



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 10:17 pm BST

PDB ID : 5FGI
Title : Yeast 20S proteasome beta1-T1A beta2-T1A double mutant in complex with Carfilzomib
Authors : Huber, E.M.; Groll, M.
Deposited on : 2015-12-20
Resolution : 2.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
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) : 2.11

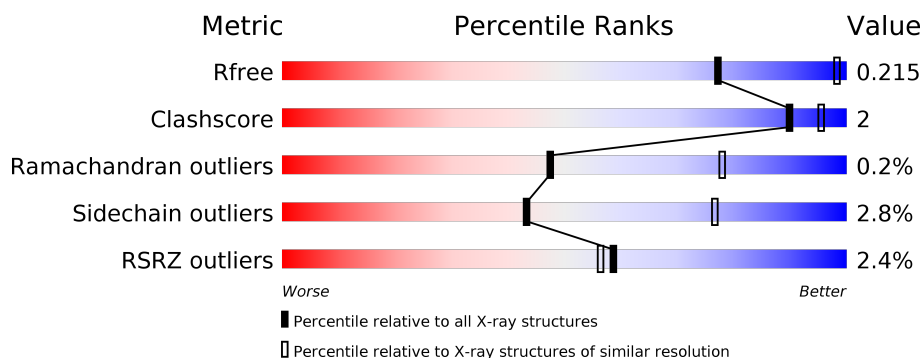
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	250	<div> <div>2%</div> <div> <div></div> <div>98%</div> <div></div> </div> <div></div> </div>
1	O	250	<div> <div>3%</div> <div> <div></div> <div>97%</div> <div></div> </div> <div></div> </div>
2	B	258	<div> <div>4%</div> <div> <div></div> <div>90%</div> <div>5%</div> <div>5%</div> </div> <div></div> </div>
2	P	258	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div></div> <div>5%</div> </div> <div></div> </div>
3	C	254	<div> <div>6%</div> <div> <div></div> <div>90%</div> <div></div> <div>6%</div> </div> <div></div> </div>
3	Q	254	<div> <div>7%</div> <div> <div></div> <div>91%</div> <div></div> <div>6%</div> </div> <div></div> </div>

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Mol	Chain	Length	Quality of chain
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	244	
8	V	244	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	213	
14	b	213	

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 50047 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	249	Total	C	N	O	S	0	0	0
			1907	1214	314	376	3			
1	O	249	Total	C	N	O	S	0	0	0
			1907	1214	314	376	3			

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	234	Total	C	N	O	S	0	0	0
			1767	1109	310	341	7			
8	V	234	Total	C	N	O	S	0	0	0
			1767	1109	310	341	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	1	ALA	THR	engineered mutation	UNP P25043
V	1	ALA	THR	engineered mutation	UNP P25043

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

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

- Molecule 10 is a protein called Proteasome subunit beta type-4.

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

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

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 subunit beta type-6.

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 subunit beta type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	232	Total	C	N	O	S	0	0	0
			1817	1150	311	349	7			
13	a	232	Total	C	N	O	S	0	0	0
			1817	1150	311	349	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	213	Total	C	N	O	S	0	0	0
			1637	1033	274	323	7			
14	b	213	Total	C	N	O	S	0	0	0
			1637	1033	274	323	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	1	ALA	THR	engineered mutation	UNP P38624

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Chain	Residue	Modelled	Actual	Comment	Reference
b	1	ALA	THR	engineered mutation	UNP P38624

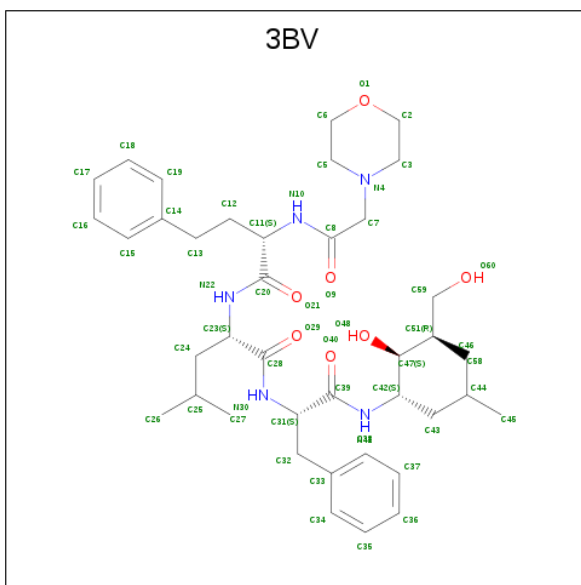
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	G	1	Total Mg 1 1	0	0
15	Z	1	Total Mg 1 1	0	0
15	I	2	Total Mg 2 2	0	0
15	K	1	Total Mg 1 1	0	0
15	N	1	Total Mg 1 1	0	0

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

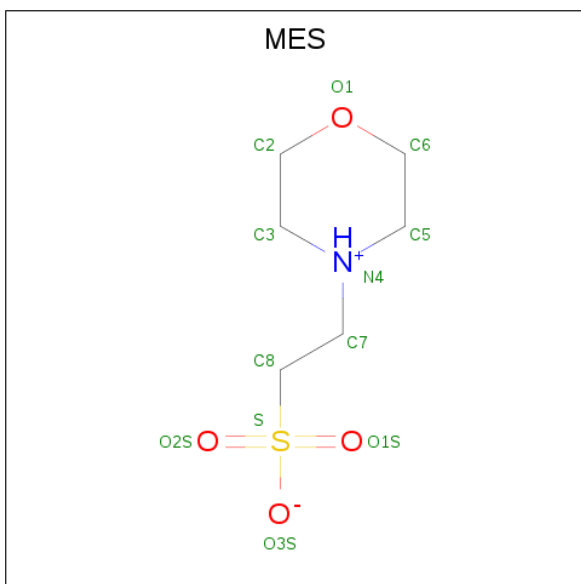
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total Cl 1 1	0	0
16	b	1	Total Cl 1 1	0	0
16	N	1	Total Cl 1 1	0	0
16	U	1	Total Cl 1 1	0	0

- Molecule 17 is N-[(2S)-2-[(morpholin-4-ylacetyl)amino]-4-phenylbutanoyl]-L-leucyl-N-[(2R,3S,4S)-1,3-dihydroxy-2,6-dimethylheptan-4-yl]-L-phenylalaninamide (three-letter code: 3BV) (formula: C₄₀H₆₁N₅O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	K	1	Total	C	N	O	0	0
			52	40	5	7		
17	Y	1	Total	C	N	O	0	0
			52	40	5	7		

- Molecule 18 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	K	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	Y	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 19 is water.

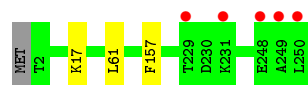
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	9	Total	O	0	0
			9	9		
19	B	19	Total	O	0	0
			19	19		
19	C	5	Total	O	0	0
			5	5		
19	D	3	Total	O	0	0
			3	3		
19	E	4	Total	O	0	0
			4	4		
19	F	10	Total	O	0	0
			10	10		
19	G	7	Total	O	0	0
			7	7		
19	H	12	Total	O	0	0
			12	12		
19	I	6	Total	O	0	0
			6	6		
19	J	9	Total	O	0	0
			9	9		
19	K	9	Total	O	0	0
			9	9		
19	L	8	Total	O	0	0
			8	8		
19	M	12	Total	O	0	0
			12	12		
19	N	6	Total	O	0	0
			6	6		
19	O	4	Total	O	0	0
			4	4		
19	P	4	Total	O	0	0
			4	4		
19	Q	5	Total	O	0	0
			5	5		
19	R	3	Total	O	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	S	4	Total 4	O 4	0	0
19	T	11	Total 11	O 11	0	0
19	U	9	Total 9	O 9	0	0
19	V	8	Total 8	O 8	0	0
19	W	8	Total 8	O 8	0	0
19	X	11	Total 11	O 11	0	0
19	Y	9	Total 9	O 9	0	0
19	Z	11	Total 11	O 11	0	0
19	a	10	Total 10	O 10	0	0
19	b	11	Total 11	O 11	0	0

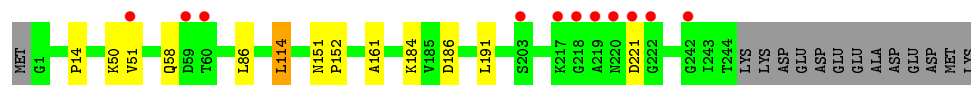
- Molecule 1: Proteasome subunit alpha type-2



- Molecule 1: Proteasome subunit alpha type-2



- Molecule 2: Proteasome subunit alpha type-3



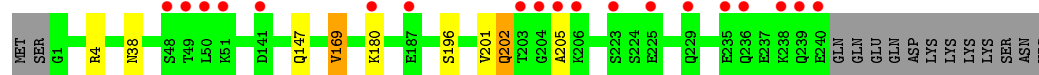
- Molecule 2: Proteasome subunit alpha type-3

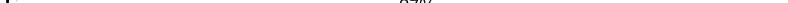


- Molecule 3: Proteasome subunit alpha type-4

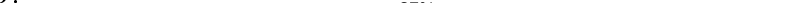


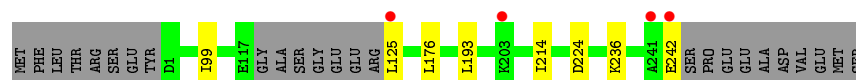
- Molecule 3: Proteasome subunit alpha type-4



- Chain D:  87% 10%



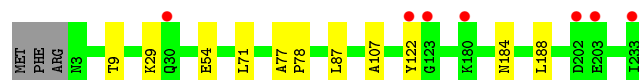
- Chain R:  2% 87% 10%




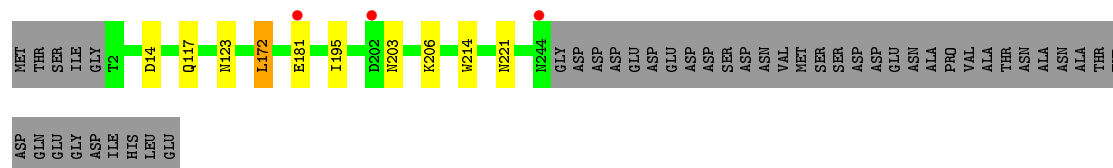
- Chain E:  2% 94%




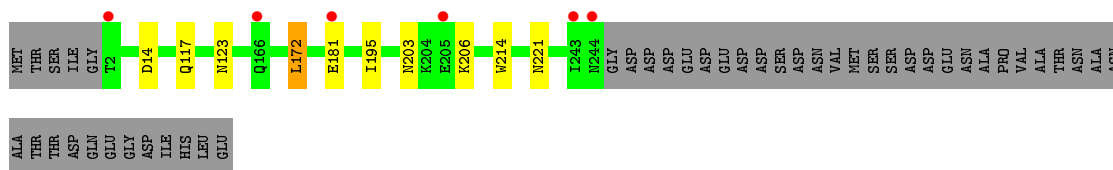
- Chain S: 



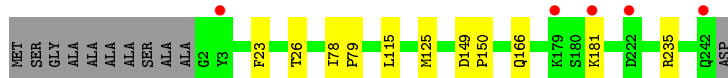
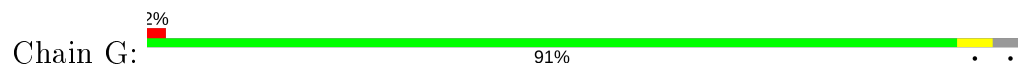
- Chain F:  81% 16% 3%



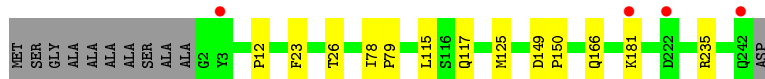
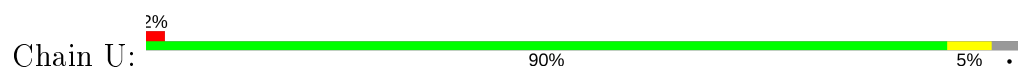
- Chain T: 



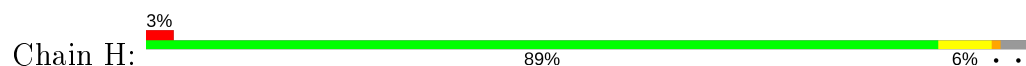
- Molecule 7: Proteasome subunit alpha type-1



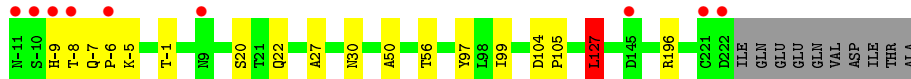
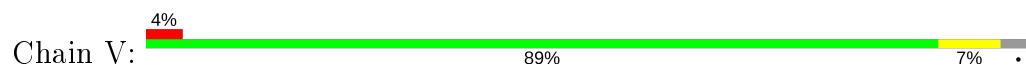
- Molecule 7: Proteasome subunit alpha type-1



- Molecule 8: Proteasome subunit beta type-2



- Molecule 8: Proteasome subunit beta type-2



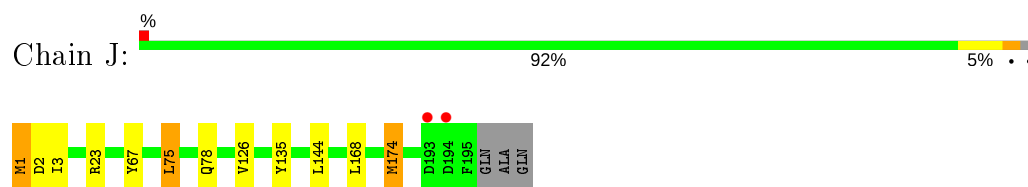
- Molecule 9: Proteasome subunit beta type-3



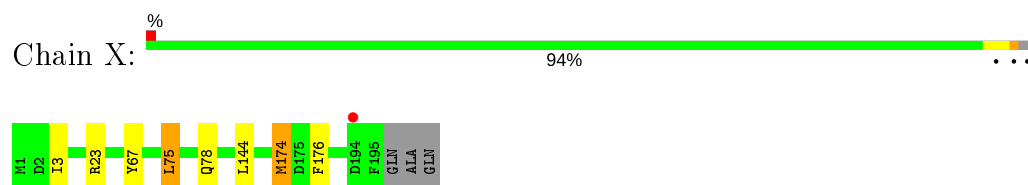
- Molecule 9: Proteasome subunit beta type-3



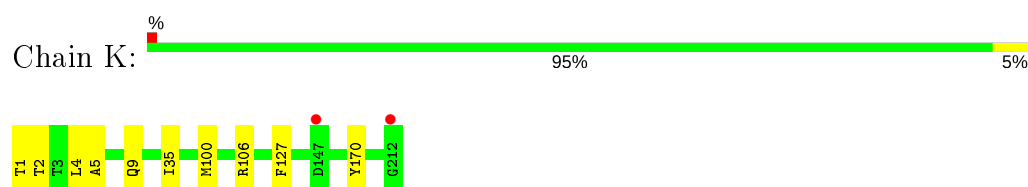
• Molecule 10: Proteasome subunit beta type-4



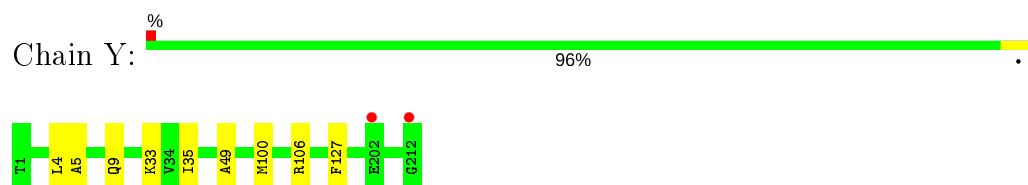
• Molecule 10: Proteasome subunit beta type-4



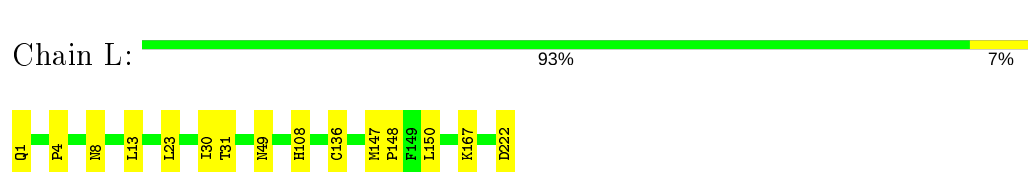
• Molecule 11: Proteasome subunit beta type-5



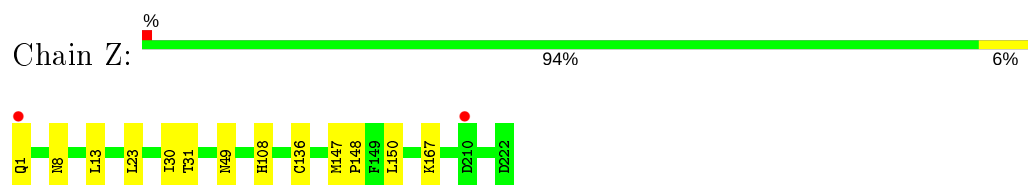
• Molecule 11: Proteasome subunit beta type-5



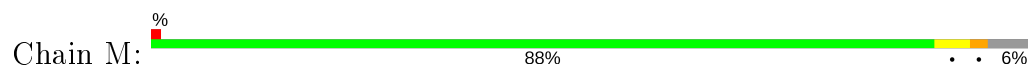
• Molecule 12: Proteasome subunit beta type-6



• Molecule 12: Proteasome subunit beta type-6

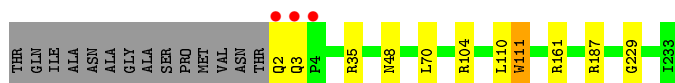
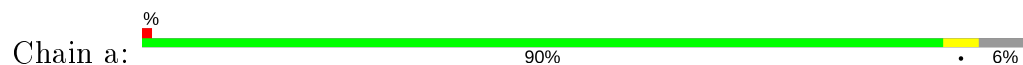


• Molecule 13: Proteasome subunit beta type-7

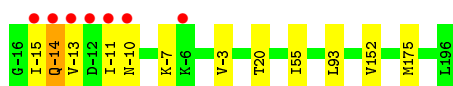




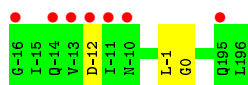
- Molecule 13: Proteasome subunit beta type-7



- Molecule 14: Proteasome subunit beta type-1



- Molecule 14: Proteasome subunit beta type-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.81Å 301.16Å 145.90Å 90.00° 113.30° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 15.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.2 (15.00-2.90) 97.2 (15.00-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.186 , 0.210 0.192 , 0.215	Depositor DCC
R_{free} test set	11524 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	61.4	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	50047	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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: MG, 3BV, MES, CL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.27	0/1944	0.46	0/2632
1	O	0.28	0/1944	0.46	0/2632
2	B	0.27	0/1934	0.47	0/2618
2	P	0.27	0/1934	0.47	0/2618
3	C	0.27	0/1910	0.50	0/2586
3	Q	0.27	0/1910	0.50	0/2586
4	D	0.27	0/1837	0.46	0/2475
4	R	0.26	0/1837	0.46	0/2475
5	E	0.27	0/1800	0.46	0/2433
5	S	0.27	0/1800	0.46	0/2433
6	F	0.28	0/1932	0.44	0/2609
6	T	0.28	0/1932	0.44	0/2609
7	G	0.27	0/1945	0.46	0/2634
7	U	0.27	0/1945	0.46	0/2634
8	H	0.39	0/1800	0.55	2/2442 (0.1%)
8	V	0.35	1/1800 (0.1%)	0.55	2/2442 (0.1%)
9	I	0.27	0/1611	0.47	0/2174
9	W	0.27	0/1611	0.47	0/2174
10	J	0.28	0/1589	0.48	0/2142
10	X	0.26	0/1589	0.48	0/2142
11	K	0.28	0/1681	0.48	0/2274
11	Y	0.28	0/1681	0.48	0/2274
12	L	0.28	0/1795	0.46	0/2420
12	Z	0.27	0/1795	0.46	0/2420
13	M	0.64	2/1848 (0.1%)	0.68	3/2504 (0.1%)
13	a	0.69	2/1848 (0.1%)	0.61	4/2504 (0.2%)
14	N	0.34	0/1666	0.48	0/2253
14	b	0.32	0/1666	0.48	0/2253
All	All	0.33	5/50584 (0.0%)	0.49	11/68392 (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
13	M	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	111	TRP	C-N	-26.17	0.73	1.34
13	M	111	TRP	C-N	-22.39	0.82	1.34
13	M	110	LEU	C-N	-7.91	1.15	1.34
13	a	110	LEU	C-N	-6.62	1.18	1.34
8	V	-6	PRO	N-CD	5.26	1.55	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	110	LEU	O-C-N	-16.09	96.95	122.70
13	a	110	LEU	O-C-N	-11.32	104.59	122.70
13	M	110	LEU	C-N-CA	11.22	149.74	121.70
13	M	110	LEU	CA-C-N	10.65	140.62	117.20
8	V	127	LEU	CD1-CG-CD2	-7.84	86.98	110.50
13	a	110	LEU	CA-C-N	7.59	133.91	117.20
13	a	110	LEU	C-N-CA	6.96	139.09	121.70
8	H	-7	GLN	C-N-CD	6.20	141.42	128.40
8	H	127	LEU	CA-CB-CG	6.06	129.24	115.30
8	V	-7	GLN	C-N-CD	5.46	139.86	128.40
13	a	111	TRP	O-C-N	-5.42	114.02	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	M	110	LEU	Mainchain

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	1907	0	1917	0	0
1	O	1907	0	1917	15	0
2	B	1904	0	1904	4	0
2	P	1904	0	1904	3	0
3	C	1881	0	1895	5	0
3	Q	1881	0	1895	3	0
4	D	1813	0	1797	0	0
4	R	1813	0	1797	0	0
5	E	1773	0	1775	2	0
5	S	1773	0	1775	12	0
6	F	1892	0	1883	1	0
6	T	1892	0	1883	1	0
7	G	1907	0	1901	3	0
7	U	1907	0	1901	4	0
8	H	1767	0	1766	17	0
8	V	1767	0	1766	10	0
9	I	1581	0	1574	7	0
9	W	1581	0	1574	4	0
10	J	1561	0	1569	9	0
10	X	1561	0	1569	3	0
11	K	1644	0	1593	7	0
11	Y	1644	0	1593	7	0
12	L	1757	0	1711	14	0
12	Z	1757	0	1711	7	0
13	M	1817	0	1820	14	0
13	a	1817	0	1820	0	0
14	N	1637	0	1618	8	0
14	b	1637	0	1618	0	0
15	G	1	0	0	0	0
15	I	2	0	0	0	0
15	K	1	0	0	0	0
15	N	1	0	0	0	0
15	Z	1	0	0	0	0
16	G	1	0	0	0	0
16	N	1	0	0	0	0
16	U	1	0	0	0	0
16	b	1	0	0	0	0
17	K	52	0	58	12	0
17	Y	52	0	58	9	0
18	K	12	0	13	1	0
18	Y	12	0	13	0	0
19	A	9	0	0	0	0
19	B	19	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	C	5	0	0	0	0
19	D	3	0	0	0	0
19	E	4	0	0	0	0
19	F	10	0	0	0	0
19	G	7	0	0	0	0
19	H	12	0	0	0	0
19	I	6	0	0	0	0
19	J	9	0	0	0	0
19	K	9	0	0	0	0
19	L	8	0	0	1	0
19	M	12	0	0	0	0
19	N	6	0	0	0	0
19	O	4	0	0	3	0
19	P	4	0	0	0	0
19	Q	5	0	0	0	0
19	R	3	0	0	0	0
19	S	4	0	0	0	0
19	T	11	0	0	0	0
19	U	9	0	0	0	0
19	V	8	0	0	0	0
19	W	8	0	0	0	0
19	X	11	0	0	0	0
19	Y	9	0	0	0	0
19	Z	11	0	0	0	0
19	a	10	0	0	0	0
19	b	11	0	0	0	0
All	All	50047	0	49588	141	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.

All (141) 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)
17:K:301:3BV:H19	12:L:108:HIS:CE1	1.44	1.53
13:M:111:TRP:C	13:M:112:ASN:CA	2.00	1.30
13:M:111:TRP:CA	13:M:112:ASN:N	2.01	1.22
13:M:111:TRP:O	13:M:112:ASN:N	1.76	1.17
17:K:301:3BV:C2	12:L:108:HIS:CE1	2.27	1.17
17:K:301:3BV:C2	12:L:108:HIS:HE1	1.58	1.16
1:O:4:ARG:NH1	5:S:122:TYR:HB3	1.65	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Y:301:3BV:H19	12:Z:108:HIS:HE1	1.15	1.09
1:O:4:ARG:NH1	5:S:122:TYR:CD2	2.21	1.06
1:O:4:ARG:NH1	5:S:122:TYR:HD2	1.53	1.06
17:Y:301:3BV:H19	12:Z:108:HIS:CE1	2.00	0.96
1:O:4:ARG:HH12	5:S:122:TYR:HB3	1.33	0.94
1:O:4:ARG:NH1	5:S:122:TYR:CB	2.32	0.92
1:O:4:ARG:HH12	5:S:122:TYR:CB	1.85	0.90
17:K:301:3BV:C3	12:L:108:HIS:NE2	2.35	0.89
13:M:111:TRP:C	13:M:112:ASN:N	0.82	0.87
8:H:91:GLN:OE1	14:N:-7:LYS:NZ	2.09	0.85
8:H:-6:PRO:HD2	8:H:-5:LYS:HD2	1.57	0.85
13:M:111:TRP:O	13:M:112:ASN:CA	2.17	0.83
8:H:-7:GLN:NE2	9:I:101:PRO:HG3	1.93	0.82
13:M:111:TRP:O	13:M:112:ASN:HA	1.80	0.81
8:H:3:ILE:CG2	8:H:44:ALA:HB1	2.12	0.80
17:K:301:3BV:H19	12:L:108:HIS:HE1	0.69	0.80
8:V:-5:LYS:NZ	9:W:2:ASP:OD1	2.17	0.77
17:K:301:3BV:C3	12:L:108:HIS:CE1	2.68	0.77
17:K:301:3BV:H16	12:L:108:HIS:NE2	1.99	0.77
13:M:35:ARG:HD2	13:M:36:PHE:CE2	2.20	0.76
1:O:4:ARG:NH1	5:S:122:TYR:CG	2.57	0.72
8:V:97:TYR:HB3	8:V:127:LEU:CD2	2.19	0.72
12:L:222:ASP:OXT	19:L:301:HOH:O	2.08	0.71
8:V:97:TYR:HB3	8:V:127:LEU:HD23	1.76	0.67
8:H:3:ILE:HG23	8:H:44:ALA:HB1	1.74	0.67
8:H:3:ILE:CG2	8:H:44:ALA:CB	2.71	0.67
8:H:3:ILE:HG21	8:H:44:ALA:HB1	1.76	0.67
17:Y:301:3BV:O9	17:Y:301:3BV:H16	1.93	0.67
8:V:99:ILE:HG13	8:V:127:LEU:CD1	2.25	0.67
8:H:3:ILE:HG21	8:H:44:ALA:CB	2.25	0.66
13:M:35:ARG:CD	13:M:36:PHE:CZ	2.79	0.65
8:V:99:ILE:HG13	8:V:127:LEU:HD12	1.78	0.65
13:M:35:ARG:HD2	13:M:36:PHE:CZ	2.34	0.63
17:K:301:3BV:O48	17:K:301:3BV:O60	2.17	0.62
1:O:2:THR:N	19:O:301:HOH:O	2.33	0.61
14:N:-13:VAL:O	14:N:-13:VAL:HG12	2.01	0.60
8:H:-7:GLN:NE2	9:I:101:PRO:CG	2.63	0.60
17:K:301:3BV:O9	17:K:301:3BV:H16	2.03	0.59
14:N:-15:ILE:O	14:N:-15:ILE:HG22	2.02	0.59
13:M:35:ARG:HD3	13:M:36:PHE:CZ	2.38	0.58
1:O:2:THR:HA	19:O:301:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.87	0.57
8:H:97:TYR:HB3	8:H:127:LEU:HD11	1.85	0.57
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.86	0.56
8:V:-1:THR:OG1	8:V:20:SER:HA	2.06	0.55
8:V:22:GLN:HG3	8:V:27:ALA:HB2	1.88	0.55
14:N:-14:GLN:O	14:N:-10:ASN:N	2.40	0.54
17:Y:301:3BV:C2	12:Z:108:HIS:CE1	2.82	0.54
10:J:1:MET:HE2	10:J:1:MET:N	2.23	0.54
8:H:-7:GLN:HE21	9:I:101:PRO:HG3	1.71	0.54
1:O:4:ARG:HH11	5:S:122:TYR:HD2	0.72	0.54
11:K:1:THR:HG22	11:K:2:THR:N	2.24	0.53
1:O:4:ARG:HH12	5:S:122:TYR:CA	2.22	0.53
11:Y:5:ALA:HB3	11:Y:100:MET:HE2	1.90	0.53
11:Y:33:LYS:HZ1	17:Y:301:3BV:H58	1.73	0.52
10:J:1:MET:CE	10:J:1:MET:N	2.73	0.52
10:X:67:TYR:CE1	10:X:75:LEU:HD13	2.45	0.52
11:Y:33:LYS:NZ	17:Y:301:3BV:H58	2.25	0.52
8:H:-7:GLN:HB2	8:H:-4:ALA:HB2	1.92	0.52
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.58	0.51
3:C:201:VAL:O	3:C:202:GLN:CB	2.59	0.51
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.45	0.51
17:K:301:3BV:H17	12:L:108:HIS:NE2	2.22	0.51
14:N:-13:VAL:HA	14:N:-10:ASN:HB2	1.92	0.51
1:O:2:THR:CA	19:O:301:HOH:O	2.58	0.51
17:K:301:3BV:O60	18:K:303:MES:O1S	2.30	0.50
1:O:4:ARG:HH12	5:S:122:TYR:C	2.14	0.50
11:K:5:ALA:HB3	11:K:100:MET:HE2	1.92	0.50
11:K:100:MET:HE3	11:K:127:PHE:HB2	1.94	0.49
10:J:174:MET:HA	10:X:174:MET:HA	1.93	0.49
11:Y:100:MET:HE3	11:Y:127:PHE:HB2	1.96	0.47
11:Y:49:ALA:HB2	17:Y:301:3BV:H52	1.96	0.47
10:J:1:MET:HE1	10:J:135:TYR:H	1.79	0.47
13:M:2:GLN:O	13:M:3:GLN:HG2	2.14	0.47
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.97	0.47
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.97	0.46
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.98	0.46
10:X:3:ILE:HD12	10:X:176:PHE:CG	2.51	0.46
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.97	0.45
7:G:23:PHE:O	7:G:26:THR:HB	2.17	0.45
8:H:97:TYR:CB	8:H:127:LEU:HD11	2.47	0.45
7:U:23:PHE:O	7:U:26:THR:HB	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:1:MET:HB2	10:J:2:ASP:H	1.52	0.45
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.99	0.45
17:Y:301:3BV:H59	17:Y:301:3BV:H44	1.74	0.45
14:N:152:VAL:HA	14:N:175:MET:HE1	1.97	0.44
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.52	0.44
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.99	0.44
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.99	0.43
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.48	0.43
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.48	0.43
7:G:78:ILE:N	7:G:79:PRO:CD	2.81	0.43
2:P:86:LEU:HB3	2:P:114:LEU:HD21	2.01	0.43
6:F:172:LEU:CD1	6:F:195:ILE:HD13	2.48	0.43
6:T:172:LEU:CD1	6:T:195:ILE:HD13	2.48	0.43
7:U:78:ILE:N	7:U:79:PRO:CD	2.81	0.43
9:W:10:ILE:HG21	9:W:141:ALA:HB3	2.01	0.43
10:J:3:ILE:HD13	10:J:168:LEU:HD13	2.01	0.43
8:V:99:ILE:CG1	8:V:127:LEU:HD12	2.46	0.43
2:B:86:LEU:HB3	2:B:114:LEU:HD21	2.01	0.43
8:H:3:ILE:HG21	8:H:44:ALA:HB3	1.99	0.43
14:N:3:VAL:CG1	14:N:20:THR:CG2	2.97	0.42
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.01	0.42
3:C:201:VAL:HG13	3:C:202:GLN:N	2.34	0.42
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.85	0.42
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.34	0.42
11:K:170:TYR:O	17:K:301:3BV:H57	2.19	0.42
14:N:55:ILE:HD11	14:N:93:LEU:HD13	2.00	0.42
8:H:50:ALA:HB2	9:I:128:CYS:HB2	2.01	0.42
9:W:20:VAL:HG13	9:W:118:PRO:HB3	2.02	0.42
12:L:4:PRO:O	13:M:104:ARG:NH1	2.50	0.42
13:M:2:GLN:C	13:M:3:GLN:HG2	2.40	0.42
17:Y:301:3BV:H16	12:Z:108:HIS:NE2	2.34	0.42
9:I:10:ILE:HG21	9:I:141:ALA:HB3	2.01	0.42
11:K:1:THR:CG2	11:K:2:THR:N	2.82	0.42
9:I:20:VAL:HG13	9:I:118:PRO:HB3	2.02	0.42
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.49	0.42
8:V:50:ALA:HB2	9:W:128:CYS:HB2	2.02	0.41
8:H:3:ILE:HD13	8:H:16:ALA:CB	2.49	0.41
11:K:100:MET:CE	11:K:127:PHE:HB2	2.51	0.41
12:L:147:MET:N	12:L:148:PRO:HD2	2.35	0.41
11:Y:5:ALA:HB3	11:Y:100:MET:CE	2.51	0.41
12:Z:147:MET:N	12:Z:148:PRO:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.20	0.41
11:Y:100:MET:CE	11:Y:127:PHE:HB2	2.51	0.41
10:J:1:MET:HE2	10:J:1:MET:H3	1.85	0.41
12:L:8:ASN:HA	12:L:30:ILE:O	2.21	0.41
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.51	0.41
2:B:161:ALA:HB3	3:C:52:LEU:HD23	2.03	0.41
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.51	0.41
11:K:5:ALA:HB3	11:K:100:MET:CE	2.51	0.41
5:E:77:ALA:N	5:E:78:PRO:CD	2.85	0.40
5:S:77:ALA:N	5:S:78:PRO:CD	2.85	0.40
2:B:14:PRO:HA	3:C:20:TYR:CD1	2.57	0.40

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	247/250 (99%)	241 (98%)	6 (2%)	0	100	100
1	O	247/250 (99%)	242 (98%)	5 (2%)	0	100	100
2	B	242/258 (94%)	234 (97%)	6 (2%)	2 (1%)	19	51
2	P	242/258 (94%)	234 (97%)	6 (2%)	2 (1%)	19	51
3	C	238/254 (94%)	231 (97%)	5 (2%)	2 (1%)	19	51
3	Q	238/254 (94%)	231 (97%)	5 (2%)	2 (1%)	19	51
4	D	231/260 (89%)	224 (97%)	7 (3%)	0	100	100
4	R	231/260 (89%)	224 (97%)	7 (3%)	0	100	100
5	E	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
5	S	229/234 (98%)	224 (98%)	5 (2%)	0	100	100
6	F	241/288 (84%)	233 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	T	241/288 (84%)	232 (96%)	9 (4%)	0	100	100
7	G	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
7	U	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
8	H	232/244 (95%)	226 (97%)	6 (3%)	0	100	100
8	V	232/244 (95%)	224 (97%)	7 (3%)	1 (0%)	34	66
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	190 (98%)	3 (2%)	0	100	100
10	X	193/198 (98%)	190 (98%)	3 (2%)	0	100	100
11	K	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
11	Y	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
12	L	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
12	Z	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
13	M	230/246 (94%)	220 (96%)	8 (4%)	2 (1%)	17	48
13	a	230/246 (94%)	220 (96%)	8 (4%)	2 (1%)	17	48
14	N	211/213 (99%)	206 (98%)	5 (2%)	0	100	100
14	b	211/213 (99%)	204 (97%)	6 (3%)	1 (0%)	29	61
All	All	6330/6672 (95%)	6157 (97%)	159 (2%)	14 (0%)	47	78

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN
13	M	111	TRP
2	P	51	VAL
3	Q	202	GLN
13	a	111	TRP
14	b	0	GLY
2	B	221	ASP
3	C	205	ALA
2	P	221	ASP
3	Q	205	ALA
8	V	-8	THR
13	M	229	GLY
13	a	229	GLY

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	208/209 (100%)	205 (99%)	3 (1%)	67	89
1	O	208/209 (100%)	205 (99%)	3 (1%)	67	89
2	B	203/216 (94%)	197 (97%)	6 (3%)	41	75
2	P	203/216 (94%)	197 (97%)	6 (3%)	41	75
3	C	212/226 (94%)	207 (98%)	5 (2%)	49	79
3	Q	212/226 (94%)	207 (98%)	5 (2%)	49	79
4	D	194/215 (90%)	186 (96%)	8 (4%)	30	64
4	R	194/215 (90%)	186 (96%)	8 (4%)	30	64
5	E	190/193 (98%)	184 (97%)	6 (3%)	39	73
5	S	190/193 (98%)	184 (97%)	6 (3%)	39	73
6	F	201/239 (84%)	192 (96%)	9 (4%)	27	61
6	T	201/239 (84%)	192 (96%)	9 (4%)	27	61
7	G	206/210 (98%)	201 (98%)	5 (2%)	49	79
7	U	206/210 (98%)	200 (97%)	6 (3%)	42	76
8	H	190/199 (96%)	184 (97%)	6 (3%)	39	73
8	V	190/199 (96%)	185 (97%)	5 (3%)	46	77
9	I	172/173 (99%)	170 (99%)	2 (1%)	71	91
9	W	172/173 (99%)	170 (99%)	2 (1%)	71	91
10	J	173/175 (99%)	167 (96%)	6 (4%)	36	70
10	X	173/175 (99%)	168 (97%)	5 (3%)	42	76
11	K	169/169 (100%)	165 (98%)	4 (2%)	49	79
11	Y	169/169 (100%)	165 (98%)	4 (2%)	49	79
12	L	185/185 (100%)	179 (97%)	6 (3%)	39	73
12	Z	185/185 (100%)	179 (97%)	6 (3%)	39	73
13	M	198/208 (95%)	191 (96%)	7 (4%)	36	70
13	a	198/208 (95%)	190 (96%)	8 (4%)	31	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	175/175 (100%)	173 (99%)	2 (1%)	73	92
14	b	175/175 (100%)	173 (99%)	2 (1%)	73	92
All	All	5352/5584 (96%)	5202 (97%)	150 (3%)	43	76

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	61	LEU
1	A	157	PHE
2	B	50	LYS
2	B	58	GLN
2	B	114	LEU
2	B	184	LYS
2	B	186	ASP
2	B	191	LEU
3	C	4	ARG
3	C	38	ASN
3	C	147	GLN
3	C	169	VAL
3	C	180	LYS
4	D	99	ILE
4	D	125	LEU
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	224	ASP
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	29	LYS
5	E	54	GLU
5	E	71	LEU
5	E	184	ASN
5	E	188	LEU
6	F	14	ASP
6	F	117	GLN
6	F	123	ASN
6	F	172	LEU
6	F	181	GLU
6	F	203	ASN

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Mol	Chain	Res	Type
6	F	206	LYS
6	F	214	TRP
6	F	221	ASN
7	G	115	LEU
7	G	125	MET
7	G	166	GLN
7	G	181	LYS
7	G	235	ARG
8	H	-8	THR
8	H	-5	LYS
8	H	30	ASN
8	H	56	THR
8	H	127	LEU
8	H	196	ARG
9	I	37	ASN
9	I	182	TRP
10	J	1	MET
10	J	23	ARG
10	J	75	LEU
10	J	78	GLN
10	J	144	LEU
10	J	174	MET
11	K	4	LEU
11	K	9	GLN
11	K	35	ILE
11	K	106	ARG
12	L	1	GLN
12	L	23	LEU
12	L	31	THR
12	L	49	ASN
12	L	136	CYS
12	L	167	LYS
13	M	2	GLN
13	M	3	GLN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
14	N	-14	GLN
14	N	-11	ILE
1	O	17	LYS

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Mol	Chain	Res	Type
1	O	61	LEU
1	O	157	PHE
2	P	50	LYS
2	P	58	GLN
2	P	114	LEU
2	P	184	LYS
2	P	186	ASP
2	P	191	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	147	GLN
3	Q	169	VAL
3	Q	180	LYS
4	R	99	ILE
4	R	125	LEU
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	224	ASP
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	54	GLU
5	S	71	LEU
5	S	184	ASN
5	S	188	LEU
6	T	14	ASP
6	T	117	GLN
6	T	123	ASN
6	T	172	LEU
6	T	181	GLU
6	T	203	ASN
6	T	206	LYS
6	T	214	TRP
6	T	221	ASN
7	U	115	LEU
7	U	117	GLN
7	U	125	MET
7	U	166	GLN
7	U	181	LYS
7	U	235	ARG

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Mol	Chain	Res	Type
8	V	-9	HIS
8	V	30	ASN
8	V	56	THR
8	V	127	LEU
8	V	196	ARG
9	W	37	ASN
9	W	182	TRP
10	X	23	ARG
10	X	75	LEU
10	X	78	GLN
10	X	144	LEU
10	X	174	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	35	ILE
11	Y	106	ARG
12	Z	1	GLN
12	Z	23	LEU
12	Z	31	THR
12	Z	49	ASN
12	Z	136	CYS
12	Z	167	LYS
13	a	2	GLN
13	a	3	GLN
13	a	35	ARG
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
14	b	-12	ASP
14	b	-1	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	119	GLN
2	B	123	GLN
3	C	38	ASN
3	C	147	GLN
3	C	160	GLN

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Mol	Chain	Res	Type
4	D	91	HIS
4	D	146	GLN
5	E	92	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	184	ASN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
6	F	240	GLN
7	G	83	ASN
7	G	117	GLN
7	G	121	GLN
8	H	-11	ASN
8	H	-7	GLN
8	H	30	ASN
8	H	66	HIS
8	H	189	ASN
10	J	55	GLN
11	K	85	ASN
11	K	176	ASN
12	L	3	ASN
12	L	70	ASN
12	L	79	HIS
12	L	158	ASN
13	M	102	GLN
14	N	-14	GLN
14	N	-10	ASN
2	P	119	GLN
2	P	123	GLN
3	Q	38	ASN
3	Q	147	GLN
3	Q	160	GLN
4	R	91	HIS
4	R	146	GLN
5	S	92	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	184	ASN

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Mol	Chain	Res	Type
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
6	T	240	GLN
7	U	83	ASN
7	U	117	GLN
7	U	121	GLN
8	V	-7	GLN
10	X	55	GLN
10	X	118	GLN
11	Y	85	ASN
11	Y	176	ASN
12	Z	70	ASN
12	Z	79	HIS
12	Z	108	HIS
12	Z	158	ASN
13	a	102	GLN
14	b	-14	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 10 are monoatomic - leaving 4 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	3BV	Y	301	11	54,54,54	1.51	4 (7%)	68,71,71	1.59	8 (11%)
17	3BV	K	301	11	54,54,54	1.43	4 (7%)	68,71,71	1.59	9 (13%)
18	MES	K	303	-	12,12,12	2.25	1 (8%)	14,16,16	1.27	1 (7%)
18	MES	Y	302	-	12,12,12	2.22	1 (8%)	14,16,16	1.25	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
17	3BV	Y	301	11	-	5/59/67/67	0/3/3/3
17	3BV	K	301	11	-	6/59/67/67	0/3/3/3
18	MES	K	303	-	-	0/6/14/14	0/1/1/1
18	MES	Y	302	-	-	0/6/14/14	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	K	303	MES	C8-S	-7.47	1.66	1.77
18	Y	302	MES	C8-S	-7.37	1.67	1.77
17	Y	301	3BV	C32-C33	-6.45	1.35	1.51
17	K	301	3BV	C32-C33	-6.26	1.36	1.51
17	Y	301	3BV	C13-C14	-4.66	1.38	1.51
17	K	301	3BV	C13-C14	-4.54	1.38	1.51
17	K	301	3BV	O48-C47	-4.04	1.33	1.43
17	Y	301	3BV	O48-C47	-4.02	1.33	1.43
17	Y	301	3BV	C59-C51	-3.05	1.49	1.52
17	K	301	3BV	C59-C51	-2.87	1.49	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	K	301	3BV	C43-C42-N41	-8.59	99.08	110.18
17	Y	301	3BV	C43-C42-N41	-8.16	99.63	110.18
17	Y	301	3BV	C58-C51-C59	-4.56	103.88	109.88
17	Y	301	3BV	C3-N4-C5	4.00	117.83	108.83
17	K	301	3BV	C58-C51-C59	-3.26	105.59	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	K	301	3BV	C3-N4-C5	3.15	115.91	108.83
17	K	301	3BV	C33-C32-C31	-3.08	104.88	113.39
18	Y	302	MES	O3S-S-C8	3.01	110.63	105.77
17	K	301	3BV	C7-N4-C3	2.82	115.47	111.09
17	Y	301	3BV	C33-C32-C31	-2.81	105.64	113.39
17	K	301	3BV	O60-C59-C51	-2.73	105.74	111.33
18	K	303	MES	O3S-S-C8	2.72	110.17	105.77
17	K	301	3BV	C24-C23-C28	-2.45	104.73	110.57
17	Y	301	3BV	C24-C23-C28	-2.45	104.74	110.57
17	K	301	3BV	C12-C11-C20	2.26	115.48	110.20
17	Y	301	3BV	C39-C31-N30	-2.07	105.51	111.16
17	K	301	3BV	O48-C47-C42	-2.06	104.06	108.98
17	Y	301	3BV	C12-C11-N10	-2.06	106.72	110.88
17	Y	301	3BV	C24-C23-N22	-2.02	105.92	110.58

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	K	301	3BV	C47-C42-C43-C44
17	K	301	3BV	O48-C47-C51-C58
17	Y	301	3BV	C47-C42-C43-C44
17	K	301	3BV	N41-C42-C43-C44
17	Y	301	3BV	N41-C42-C43-C44
17	Y	301	3BV	N41-C42-C47-C51
17	K	301	3BV	N30-C31-C39-O40
17	Y	301	3BV	N41-C42-C47-O48
17	K	301	3BV	C11-C12-C13-C14
17	Y	301	3BV	N30-C31-C39-O40
17	K	301	3BV	N30-C31-C39-N41

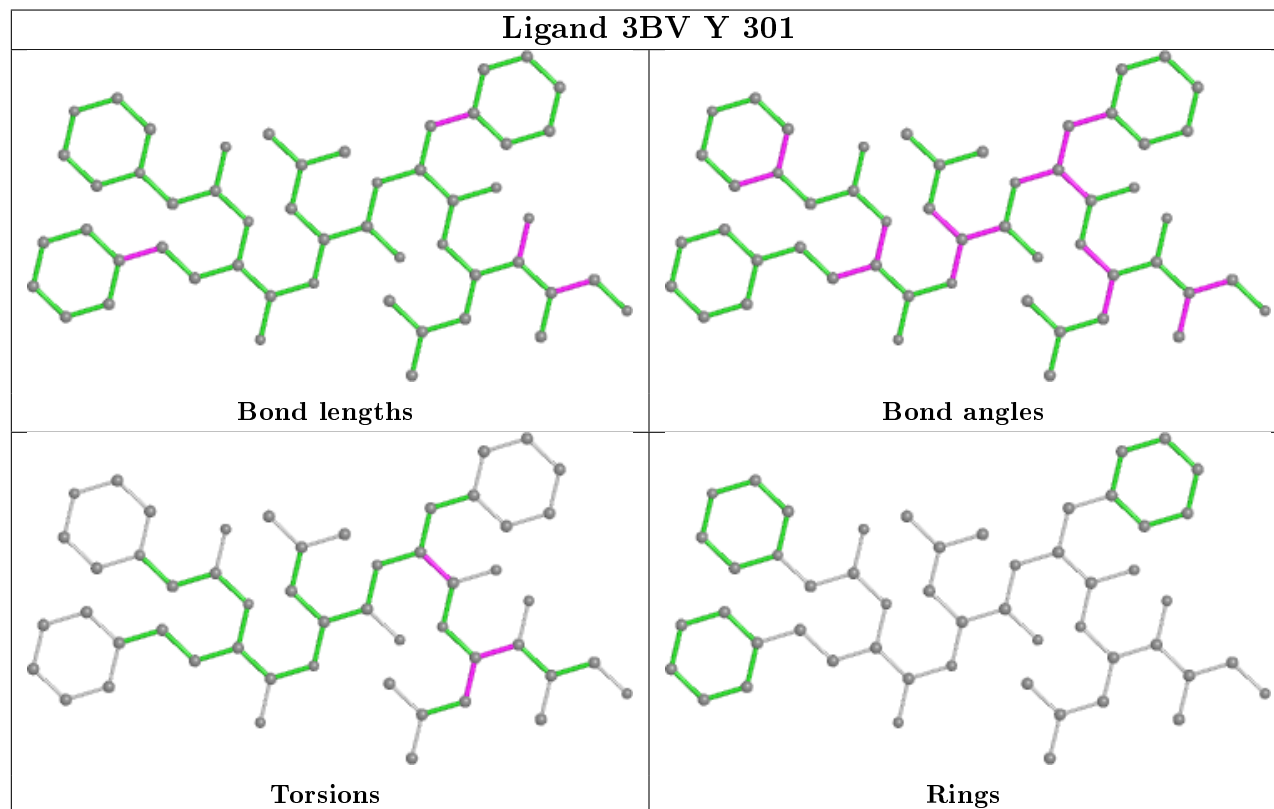
There are no ring outliers.

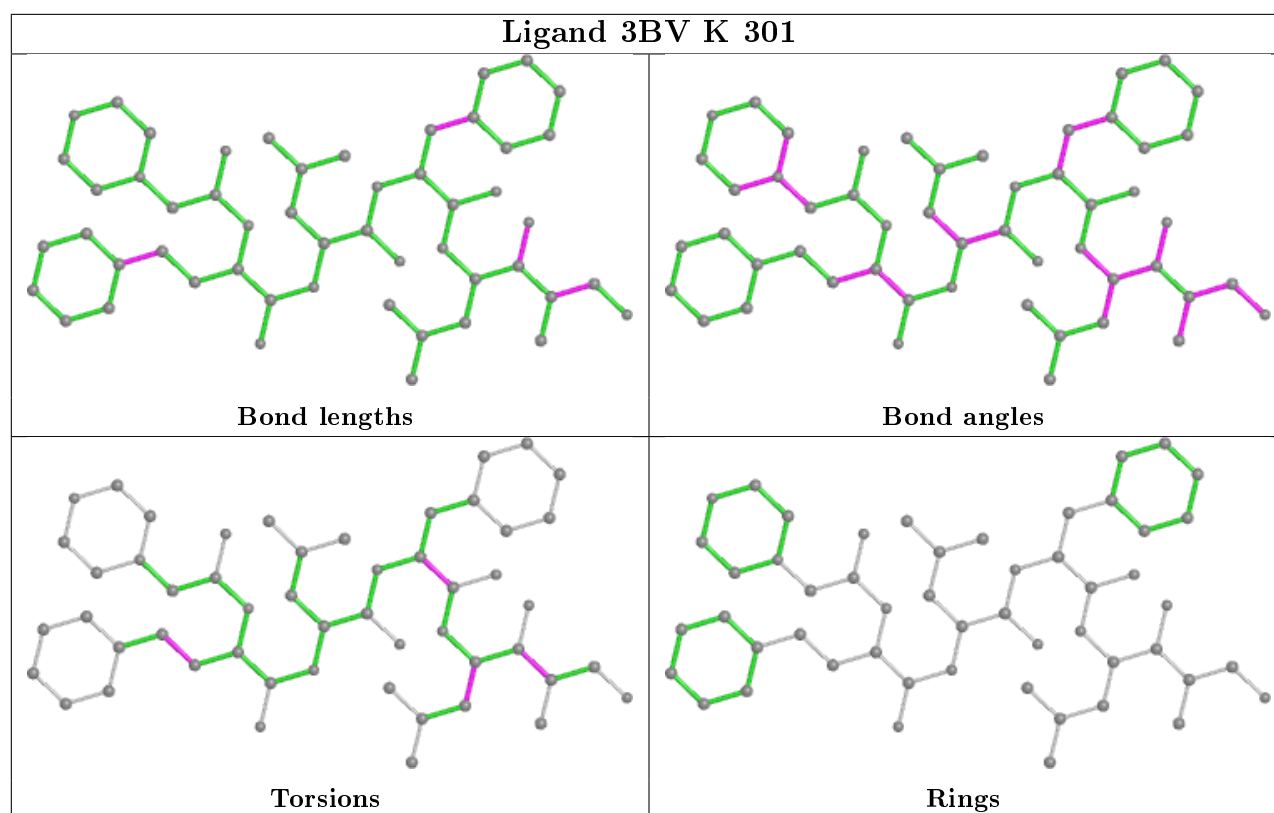
3 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	Y	301	3BV	9	0
17	K	301	3BV	12	0
18	K	303	MES	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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
13	a	2
13	M	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	a	110:LEU	C	111:TRP	N	1.18
1	M	110:LEU	C	111:TRP	N	1.15
1	M	111:TRP	C	112:ASN	N	0.82
1	a	111:TRP	C	112:ASN	N	0.73

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, 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	249/250 (99%)	-0.40	5 (2%) 65 63	40, 55, 94, 128	0
1	O	249/250 (99%)	-0.28	8 (3%) 47 43	43, 64, 111, 141	0
2	B	244/258 (94%)	-0.22	11 (4%) 33 29	40, 61, 105, 155	0
2	P	244/258 (94%)	-0.22	9 (3%) 41 37	43, 65, 112, 160	0
3	C	240/254 (94%)	-0.15	15 (6%) 20 16	39, 66, 132, 166	0
3	Q	240/254 (94%)	0.07	19 (7%) 12 10	45, 78, 159, 181	0
4	D	235/260 (90%)	-0.30	3 (1%) 77 77	49, 71, 100, 145	0
4	R	235/260 (90%)	-0.27	4 (1%) 70 69	51, 71, 110, 155	0
5	E	231/234 (98%)	-0.22	4 (1%) 70 69	50, 73, 109, 151	0
5	S	231/234 (98%)	-0.18	7 (3%) 50 45	49, 76, 116, 150	0
6	F	243/288 (84%)	-0.40	3 (1%) 79 79	40, 63, 109, 137	0
6	T	243/288 (84%)	-0.36	6 (2%) 57 55	42, 67, 117, 155	0
7	G	241/252 (95%)	-0.41	5 (2%) 63 61	39, 58, 96, 142	0
7	U	241/252 (95%)	-0.41	4 (1%) 70 69	36, 58, 91, 130	0
8	H	234/244 (95%)	-0.17	8 (3%) 45 40	37, 57, 98, 130	0
8	V	234/244 (95%)	-0.14	9 (3%) 40 36	40, 63, 97, 142	0
9	I	204/205 (99%)	-0.62	2 (0%) 82 82	32, 50, 81, 102	0
9	W	204/205 (99%)	-0.61	2 (0%) 82 82	36, 54, 84, 110	0
10	J	195/198 (98%)	-0.56	2 (1%) 82 82	35, 52, 82, 123	0
10	X	195/198 (98%)	-0.54	1 (0%) 91 91	38, 55, 82, 128	0
11	K	212/212 (100%)	-0.54	2 (0%) 84 84	36, 53, 81, 109	0
11	Y	212/212 (100%)	-0.55	2 (0%) 84 84	38, 53, 81, 106	0
12	L	222/222 (100%)	-0.47	0 100 100	32, 58, 90, 120	0
12	Z	222/222 (100%)	-0.49	2 (0%) 84 84	38, 57, 88, 109	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
13	M	232/246 (94%)	-0.50	3 (1%)	77 77	37, 57, 82, 92	0
13	a	232/246 (94%)	-0.53	3 (1%)	77 77	38, 54, 79, 88	0
14	N	213/213 (100%)	-0.44	7 (3%)	46 41	38, 53, 81, 109	0
14	b	213/213 (100%)	-0.45	7 (3%)	46 41	38, 52, 81, 106	0
All	All	6390/6672 (95%)	-0.36	153 (2%)	59 56	32, 60, 105, 181	0

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	49	THR	8.5
8	V	-8	THR	6.1
3	Q	50	LEU	6.0
8	V	-9	HIS	6.0
2	B	220	ASN	5.8
2	P	219	ALA	5.4
3	Q	240	GLU	5.1
3	C	206	LYS	5.1
3	Q	206	LYS	5.1
3	C	49	THR	5.0
14	b	-16	GLY	5.0
2	P	51	VAL	5.0
2	P	220	ASN	4.7
8	V	222	ASP	4.7
8	H	-11	ASN	4.7
1	O	231	LYS	4.3
3	Q	236	GLN	4.3
5	S	202	ASP	4.3
3	C	238	LYS	4.3
8	H	-6	PRO	4.3
2	B	218	GLY	4.2
2	P	59	ASP	4.2
2	B	51	VAL	4.2
8	V	-10	SER	4.2
14	N	-13	VAL	4.1
2	B	221	ASP	4.1
8	H	221	CYS	4.1
1	O	249	ALA	4.0
8	H	-10	SER	4.0
2	P	221	ASP	4.0
3	C	50	LEU	3.9
3	Q	238	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
11	Y	212	GLY	3.8
8	H	-8	THR	3.8
9	W	1	SER	3.8
5	E	202	ASP	3.8
10	J	194	ASP	3.7
8	H	-9	HIS	3.7
8	V	-11	ASN	3.7
1	O	52	SER	3.7
13	M	2	GLN	3.7
13	M	4	PRO	3.6
3	C	240	GLU	3.5
3	Q	48	SER	3.5
4	R	241	ALA	3.4
2	B	59	ASP	3.4
14	N	-12	ASP	3.3
10	X	194	ASP	3.3
4	D	242	GLU	3.3
8	H	222	ASP	3.3
3	C	202	GLN	3.3
3	Q	239	GLN	3.2
14	N	-10	ASN	3.2
12	Z	1	GLN	3.2
1	A	231	LYS	3.2
3	C	239	GLN	3.2
2	P	218	GLY	3.1
2	P	52	THR	3.1
14	N	-14	GLN	3.1
3	Q	180	LYS	3.1
13	a	2	GLN	3.1
6	F	181	GLU	3.1
3	Q	204	GLY	3.0
8	V	221	CYS	3.0
11	K	212	GLY	3.0
3	C	236	GLN	3.0
14	b	-14	GLN	2.9
10	J	193	ASP	2.9
2	P	222	GLY	2.9
13	M	3	GLN	2.9
5	S	122	TYR	2.9
3	C	181	GLU	2.9
2	B	219	ALA	2.8
3	Q	141	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
4	R	242	GLU	2.8
12	Z	210	ASP	2.8
3	Q	205	ALA	2.8
1	A	229	THR	2.8
14	b	-12	ASP	2.8
1	A	249	ALA	2.8
6	T	2	THR	2.7
2	B	242	GLY	2.7
2	B	60	THR	2.7
14	b	-11	ILE	2.7
7	U	181	LYS	2.7
1	O	2	THR	2.7
3	C	225	GLU	2.6
1	O	201	GLU	2.6
1	O	229	THR	2.6
14	b	-13	VAL	2.6
14	N	-6	LYS	2.6
7	U	242	GLN	2.6
1	O	248	GLU	2.6
1	A	248	GLU	2.6
1	A	250	LEU	2.6
3	Q	187	GLU	2.5
5	E	54	GLU	2.5
7	U	222	ASP	2.5
13	a	3	GLN	2.5
3	Q	225	GLU	2.5
9	I	133	LYS	2.5
6	T	243	ILE	2.4
8	V	-6	PRO	2.4
4	R	125	LEU	2.4
13	a	4	PRO	2.4
14	b	-10	ASN	2.4
2	B	222	GLY	2.4
2	P	60	THR	2.4
2	B	203	SER	2.4
6	T	166	GLN	2.3
7	G	179	LYS	2.3
3	C	60	SER	2.3
6	F	202	ASP	2.3
8	V	9	ASN	2.3
5	S	180	LYS	2.3
14	N	-15	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	217	LYS	2.3
3	Q	203	THR	2.3
14	b	195	GLN	2.3
5	S	233	ILE	2.3
5	S	30	GLN	2.3
9	W	133	LYS	2.3
3	C	205	ALA	2.2
4	R	203	LYS	2.2
5	S	123	GLY	2.2
6	F	244	ASN	2.2
11	K	147	ASP	2.2
6	T	205	GLU	2.2
7	G	222	ASP	2.2
3	C	235	GLU	2.2
6	T	244	ASN	2.2
5	E	180	LYS	2.2
3	C	216	ASP	2.2
14	N	-11	ILE	2.2
3	Q	223	SER	2.2
4	D	117	GLU	2.2
7	G	3	TYR	2.1
5	S	203	GLU	2.1
3	Q	51	LYS	2.1
7	G	242	GLN	2.1
3	Q	235	GLU	2.1
1	O	230	ASP	2.1
9	I	1	SER	2.1
8	V	145	ASP	2.1
4	D	241	ALA	2.1
3	Q	229	GLN	2.1
11	Y	202	GLU	2.1
7	U	3	TYR	2.0
7	G	181	LYS	2.0
5	E	3	ASN	2.0
6	T	181	GLU	2.0
3	C	180	LYS	2.0
8	H	-7	GLN	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

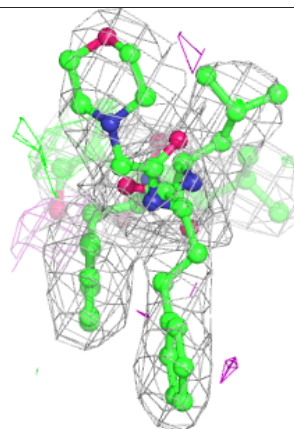
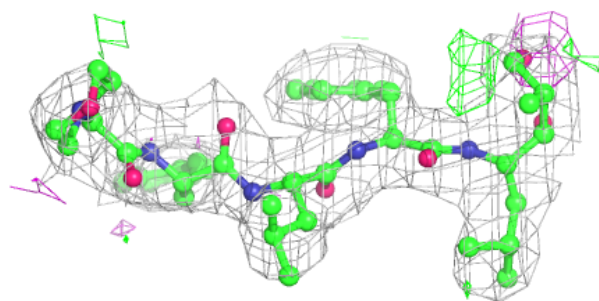
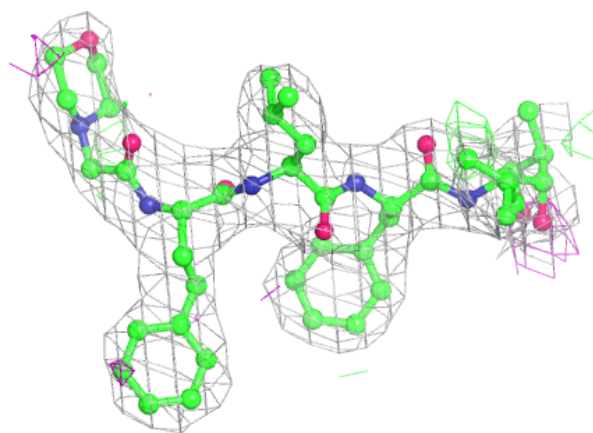
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	3BV	K	301	52/52	0.93	0.18	40,49,113,119	0
17	3BV	Y	301	52/52	0.94	0.18	39,49,109,116	0
15	MG	G	301	1/1	0.95	0.13	56,56,56,56	0
15	MG	N	201	1/1	0.95	0.07	48,48,48,48	0
15	MG	Z	301	1/1	0.96	0.16	52,52,52,52	0
18	MES	Y	302	12/12	0.97	0.23	46,47,58,61	0
15	MG	I	302	1/1	0.97	0.13	44,44,44,44	0
18	MES	K	303	12/12	0.97	0.27	47,49,62,62	0
16	CL	U	301	1/1	0.98	0.14	49,49,49,49	0
15	MG	I	301	1/1	0.98	0.08	55,55,55,55	0
16	CL	b	201	1/1	0.98	0.09	62,62,62,62	0
16	CL	N	202	1/1	0.99	0.10	56,56,56,56	0
16	CL	G	302	1/1	0.99	0.14	42,42,42,42	0
15	MG	K	302	1/1	0.99	0.05	45,45,45,45	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

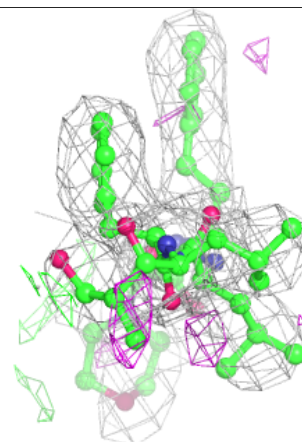
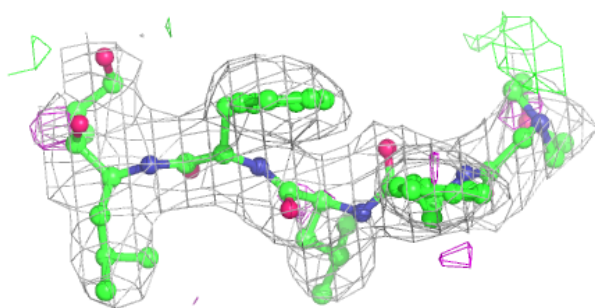
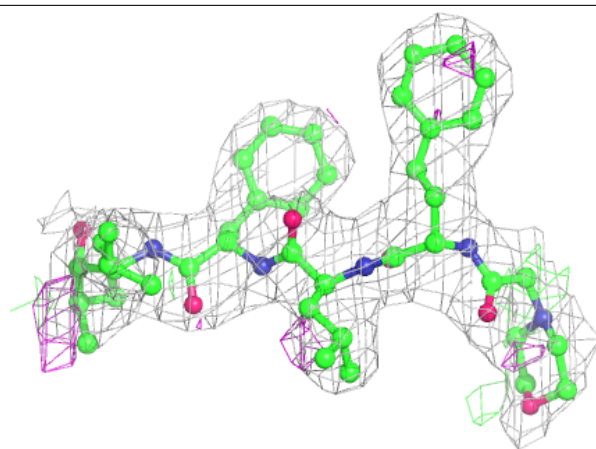
Electron density around 3BV K 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 3BV Y 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.