



wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 03:59 am BST

PDB ID : 1G65
Title : Crystal structure of epoxomicin:20s proteasome reveals a molecular basis for selectivity of alpha,beta-epoxyketone proteasome inhibitors
Authors : Groll, M.; Kim, K.B.; Kairies, N.; Huber, R.; Crews, C.
Deposited on : 2000-11-03
Resolution : 2.25 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

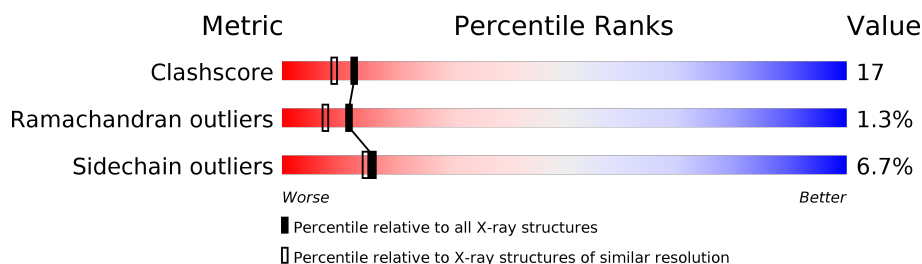
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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))
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)























The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	250	
1	O	250	
2	B	244	
2	P	244	
3	C	241	
3	Q	241	
4	D	242	
4	R	242	

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Mol	Chain	Length	Quality of chain
5	E	233	
5	S	233	
6	F	244	
6	T	244	
7	G	243	
7	U	243	
8	H	222	
8	V	222	
9	I	204	
9	W	204	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	1	233	
13	M	233	
14	2	196	
14	N	196	
15	3	5	
15	4	5	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 52508 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 component Y7.

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

- Molecule 2 is a protein called Proteasome component Y13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	0	0
			1905	1201	321	380	3			
2	P	244	Total	C	N	O	S	0	0	0
			1905	1201	321	380	3			

- Molecule 3 is a protein called Proteasome component PRE6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	241	Total	C	N	O	S	0	0	0
			1891	1181	331	375	4			
3	Q	241	Total	C	N	O	S	0	0	0
			1891	1181	331	375	4			

- Molecule 4 is a protein called Proteasome component PUP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	242	Total	C	N	O	S	0	0	0
			1862	1162	314	379	7			
4	R	242	Total	C	N	O	S	0	0	0
			1862	1162	314	379	7			

- Molecule 5 is a protein called Proteasome component PRE5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			
5	S	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			

- Molecule 6 is a protein called Proteasome component C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	244	Total	C	N	O	S	0	0	0
			1897	1205	330	358	4			
6	T	244	Total	C	N	O	S	0	0	0
			1897	1205	330	358	4			

- Molecule 7 is a protein called Proteasome component C7-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			
7	U	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			

- Molecule 8 is a protein called Proteasome component PUP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			
8	V	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			

- Molecule 9 is a protein called Proteasome component PUP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			
9	W	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

- Molecule 10 is a protein called Proteasome component C11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

- Molecule 11 is a protein called Proteasome component PRE2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			

- Molecule 12 is a protein called Proteasome component C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
12	Z	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

- Molecule 13 is a protein called Proteasome component PRE4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	1	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

- Molecule 14 is a protein called Proteasome component PRE3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
14	2	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

- Molecule 15 is a protein called EPOXOMICIN (peptide inhibitor).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	3	5	Total	C	N	O	0	0	0
			39	28	4	7			
15	4	5	Total	C	N	O	0	0	0
			39	28	4	7			

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	G	1	Total 1	Mg 1	0	0
16	D	1	Total 1	Mg 1	0	0
16	K	1	Total 1	Mg 1	0	0
16	H	1	Total 1	Mg 1	0	0
16	I	2	Total 2	Mg 2	0	0
16	N	1	Total 1	Mg 1	0	0
16	L	1	Total 1	Mg 1	0	0
16	F	2	Total 2	Mg 2	0	0

- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	100	Total 100	O 100	0	0
17	B	72	Total 72	O 72	0	0
17	C	71	Total 71	O 71	0	0
17	D	86	Total 86	O 86	0	0
17	E	57	Total 57	O 57	0	0
17	F	98	Total 98	O 98	0	0
17	G	106	Total 106	O 106	0	0
17	H	129	Total 129	O 129	0	0
17	I	109	Total 109	O 109	0	0
17	J	114	Total 114	O 114	0	0
17	K	94	Total 94	O 94	0	0

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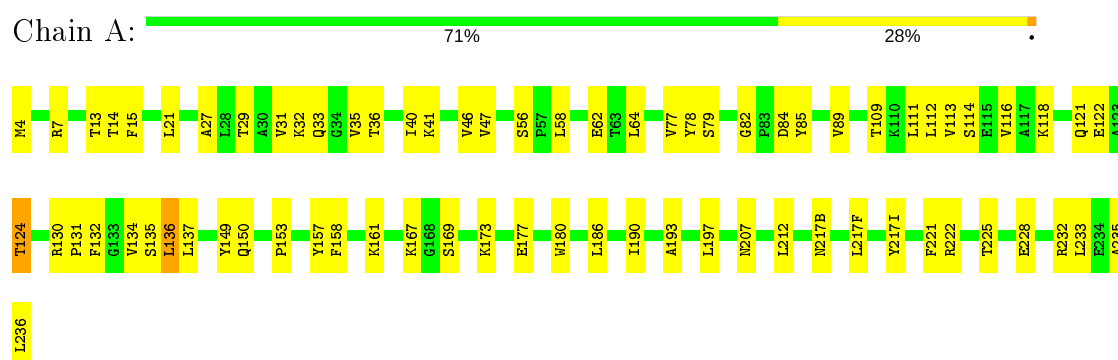
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	L	147	Total 147	O 147	0	0
17	M	130	Total 130	O 130	0	0
17	N	115	Total 115	O 115	0	0
17	O	99	Total 99	O 99	0	0
17	P	72	Total 72	O 72	0	0
17	Q	68	Total 68	O 68	0	0
17	R	87	Total 87	O 87	0	0
17	S	56	Total 56	O 56	0	0
17	T	95	Total 95	O 95	0	0
17	U	111	Total 111	O 111	0	0
17	V	124	Total 124	O 124	0	0
17	W	111	Total 111	O 111	0	0
17	X	119	Total 119	O 119	0	0
17	Y	93	Total 93	O 93	0	0
17	Z	142	Total 142	O 142	0	0
17	1	142	Total 142	O 142	0	0
17	2	124	Total 124	O 124	0	0
17	3	1	Total 1	O 1	0	0

3 Residue-property plots

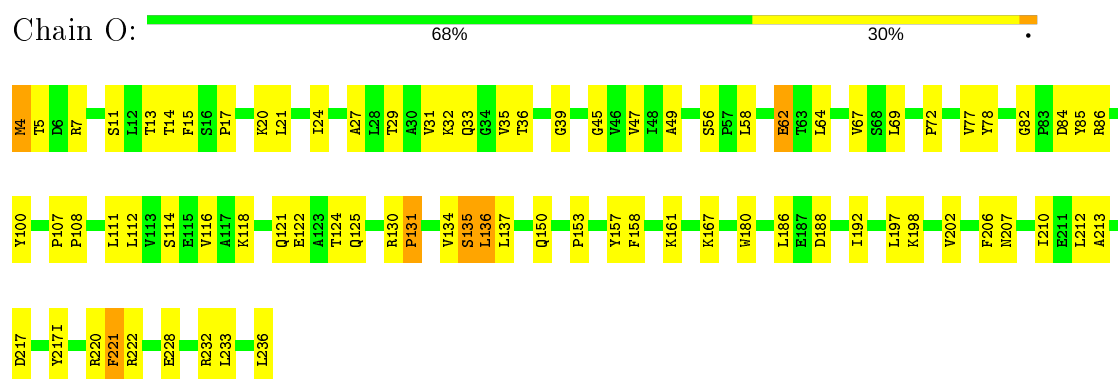
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

Note EDS was not executed.

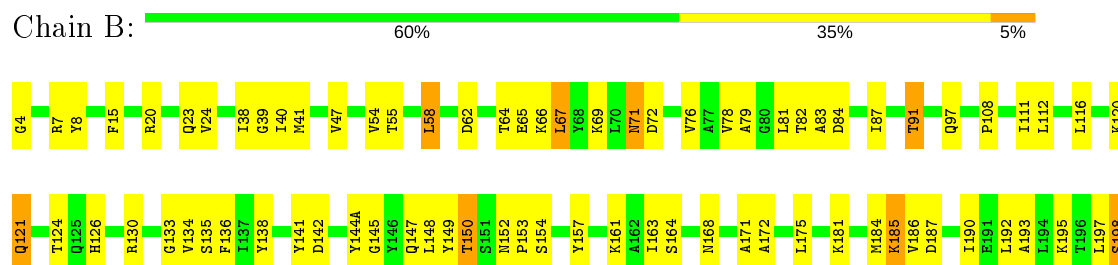
• Molecule 1: Proteasome component Y7



• Molecule 1: Proteasome component Y7



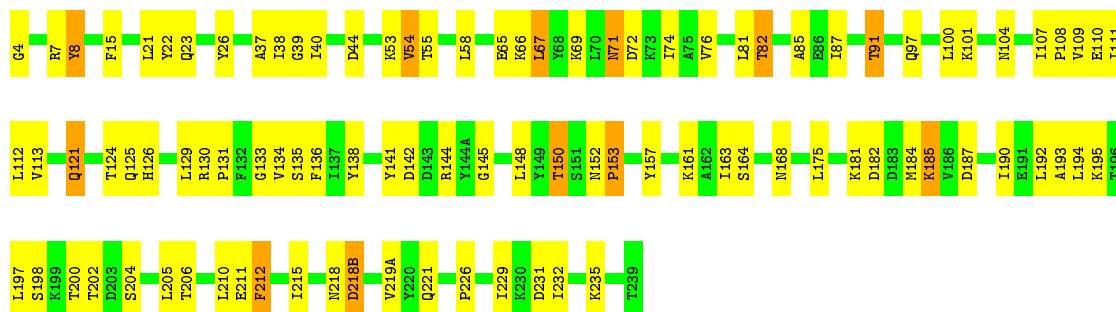
• Molecule 2: Proteasome component Y13





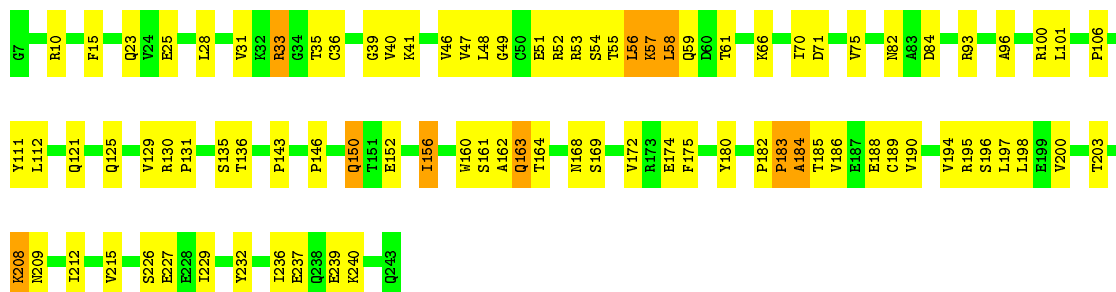
• Molecule 2: Proteasome component Y13

Chain P: 60% 35% 5%



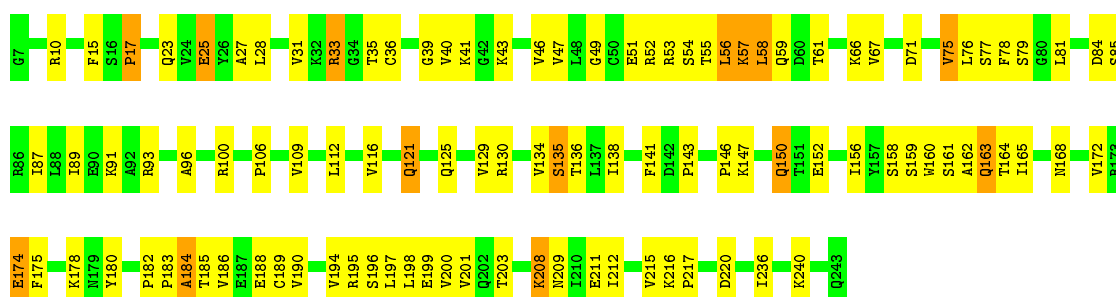
• Molecule 3: Proteasome component PRE6

Chain C: 63% 33% 4%



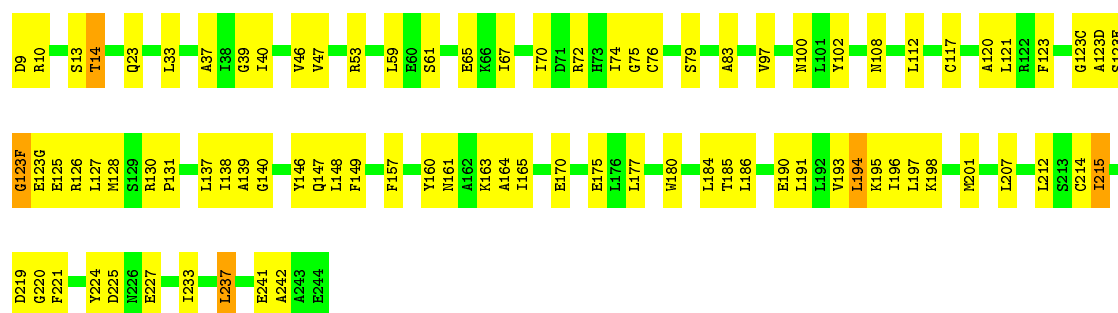
• Molecule 3: Proteasome component PRE6

Chain Q: 56% 38% 6%



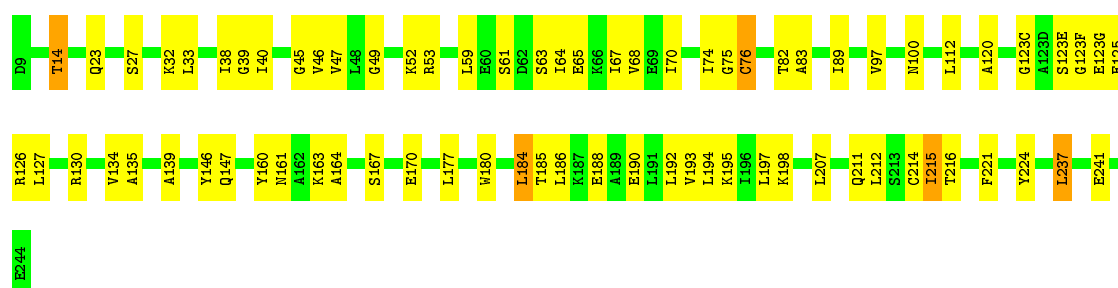
• Molecule 4: Proteasome component PUP2

Chain D: 64% 34% 2%



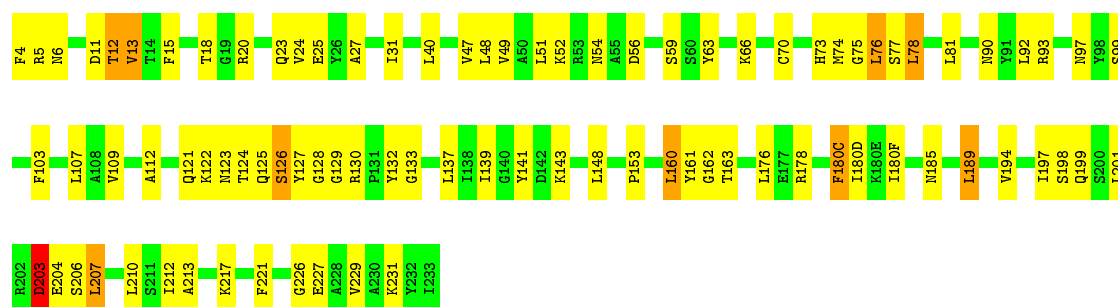
• Molecule 4: Proteasome component PUP2

Chain R: 69% 29%



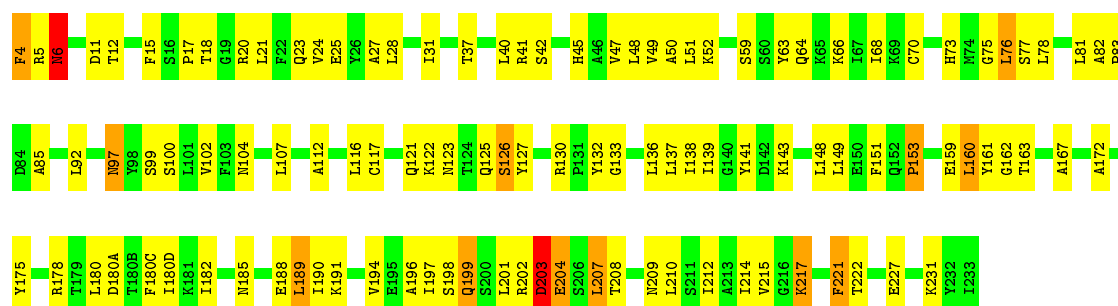
• Molecule 5: Proteasome component PRE5

Chain E: 62% 34%

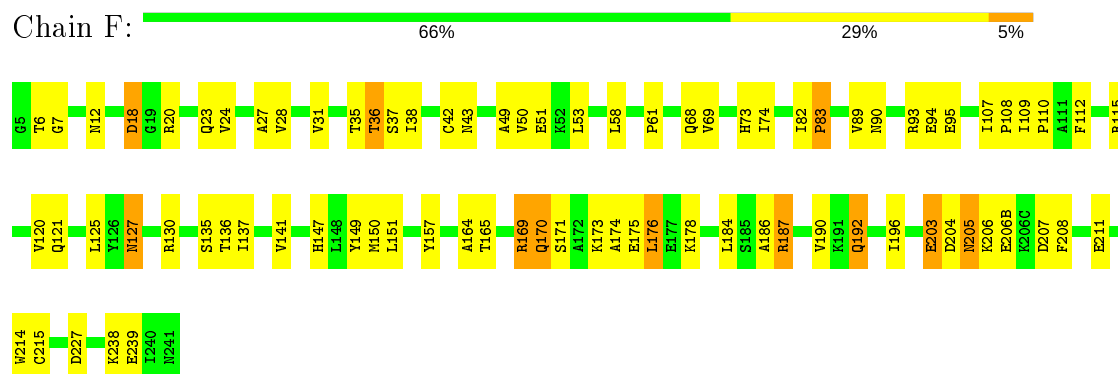


• Molecule 5: Proteasome component PRE5

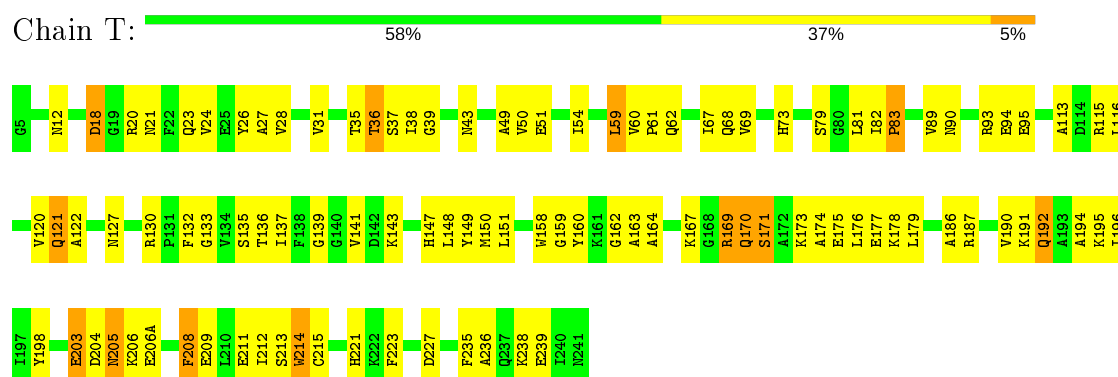
Chain S: 52% 42% 5%



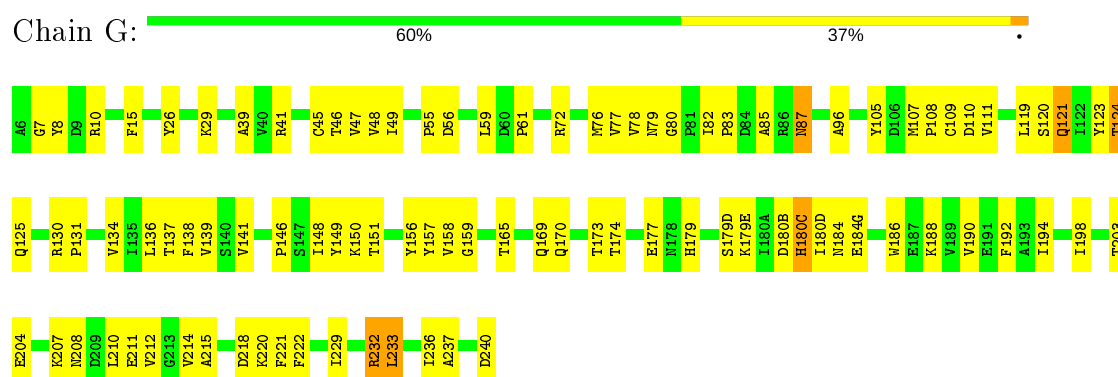
- Molecule 6: Proteasome component C1



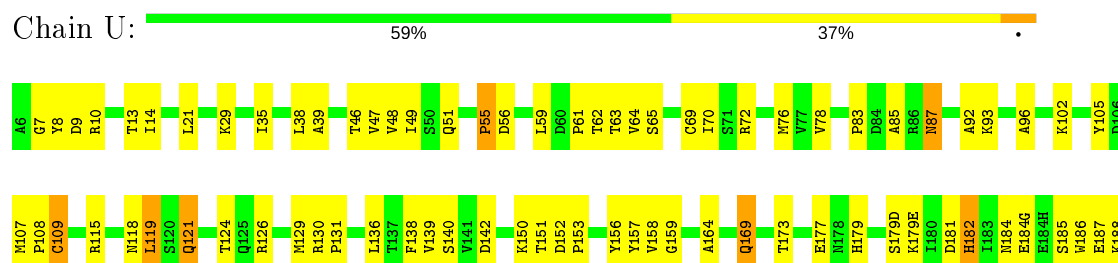
- Molecule 6: Proteasome component C1

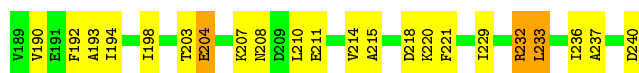


- Molecule 7: Proteasome component C7-alpha

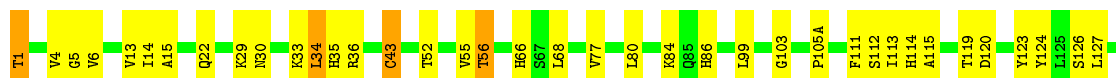


- Molecule 7: Proteasome component C7-alpha

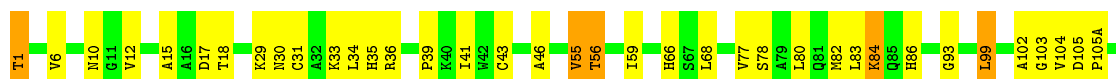




• Molecule 8: Proteasome component PUP1



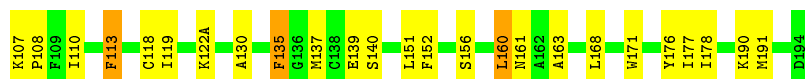
• Molecule 8: Proteasome component PUP1



• Molecule 9: Proteasome component PUP3

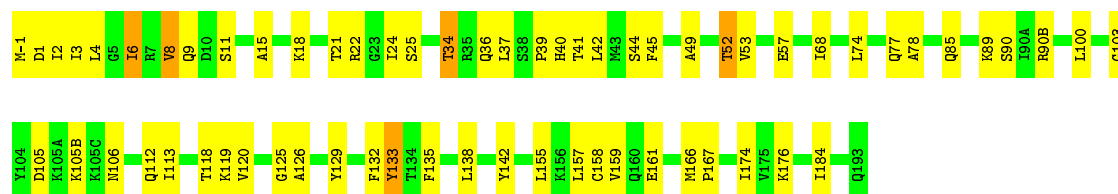


• Molecule 9: Proteasome component PUP3



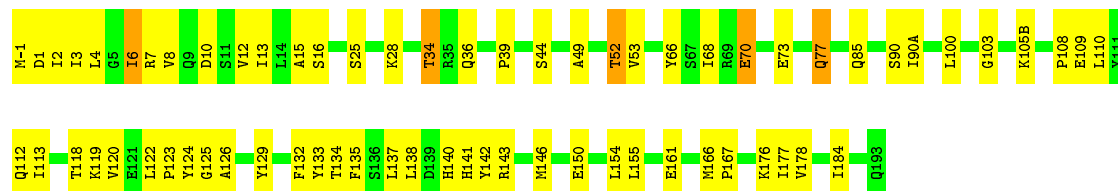
• Molecule 10: Proteasome component C11





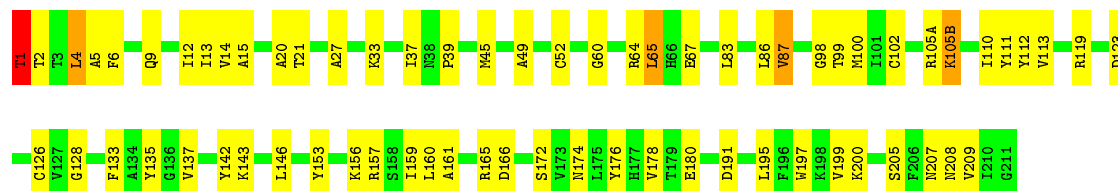
• Molecule 10: Proteasome component C11

Chain X: 66% 32%



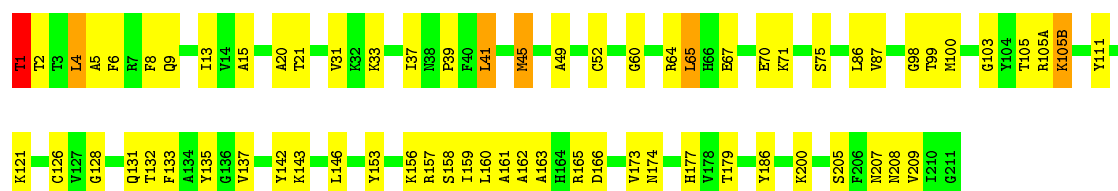
• Molecule 11: Proteasome component PRE2

Chain K: 68% 30%



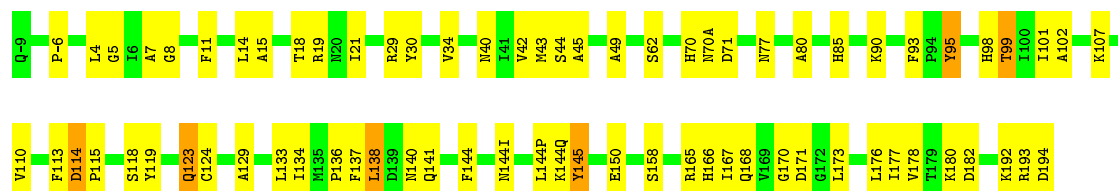
• Molecule 11: Proteasome component PRE2

Chain Y: 68% 29%




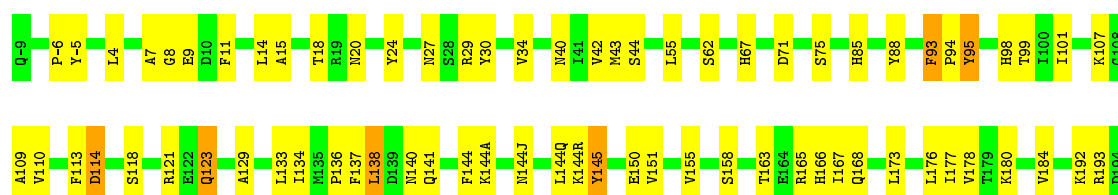
• Molecule 12: Proteasome component C5

Chain L: 67% 30%



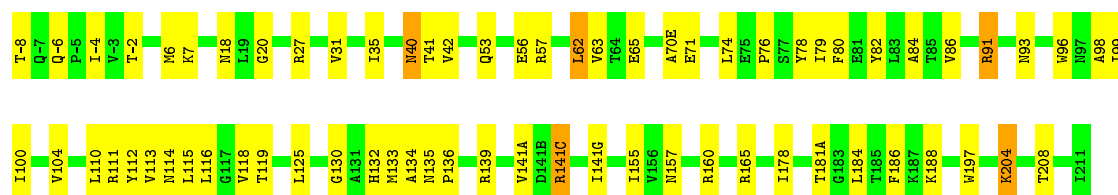
• Molecule 12: Proteasome component C5

Chain Z:  68% 30%



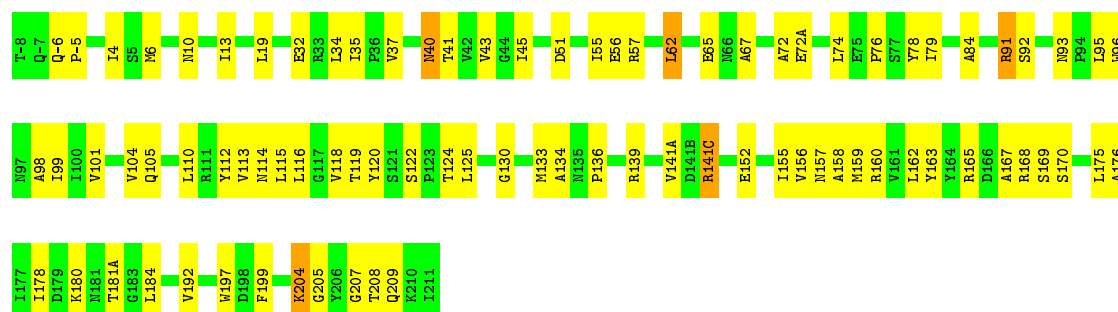
- Molecule 13: Proteasome component PRE4

Chain M:  70% 27%



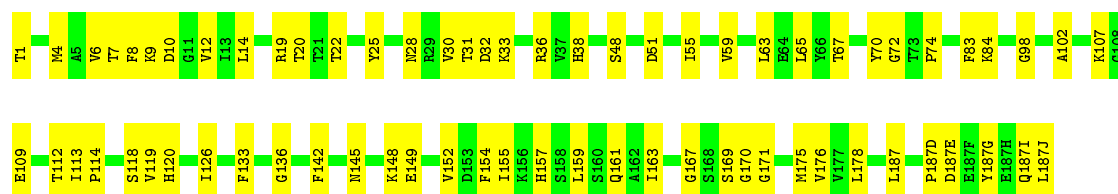
- Molecule 13: Proteasome component PRE4

Chain 1:  63% 35%



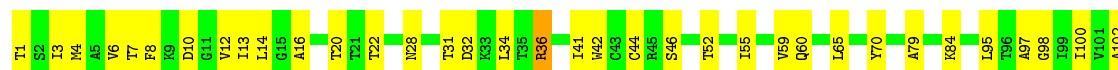
- Molecule 14: Proteasome component PRE3

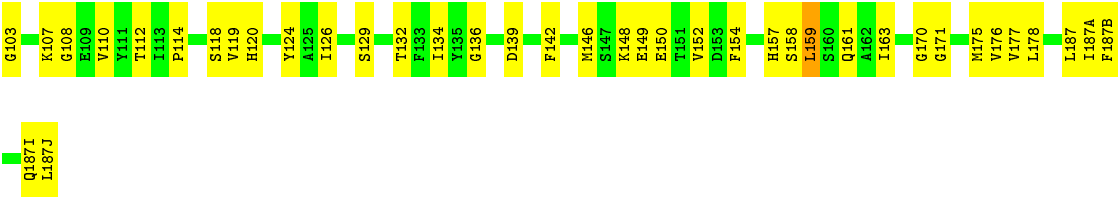
Chain N:  65% 35%



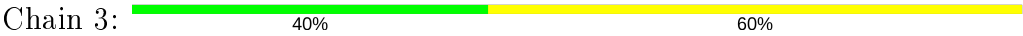
- Molecule 14: Proteasome component PRE3

Chain 2:  62% 37%





- Molecule 15: EPOXOMICIN (peptide inhibitor)



- Molecule 15: EPOXOMICIN (peptide inhibitor)



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.20Å 300.20Å 144.02Å 90.00° 112.98° 90.00°	Depositor
Resolution (Å)	20.00 – 2.25	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.25)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.283 , 0.336	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	52508	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 04D, IML, ACE

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	0.60	0/1952	0.80	0/2642
1	O	0.59	0/1952	0.79	0/2642
2	B	0.59	0/1935	0.76	0/2618
2	P	0.58	0/1935	0.77	0/2618
3	C	0.59	0/1920	0.78	1/2598 (0.0%)
3	Q	0.57	0/1920	0.78	1/2598 (0.0%)
4	D	0.59	0/1887	0.78	0/2541
4	R	0.58	0/1887	0.75	0/2541
5	E	0.53	0/1823	0.73	0/2463
5	S	0.55	0/1823	0.74	0/2463
6	F	0.54	0/1937	0.76	1/2614 (0.0%)
6	T	0.59	0/1937	0.79	1/2614 (0.0%)
7	G	0.61	0/1959	0.79	0/2652
7	U	0.65	1/1959 (0.1%)	0.80	0/2652
8	H	0.64	2/1716 (0.1%)	0.94	4/2326 (0.2%)
8	V	0.62	1/1716 (0.1%)	0.87	3/2326 (0.1%)
9	I	0.61	0/1611	0.81	0/2174
9	W	0.64	0/1611	0.83	1/2174 (0.0%)
10	J	0.62	0/1613	0.80	0/2173
10	X	0.63	0/1613	0.81	0/2173
11	K	0.64	1/1681 (0.1%)	0.83	4/2274 (0.2%)
11	Y	0.63	1/1681 (0.1%)	0.81	3/2274 (0.1%)
12	L	0.64	0/1795	0.78	2/2420 (0.1%)
12	Z	0.59	0/1795	0.78	1/2420 (0.0%)
13	1	0.64	0/1855	0.84	2/2514 (0.1%)
13	M	0.60	0/1855	0.79	2/2514 (0.1%)
14	2	0.64	0/1541	0.76	1/2087 (0.0%)
14	N	0.63	0/1541	0.80	2/2087 (0.1%)
15	3	1.51	0/14	1.53	0/18
15	4	1.25	0/14	1.38	0/18
All	All	0.61	6/50478 (0.0%)	0.80	29/68228 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	1	THR	C-N	-8.54	1.14	1.34
8	H	43	CYS	CB-SG	-5.80	1.72	1.81
11	K	1	THR	C-N	5.80	1.47	1.34
7	U	109	CYS	CB-SG	-5.53	1.72	1.81
8	V	31	CYS	CB-SG	-5.18	1.73	1.81

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	1	THR	O-C-N	-16.55	96.21	122.70
8	H	1	THR	C-N-CA	12.88	153.89	121.70
8	V	1	THR	O-C-N	-12.00	103.51	122.70
8	H	1	THR	CA-C-N	11.83	143.22	117.20
8	V	1	THR	C-N-CA	9.97	146.62	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	144(A)	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1926	55	0
1	O	1915	0	1926	61	0
2	B	1905	0	1901	76	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	1905	0	1901	85	0
3	C	1891	0	1900	74	0
3	Q	1891	0	1900	102	0
4	D	1862	0	1836	70	0
4	R	1862	0	1836	61	0
5	E	1795	0	1797	70	0
5	S	1795	0	1797	92	0
6	F	1897	0	1886	57	0
6	T	1897	0	1886	79	0
7	G	1921	0	1910	79	0
7	U	1921	0	1910	79	0
8	H	1685	0	1687	46	0
8	V	1685	0	1687	63	0
9	I	1581	0	1573	38	0
9	W	1581	0	1574	50	0
10	J	1585	0	1590	52	0
10	X	1585	0	1590	55	0
11	K	1644	0	1592	59	0
11	Y	1644	0	1593	60	0
12	L	1757	0	1711	70	0
12	Z	1757	0	1711	62	0
13	1	1824	0	1832	65	0
13	M	1824	0	1832	48	0
14	2	1512	0	1481	59	0
14	N	1512	0	1481	50	0
15	3	39	0	51	4	0
15	4	39	0	51	3	0
16	D	1	0	0	0	0
16	F	2	0	0	0	0
16	G	1	0	0	0	0
16	H	1	0	0	0	0
16	I	2	0	0	0	0
16	K	1	0	0	0	0
16	L	1	0	0	0	0
16	N	1	0	0	0	0
17	1	142	0	0	1	0
17	2	124	0	0	0	0
17	3	1	0	0	0	0
17	A	100	0	0	2	0
17	B	72	0	0	1	0
17	C	71	0	0	0	0
17	D	86	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	E	57	0	0	1	0
17	F	98	0	0	2	0
17	G	106	0	0	4	0
17	H	129	0	0	2	0
17	I	109	0	0	1	0
17	J	114	0	0	3	0
17	K	94	0	0	5	0
17	L	147	0	0	4	0
17	M	130	0	0	0	0
17	N	115	0	0	1	0
17	O	99	0	0	1	0
17	P	72	0	0	2	0
17	Q	68	0	0	0	0
17	R	87	0	0	3	0
17	S	56	0	0	3	0
17	T	95	0	0	5	0
17	U	111	0	0	6	0
17	V	124	0	0	8	0
17	W	111	0	0	3	0
17	X	119	0	0	5	0
17	Y	93	0	0	9	0
17	Z	142	0	0	6	0
All	All	52508	0	49348	1644	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 17.

The worst 5 of 1644 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)
14:N:136:GLY:HA2	14:2:161:GLN:HE21	1.09	1.09
14:N:161:GLN:HE21	14:2:136:GLY:HA2	1.13	1.05
11:K:4:LEU:HD12	11:K:159:ILE:HD11	1.44	1.00
7:G:96:ALA:HA	7:G:107:MET:HE2	1.40	0.99
12:L:18:THR:CG2	12:L:30:TYR:HA	1.95	0.97

There are no symmetry-related clashes.

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	A	248/250 (99%)	220 (89%)	26 (10%)	2 (1%)	19	17
1	O	248/250 (99%)	218 (88%)	28 (11%)	2 (1%)	19	17
2	B	242/244 (99%)	217 (90%)	21 (9%)	4 (2%)	9	4
2	P	242/244 (99%)	223 (92%)	15 (6%)	4 (2%)	9	4
3	C	239/241 (99%)	218 (91%)	16 (7%)	5 (2%)	7	3
3	Q	239/241 (99%)	214 (90%)	18 (8%)	7 (3%)	4	2
4	D	240/242 (99%)	215 (90%)	19 (8%)	6 (2%)	5	3
4	R	240/242 (99%)	213 (89%)	22 (9%)	5 (2%)	7	3
5	E	231/233 (99%)	207 (90%)	19 (8%)	5 (2%)	6	3
5	S	231/233 (99%)	207 (90%)	15 (6%)	9 (4%)	3	1
6	F	242/244 (99%)	220 (91%)	21 (9%)	1 (0%)	34	37
6	T	242/244 (99%)	220 (91%)	20 (8%)	2 (1%)	19	17
7	G	241/243 (99%)	224 (93%)	15 (6%)	2 (1%)	19	17
7	U	241/243 (99%)	222 (92%)	15 (6%)	4 (2%)	9	4
8	H	220/222 (99%)	204 (93%)	15 (7%)	1 (0%)	29	29
8	V	220/222 (99%)	205 (93%)	14 (6%)	1 (0%)	29	29
9	I	202/204 (99%)	189 (94%)	13 (6%)	0	100	100
9	W	202/204 (99%)	192 (95%)	9 (4%)	1 (0%)	29	29
10	J	196/198 (99%)	184 (94%)	9 (5%)	3 (2%)	10	6
10	X	196/198 (99%)	185 (94%)	9 (5%)	2 (1%)	15	13
11	K	210/212 (99%)	199 (95%)	10 (5%)	1 (0%)	29	29
11	Y	210/212 (99%)	201 (96%)	8 (4%)	1 (0%)	29	29
12	L	220/222 (99%)	205 (93%)	13 (6%)	2 (1%)	17	14
12	Z	220/222 (99%)	206 (94%)	13 (6%)	1 (0%)	29	29
13	1	231/233 (99%)	214 (93%)	14 (6%)	3 (1%)	12	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	M	231/233 (99%)	213 (92%)	13 (6%)	5 (2%)	6	3
14	2	194/196 (99%)	183 (94%)	11 (6%)	0	100	100
14	N	194/196 (99%)	184 (95%)	10 (5%)	0	100	100
15	3	1/5 (20%)	1 (100%)	0	0	100	100
15	4	1/5 (20%)	1 (100%)	0	0	100	100
All	All	6314/6378 (99%)	5804 (92%)	431 (7%)	79 (1%)	12	8

5 of 79 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	LYS
2	B	218(C)	ASP
3	C	58	LEU
3	C	184	ALA
4	D	123(E)	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	197 (94%)	12 (6%)	20	20
1	O	209/209 (100%)	198 (95%)	11 (5%)	22	23
2	B	203/203 (100%)	189 (93%)	14 (7%)	15	14
2	P	203/203 (100%)	187 (92%)	16 (8%)	12	10
3	C	213/213 (100%)	193 (91%)	20 (9%)	8	6
3	Q	213/213 (100%)	198 (93%)	15 (7%)	15	13
4	D	198/198 (100%)	181 (91%)	17 (9%)	10	9
4	R	198/198 (100%)	187 (94%)	11 (6%)	21	21
5	E	192/192 (100%)	171 (89%)	21 (11%)	6	4
5	S	192/192 (100%)	170 (88%)	22 (12%)	5	3
6	F	201/201 (100%)	181 (90%)	20 (10%)	7	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	T	201/201 (100%)	180 (90%)	21 (10%)	7	5
7	G	207/207 (100%)	196 (95%)	11 (5%)	22	23
7	U	207/207 (100%)	196 (95%)	11 (5%)	22	23
8	H	181/181 (100%)	168 (93%)	13 (7%)	14	12
8	V	181/181 (100%)	167 (92%)	14 (8%)	13	11
9	I	172/172 (100%)	164 (95%)	8 (5%)	26	29
9	W	172/172 (100%)	166 (96%)	6 (4%)	36	43
10	J	175/175 (100%)	167 (95%)	8 (5%)	27	30
10	X	175/175 (100%)	167 (95%)	8 (5%)	27	30
11	K	169/169 (100%)	161 (95%)	8 (5%)	26	29
11	Y	169/169 (100%)	160 (95%)	9 (5%)	22	23
12	L	185/185 (100%)	173 (94%)	12 (6%)	17	16
12	Z	185/185 (100%)	172 (93%)	13 (7%)	15	13
13	1	199/199 (100%)	189 (95%)	10 (5%)	24	26
13	M	199/199 (100%)	188 (94%)	11 (6%)	21	21
14	2	162/162 (100%)	155 (96%)	7 (4%)	29	33
14	N	162/162 (100%)	155 (96%)	7 (4%)	29	33
15	3	2/2 (100%)	2 (100%)	0	100	100
15	4	2/2 (100%)	2 (100%)	0	100	100
All	All	5336/5336 (100%)	4980 (93%)	356 (7%)	16	15

5 of 356 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	L	144(P)	LEU
2	P	91	THR
12	Z	93	PHE
13	M	40	ASN
14	N	187(E)	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 175 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	93	ASN

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Mol	Chain	Res	Type
3	Q	82	ASN
12	Z	144(J)	ASN
13	M	157	ASN
2	P	23	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	$\# Z > 2$
15	IML	4	2	15	7,8,9	2.22	1 (14%)	8,9,11	1.46	2 (25%)
15	IML	3	2	15	7,8,9	2.36	2 (28%)	8,9,11	1.46	2 (25%)

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
15	IML	4	2	15	-	0/10/10/12	-
15	IML	3	2	15	-	0/10/10/12	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	4	2	IML	OXT-C	-5.18	1.20	1.42
15	3	2	IML	OXT-C	-4.96	1.21	1.42
15	3	2	IML	CB-CA	2.31	1.59	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	4	2	IML	OXT-C-CA	3.13	118.69	111.09
15	3	2	IML	C-CA-CB	2.74	122.88	114.25
15	3	2	IML	OXT-C-CA	2.65	117.53	111.09
15	4	2	IML	C-CA-CB	2.31	121.52	114.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	1:THR	C	2:THR	N	1.14

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.