (0.2%)
5	E	0.75	1/1851 (0.1%)	0.91	3/2502 (0.1%)
5	S	0.71	0/1908	0.91	6/2577 (0.2%)
6	F	0.91	1/1937 (0.1%)	1.01	9/2607 (0.3%)
6	T	0.77	0/1905	0.96	8/2567 (0.3%)
7	G	0.91	1/1925 (0.1%)	0.92	8/2598 (0.3%)
7	U	0.69	0/1806	0.84	4/2438 (0.2%)
8	H	0.85	1/1705 (0.1%)	0.98	6/2307 (0.3%)
8	V	0.68	0/1688	0.90	4/2288 (0.2%)
9	I	0.82	0/1668	0.97	5/2247 (0.2%)
9	W	0.68	0/1636	1.00	9/2205 (0.4%)
10	J	0.95	3/1605 (0.2%)	0.99	2/2170 (0.1%)
10	X	0.84	2/1613 (0.1%)	0.98	8/2180 (0.4%)
11	K	0.79	0/1574	1.00	7/2128 (0.3%)
11	Y	0.85	0/1604	1.04	10/2165 (0.5%)
12	L	0.73	1/1692 (0.1%)	0.87	3/2281 (0.1%)
12	Z	0.84	2/1677 (0.1%)	1.06	4/2260 (0.2%)
13	M	0.82	1/1720 (0.1%)	0.97	4/2328 (0.2%)
13	a	0.86	0/1724	0.98	7/2334 (0.3%)
14	N	0.94	4/1544 (0.3%)	0.94	4/2090 (0.2%)
14	b	0.86	4/1556 (0.3%)	0.91	2/2107 (0.1%)
All	All	0.82	29/49226 (0.1%)	0.94	142/66519 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	P	0	1
3	C	0	1
3	Q	0	2
4	D	0	3
7	U	1	0
9	I	0	1
10	X	0	1
12	Z	0	1
All	All	1	10

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	182	GLU	CG-CD	27.93	1.93	1.51
3	C	182	GLU	CD-OE2	-24.47	0.98	1.25
7	G	108	GLU	CD-OE1	14.97	1.42	1.25
3	Q	189	LYS	C-O	11.20	1.44	1.23
14	b	150	GLU	CD-OE1	9.45	1.36	1.25

The worst 5 of 142 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	Z	99	ARG	NE-CZ-NH2	-17.26	111.67	120.30
12	Z	99	ARG	NE-CZ-NH1	16.34	128.47	120.30
9	W	69	ARG	NE-CZ-NH1	14.69	127.64	120.30
9	W	69	ARG	NE-CZ-NH2	-12.94	113.83	120.30
13	M	151	ARG	NE-CZ-NH1	11.86	126.23	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	202	GLY	Peptide
4	D	175[A]	GLU	Peptide
4	D	175[B]	GLU	Mainchain,Peptide

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Mol	Chain	Res	Type	Group
9	I	78[B]	GLY	Peptide
2	P	54	LYS	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	1799	0	1793	8	0
1	O	1779	0	1747	13	0
2	B	1942	0	1938	6	0
2	P	1919	0	1895	16	0
3	C	1836	0	1821	20	0
3	Q	1821	0	1788	12	0
4	D	1783	0	1751	6	0
4	R	1773	0	1760	9	0
5	E	1833	0	1797	8	0
5	S	1880	0	1850	10	0
6	F	1890	0	1886	11	0
6	T	1867	0	1847	8	0
7	G	1928	0	1905	10	0
7	U	1820	0	1792	10	0
8	H	1672	0	1703	5	0
8	V	1655	0	1661	9	0
9	I	1633	0	1660	4	0
9	W	1604	0	1626	3	0
10	J	1585	0	1568	19	0
10	X	1590	0	1580	7	0
11	K	1543	0	1495	4	0
11	Y	1564	0	1539	9	0
12	L	1656	0	1655	7	0
12	Z	1644	0	1644	3	0
13	M	1687	0	1666	4	0
13	a	1688	0	1666	0	0
14	N	1515	0	1492	2	0
14	b	1526	0	1503	0	0
15	A	4	0	0	0	0
15	B	2	0	0	1	0
15	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	D	2	0	0	0	0
15	E	3	0	0	0	0
15	F	1	0	0	0	0
15	G	2	0	0	0	0
15	H	2	0	0	1	0
15	I	1	0	0	0	0
15	K	4	0	0	0	0
15	M	4	0	0	1	0
15	N	3	0	0	0	0
15	O	4	0	0	0	0
15	P	1	0	0	0	0
15	Q	2	0	0	0	0
15	R	2	0	0	1	0
15	S	3	0	0	0	0
15	U	1	0	0	0	0
15	V	2	0	0	0	0
15	W	1	0	0	0	0
15	Y	5	0	0	1	0
15	a	3	0	0	0	0
15	b	3	0	0	0	0
16	G	16	0	22	1	0
16	I	32	0	44	0	0
16	L	16	0	22	0	0
16	W	16	0	22	0	0
16	Z	16	0	22	0	0
16	a	16	0	22	0	0
16	b	32	0	44	0	0
17	G	1	0	0	0	0
17	L	1	0	0	0	0
17	N	1	0	0	0	0
17	U	1	0	0	0	0
17	Z	1	0	0	0	0
17	b	1	0	0	0	0
18	H	2	0	0	0	0
18	I	2	0	0	0	0
18	J	1	0	0	0	0
18	K	1	0	0	0	0
18	L	1	0	0	0	0
18	V	1	0	0	0	0
18	W	1	0	0	0	0
18	X	1	0	0	0	0
19	A	112	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	B	123	0	0	0	0
19	C	75	0	0	0	0
19	D	83	0	0	0	0
19	E	134	0	0	1	0
19	F	189	0	0	5	0
19	G	190	0	0	4	0
19	H	151	0	0	2	0
19	I	149	0	0	1	0
19	J	127	0	0	1	0
19	K	108	0	0	0	0
19	L	115	0	0	1	0
19	M	155	0	0	0	0
19	N	164	0	0	0	0
19	O	85	0	0	1	0
19	P	111	0	0	1	0
19	Q	66	0	0	0	0
19	R	126	0	0	2	0
19	S	115	0	0	3	0
19	T	85	0	0	1	0
19	U	100	0	0	0	0
19	V	108	0	0	2	0
19	W	117	0	0	3	0
19	X	120	0	0	1	0
19	Y	145	0	0	0	0
19	Z	168	0	0	0	0
19	a	164	0	0	0	0
19	b	127	0	0	0	0
All	All	52161	0	48226	213	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 2.

The worst 5 of 213 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)
3:C:182:GLU:CD	3:C:182:GLU:CG	1.93	1.34
10:J:1:MET:HG3	10:J:134:TYR:CD2	1.92	1.04
10:J:183:ILE:O	10:J:184:ASP:OD1	1.83	0.97
9:I:16[A]:LYS:O	19:I:401:HOH:O	1.85	0.95
10:J:1:MET:HG3	10:J:134:TYR:HD2	1.36	0.91

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	230/234 (98%)	220 (96%)	6 (3%)	4 (2%)	9 2
1	O	228/234 (97%)	214 (94%)	7 (3%)	7 (3%)	4 0
2	B	247/261 (95%)	238 (96%)	9 (4%)	0	100 100
2	P	247/261 (95%)	234 (95%)	11 (4%)	2 (1%)	19 7
3	C	234/248 (94%)	224 (96%)	6 (3%)	4 (2%)	9 2
3	Q	229/248 (92%)	218 (95%)	6 (3%)	5 (2%)	6 1
4	D	233/241 (97%)	223 (96%)	6 (3%)	4 (2%)	9 2
4	R	232/241 (96%)	223 (96%)	6 (3%)	3 (1%)	12 3
5	E	231/263 (88%)	226 (98%)	4 (2%)	1 (0%)	34 21
5	S	238/263 (90%)	234 (98%)	4 (2%)	0	100 100
6	F	241/255 (94%)	238 (99%)	3 (1%)	0	100 100
6	T	239/255 (94%)	233 (98%)	4 (2%)	2 (1%)	19 7
7	G	241/246 (98%)	237 (98%)	4 (2%)	0	100 100
7	U	228/246 (93%)	224 (98%)	4 (2%)	0	100 100
8	H	220/234 (94%)	217 (99%)	3 (1%)	0	100 100
8	V	220/234 (94%)	215 (98%)	4 (2%)	1 (0%)	29 15
9	I	208/205 (102%)	204 (98%)	4 (2%)	0	100 100
9	W	204/205 (100%)	198 (97%)	6 (3%)	0	100 100
10	J	195/201 (97%)	192 (98%)	3 (2%)	0	100 100
10	X	195/201 (97%)	192 (98%)	3 (2%)	0	100 100
11	K	199/204 (98%)	195 (98%)	4 (2%)	0	100 100
11	Y	200/204 (98%)	197 (98%)	3 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	L	213/213 (100%)	211 (99%)	2 (1%)	0	100	100
12	Z	212/213 (100%)	210 (99%)	2 (1%)	0	100	100
13	M	214/219 (98%)	208 (97%)	6 (3%)	0	100	100
13	a	215/219 (98%)	209 (97%)	6 (3%)	0	100	100
14	N	201/205 (98%)	198 (98%)	3 (2%)	0	100	100
14	b	202/205 (98%)	199 (98%)	3 (2%)	0	100	100
All	All	6196/6458 (96%)	6031 (97%)	132 (2%)	33 (0%)	29	15

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	LYS
1	A	53	SER
4	D	127	ASP
4	D	176	GLY
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	188/191 (98%)	177 (94%)	11 (6%)	19	7
1	O	184/191 (96%)	172 (94%)	12 (6%)	17	6
2	B	205/221 (93%)	198 (97%)	7 (3%)	37	22
2	P	201/221 (91%)	190 (94%)	11 (6%)	21	8
3	C	189/210 (90%)	181 (96%)	8 (4%)	30	15
3	Q	189/210 (90%)	176 (93%)	13 (7%)	15	5
4	D	194/203 (96%)	187 (96%)	7 (4%)	35	20
4	R	192/203 (95%)	189 (98%)	3 (2%)	62	54
5	E	195/223 (87%)	188 (96%)	7 (4%)	35	20
5	S	201/223 (90%)	194 (96%)	7 (4%)	36	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	F	200/212 (94%)	192 (96%)	8 (4%)	31 16
6	T	194/212 (92%)	184 (95%)	10 (5%)	23 10
7	G	206/207 (100%)	201 (98%)	5 (2%)	49 36
7	U	192/207 (93%)	187 (97%)	5 (3%)	46 32
8	H	183/195 (94%)	179 (98%)	4 (2%)	52 39
8	V	180/195 (92%)	172 (96%)	8 (4%)	28 14
9	I	178/174 (102%)	178 (100%)	0	100 100
9	W	174/174 (100%)	174 (100%)	0	100 100
10	J	166/170 (98%)	160 (96%)	6 (4%)	35 20
10	X	168/170 (99%)	164 (98%)	4 (2%)	49 36
11	K	153/159 (96%)	144 (94%)	9 (6%)	19 7
11	Y	157/159 (99%)	152 (97%)	5 (3%)	39 25
12	L	179/178 (101%)	170 (95%)	9 (5%)	24 10
12	Z	176/178 (99%)	171 (97%)	5 (3%)	43 30
13	M	179/181 (99%)	175 (98%)	4 (2%)	52 39
13	a	179/181 (99%)	174 (97%)	5 (3%)	43 30
14	N	157/159 (99%)	155 (99%)	2 (1%)	69 62
14	b	159/159 (100%)	158 (99%)	1 (1%)	86 84
All	All	5118/5366 (95%)	4942 (97%)	176 (3%)	37 22

5 of 176 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	Q	166	LYS
7	U	42	VAL
3	Q	208	LEU
5	S	181	GLU
8	V	68	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
5	S	185	ASN
10	X	24	ASN
6	T	63	ASN

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Mol	Chain	Res	Type
8	V	116	HIS
10	X	174	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

12 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	6V1	G	161	7	12,15,16	1.93	4 (33%)	9,20,22	2.13	3 (33%)
5	6V1	E	148	5	12,15,16	1.79	4 (33%)	9,20,22	3.07	3 (33%)
7	YCM	U	137	7	7,9,10	1.25	1 (14%)	4,10,12	1.92	2 (50%)
7	6V1	G	47	7	12,15,16	3.22	5 (41%)	9,20,22	2.27	3 (33%)
10	6V1	X	91	10	12,15,16	2.73	4 (33%)	9,20,22	5.55	7 (77%)
3	YCM	C	63	3	7,9,10	1.07	1 (14%)	4,10,12	0.73	0
10	6V1	J	91	10	12,15,16	2.43	2 (16%)	9,20,22	5.84	7 (77%)
7	6V1	U	47	7	12,15,16	2.14	2 (16%)	9,20,22	3.01	3 (33%)
5	6V1	S	148	5	12,15,16	1.88	2 (16%)	9,20,22	3.32	5 (55%)
3	YCM	Q	63	3	7,9,10	1.64	1 (14%)	4,10,12	3.94	3 (75%)
7	YCM	G	137	7	7,9,10	2.19	3 (42%)	4,10,12	2.50	3 (75%)
7	6V1	U	161	7	12,15,16	1.85	4 (33%)	9,20,22	2.47	4 (44%)

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	6V1	G	161	7	-	1/6/25/27	0/1/1/1
5	6V1	E	148	5	-	2/6/25/27	0/1/1/1
7	YCM	U	137	7	-	1/6/8/10	-
7	6V1	G	47	7	-	0/6/25/27	0/1/1/1
10	6V1	X	91	10	-	2/6/25/27	0/1/1/1
3	YCM	C	63	3	-	1/6/8/10	-
10	6V1	J	91	10	-	3/6/25/27	0/1/1/1
7	6V1	U	47	7	1/1/5/6	2/6/25/27	0/1/1/1
5	6V1	S	148	5	-	2/6/25/27	0/1/1/1
3	YCM	Q	63	3	-	3/6/8/10	-
7	YCM	G	137	7	-	2/6/8/10	-
7	6V1	U	161	7	-	1/6/25/27	0/1/1/1

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	47	6V1	CB-SG	-8.11	1.73	1.82
10	X	91	6V1	C1-SG	-7.84	1.74	1.83
10	J	91	6V1	C1-SG	-7.47	1.75	1.83
7	U	47	6V1	CB-SG	-6.21	1.75	1.82
5	S	148	6V1	CB-SG	-4.55	1.77	1.82

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	J	91	6V1	C5-C4-N3	10.03	114.04	108.13
10	J	91	6V1	C6-N3-C2	9.25	135.09	123.36
10	X	91	6V1	C5-C4-N3	9.05	113.46	108.13
10	X	91	6V1	C6-N3-C2	8.49	134.12	123.36
3	Q	63	YCM	CE-CD-SG	-6.49	94.49	113.59

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	63	YCM	CE-CD-SG-CB
5	E	148	6V1	C3-C6-N3-C2

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Mol	Chain	Res	Type	Atoms
5	E	148	6V1	C3-C6-N3-C4
7	G	137	YCM	CE-CD-SG-CB
7	G	137	YCM	SG-CD-CE-NZ2

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 82 ligands modelled in this entry, 73 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	$\#\|Z\| > 2$
16	1PE	W	303	-	15,15,15	0.56	0	14,14,14	0.50	0
16	1PE	a	304	-	15,15,15	0.53	0	14,14,14	0.57	0
16	1PE	G	303	-	15,15,15	0.57	0	14,14,14	0.70	0
16	1PE	Z	301	-	15,15,15	0.62	0	14,14,14	0.62	0
16	1PE	b	505	-	15,15,15	0.66	0	14,14,14	0.39	0
16	1PE	I	304	-	15,15,15	0.53	0	14,14,14	0.64	0
16	1PE	b	504	-	15,15,15	0.61	0	14,14,14	0.77	0
16	1PE	I	303	-	15,15,15	0.55	0	14,14,14	0.86	1 (7%)
16	1PE	L	301	-	15,15,15	0.61	0	14,14,14	0.73	1 (7%)

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
16	1PE	W	303	-	-	6/13/13/13	-
16	1PE	a	304	-	-	4/13/13/13	-
16	1PE	G	303	-	-	3/13/13/13	-
16	1PE	Z	301	-	-	6/13/13/13	-
16	1PE	b	505	-	-	9/13/13/13	-
16	1PE	I	304	-	-	5/13/13/13	-
16	1PE	b	504	-	-	5/13/13/13	-
16	1PE	I	303	-	-	8/13/13/13	-
16	1PE	L	301	-	-	6/13/13/13	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	I	303	1PE	C25-OH5-C14	2.12	122.49	113.29
16	L	301	1PE	C26-OH6-C15	2.11	122.45	113.29

There are no chirality outliers.

5 of 52 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	I	304	1PE	C24-C14-OH5-C25
16	I	303	1PE	C15-C25-OH5-C14
16	b	505	1PE	OH5-C14-C24-OH4
16	L	301	1PE	OH6-C15-C25-OH5
16	W	303	1PE	OH6-C15-C25-OH5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	G	303	1PE	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	230/234 (98%)	-0.11	4 (1%) 70 66	27, 42, 75, 87	0
1	O	230/234 (98%)	0.34	17 (7%) 14 11	36, 56, 92, 119	0
2	B	248/261 (95%)	0.11	9 (3%) 42 37	31, 48, 85, 130	0
2	P	247/261 (94%)	0.25	18 (7%) 15 11	35, 53, 91, 133	0
3	C	236/248 (95%)	0.47	20 (8%) 10 8	32, 57, 97, 128	0
3	Q	233/248 (93%)	0.28	15 (6%) 19 15	31, 54, 95, 127	0
4	D	233/241 (96%)	0.23	13 (5%) 24 19	35, 55, 85, 106	0
4	R	233/241 (96%)	-0.11	5 (2%) 63 59	29, 40, 62, 82	0
5	E	233/263 (88%)	0.09	14 (6%) 21 17	25, 39, 82, 98	0
5	S	237/263 (90%)	-0.05	8 (3%) 45 39	31, 43, 72, 94	0
6	F	239/255 (93%)	-0.15	0 100 100	22, 32, 52, 72	0
6	T	240/255 (94%)	0.17	11 (4%) 32 26	32, 49, 79, 105	0
7	G	241/246 (97%)	-0.10	3 (1%) 79 76	23, 35, 65, 89	0
7	U	232/246 (94%)	0.23	14 (6%) 21 17	38, 56, 86, 122	0
8	H	220/234 (94%)	-0.00	4 (1%) 68 64	25, 32, 62, 87	0
8	V	220/234 (94%)	-0.07	6 (2%) 54 49	34, 44, 78, 100	0
9	I	204/205 (99%)	-0.25	0 100 100	25, 32, 51, 64	0
9	W	204/205 (99%)	-0.22	2 (0%) 82 80	32, 44, 66, 72	0
10	J	195/201 (97%)	-0.16	1 (0%) 91 89	28, 38, 55, 70	0
10	X	195/201 (97%)	-0.22	0 100 100	30, 38, 54, 69	0
11	K	201/204 (98%)	-0.28	0 100 100	32, 41, 65, 90	0
11	Y	199/204 (97%)	-0.26	0 100 100	26, 33, 51, 62	0
12	L	213/213 (100%)	-0.11	0 100 100	29, 45, 65, 83	0
12	Z	213/213 (100%)	-0.16	1 (0%) 91 89	24, 34, 55, 73	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	M	216/219 (98%)	-0.10	2 (0%)	84	82	24, 35, 59, 94	0
13	a	216/219 (98%)	-0.14	2 (0%)	84	82	24, 36, 57, 82	0
14	N	202/205 (98%)	-0.08	3 (1%)	73	70	23, 32, 52, 91	0
14	b	203/205 (99%)	-0.13	4 (1%)	65	61	30, 38, 63, 90	0
All	All	6213/6458 (96%)	-0.01	176 (2%)	53	47	22, 42, 78, 133	0

The worst 5 of 176 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	232	ILE	13.9
2	B	203	VAL	10.3
4	D	241	ILE	9.3
2	P	204	SER	9.0
2	P	203	VAL	9.0

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	6V1	U	47	15/16	0.83	0.29	64,96,103,104	0
7	YCM	U	137	10/11	0.83	0.15	46,54,72,72	0
3	YCM	C	63	10/11	0.87	0.11	48,50,59,60	0
7	YCM	G	137	10/11	0.89	0.12	27,34,48,49	0
5	6V1	S	148	15/16	0.89	0.18	35,56,62,64	0
5	6V1	E	148	15/16	0.89	0.15	29,45,55,55	0
7	6V1	G	47	15/16	0.89	0.17	33,52,55,55	0
3	YCM	Q	63	10/11	0.90	0.09	45,48,59,60	0
10	6V1	J	91	15/16	0.90	0.19	31,44,50,50	0
10	6V1	X	91	15/16	0.92	0.16	32,47,53,53	0
7	6V1	U	161	15/16	0.94	0.11	48,62,69,70	0
7	6V1	G	161	15/16	0.94	0.12	28,44,50,52	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
18	MG	H	301	1/1	0.71	0.10	45,45,45,45	0
18	MG	V	301	1/1	0.74	0.18	48,48,48,48	0
16	1PE	a	304	16/16	0.78	0.22	57,62,69,71	0
15	CL	b	502	1/1	0.79	0.10	59,59,59,59	0
16	1PE	b	505	16/16	0.79	0.23	64,67,78,78	0
15	CL	O	303	1/1	0.80	0.37	74,74,74,74	0
16	1PE	I	304	16/16	0.80	0.25	48,61,71,75	0
16	1PE	L	301	16/16	0.84	0.17	49,62,66,69	0
16	1PE	W	303	16/16	0.84	0.14	55,58,64,66	0
16	1PE	b	504	16/16	0.85	0.13	41,50,67,68	0
16	1PE	I	303	16/16	0.85	0.14	48,52,60,68	0
16	1PE	Z	301	16/16	0.86	0.14	51,61,64,64	0
15	CL	M	302	1/1	0.86	0.18	62,62,62,62	0
15	CL	C	302	1/1	0.87	0.15	63,63,63,63	0
15	CL	H	303	1/1	0.88	0.11	51,51,51,51	0
18	MG	X	301	1/1	0.89	0.07	44,44,44,44	0
16	1PE	G	303	16/16	0.91	0.12	34,42,51,56	0
15	CL	A	302	1/1	0.91	0.07	61,61,61,61	0
15	CL	K	304	1/1	0.91	0.15	52,52,52,52	0
15	CL	V	303	1/1	0.91	0.09	59,59,59,59	0
18	MG	J	301	1/1	0.91	0.06	41,41,41,41	0
15	CL	Y	305	1/1	0.91	0.09	54,54,54,54	0
15	CL	K	305	1/1	0.91	0.29	60,60,60,60	0
15	CL	D	302	1/1	0.92	0.10	53,53,53,53	0
15	CL	C	301	1/1	0.92	0.11	56,56,56,56	0
15	CL	O	304	1/1	0.92	0.14	55,55,55,55	0
15	CL	V	302	1/1	0.92	0.10	50,50,50,50	0
15	CL	M	301	1/1	0.92	0.18	52,52,52,52	0
15	CL	G	302	1/1	0.93	0.05	56,56,56,56	0
18	MG	K	301	1/1	0.93	0.07	33,33,33,33	0
15	CL	S	302	1/1	0.93	0.12	54,54,54,54	0
15	CL	Y	304	1/1	0.93	0.07	51,51,51,51	0
15	CL	P	301	1/1	0.94	0.06	45,45,45,45	0
15	CL	B	302	1/1	0.94	0.17	54,54,54,54	0
15	CL	F	301	1/1	0.94	0.06	46,46,46,46	0
15	CL	E	303	1/1	0.95	0.15	54,54,54,54	0
15	CL	A	301	1/1	0.95	0.07	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	CL	O	301	1/1	0.95	0.05	49,49,49,49	0
15	CL	Y	303	1/1	0.95	0.06	56,56,56,56	0
17	K	b	506	1/1	0.95	0.07	38,38,38,38	0
15	CL	O	302	1/1	0.96	0.07	59,59,59,59	0
15	CL	E	302	1/1	0.96	0.07	49,49,49,49	0
15	CL	D	301	1/1	0.96	0.19	61,61,61,61	0
15	CL	I	302	1/1	0.96	0.06	40,40,40,40	0
15	CL	a	301	1/1	0.96	0.13	53,53,53,53	0
17	K	U	302	1/1	0.96	0.06	38,38,38,38	0
15	CL	a	303	1/1	0.96	0.08	52,52,52,52	0
15	CL	Q	302	1/1	0.96	0.21	54,54,54,54	0
18	MG	I	301	1/1	0.96	0.08	29,29,29,29	0
15	CL	R	302	1/1	0.96	0.15	48,48,48,48	0
15	CL	S	301	1/1	0.96	0.29	59,59,59,59	0
15	CL	M	304	1/1	0.96	0.04	49,49,49,49	0
18	MG	W	301	1/1	0.96	0.07	34,34,34,34	0
15	CL	B	301	1/1	0.96	0.09	37,37,37,37	0
15	CL	Q	301	1/1	0.97	0.16	62,62,62,62	0
15	CL	S	303	1/1	0.97	0.06	48,48,48,48	0
15	CL	N	501	1/1	0.97	0.07	42,42,42,42	0
15	CL	a	302	1/1	0.97	0.06	42,42,42,42	0
15	CL	K	303	1/1	0.97	0.12	62,62,62,62	0
15	CL	b	501	1/1	0.97	0.07	44,44,44,44	0
18	MG	L	303	1/1	0.97	0.08	33,33,33,33	0
15	CL	W	302	1/1	0.97	0.05	49,49,49,49	0
15	CL	K	302	1/1	0.97	0.07	41,41,41,41	0
17	K	N	504	1/1	0.97	0.06	37,37,37,37	0
15	CL	Y	301	1/1	0.98	0.09	33,33,33,33	0
15	CL	U	301	1/1	0.98	0.10	51,51,51,51	0
17	K	L	302	1/1	0.98	0.05	42,42,42,42	0
15	CL	G	301	1/1	0.98	0.10	41,41,41,41	0
15	CL	R	301	1/1	0.98	0.09	50,50,50,50	0
15	CL	b	503	1/1	0.98	0.07	44,44,44,44	0
15	CL	A	304	1/1	0.98	0.12	52,52,52,52	0
15	CL	N	503	1/1	0.99	0.06	40,40,40,40	0
15	CL	A	303	1/1	0.99	0.07	42,42,42,42	0
18	MG	H	302	1/1	0.99	0.05	29,29,29,29	0
15	CL	M	303	1/1	0.99	0.05	38,38,38,38	0
18	MG	I	305	1/1	0.99	0.07	26,26,26,26	0
15	CL	E	301	1/1	0.99	0.08	54,54,54,54	0
17	K	G	304	1/1	0.99	0.07	28,28,28,28	0
15	CL	H	304	1/1	0.99	0.06	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	CL	N	502	1/1	0.99	0.05	43,43,43,43	0
15	CL	Y	302	1/1	0.99	0.07	47,47,47,47	0
17	K	Z	302	1/1	0.99	0.06	34,34,34,34	0

6.5 Other polymers (i)

There are no such residues in this entry.