



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 30, 2026 – 02:12 PM UTC

PDB ID : 5L61 / pdb_00005l61
Title : Yeast 20S proteasome with human beta5c (1-138) and human beta6 (99-132)
in complex with epoxyketone inhibitor 14
Authors : Groll, M.; Huber, E.M.
Deposited on : 2016-05-28
Resolution : 2.80 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

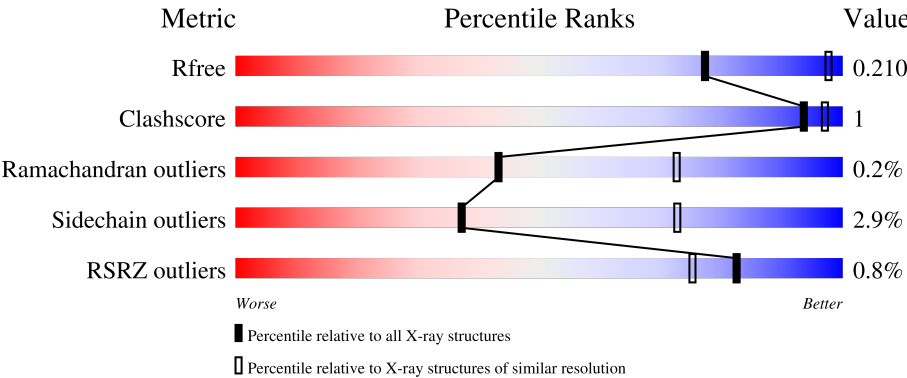
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.



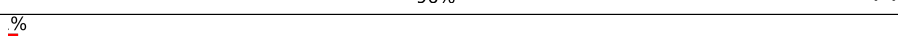
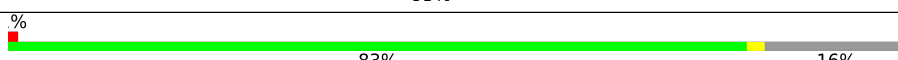
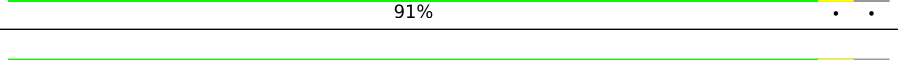
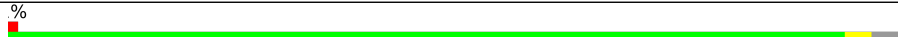
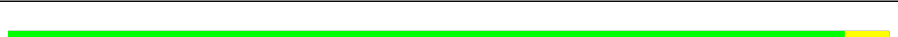
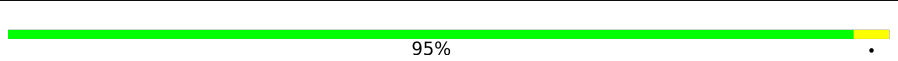
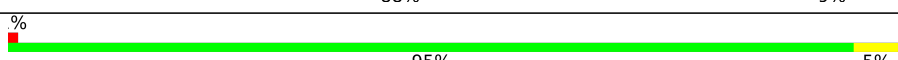
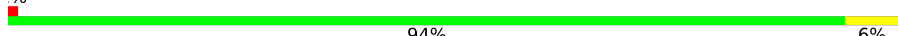
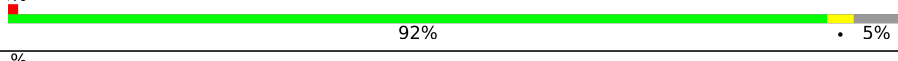
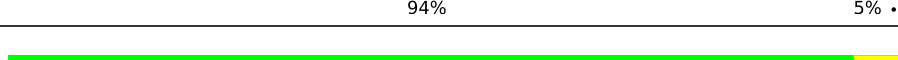
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 $\leq 5\%$. 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	98%
1	O	250	% 98%
2	B	258	2% 89% 5% • 5%
2	P	258	% 89% 5% • 5%
3	C	254	2% 87% 6% • 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	
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	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	211	
11	Y	211	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	196	

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 49776 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	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 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	226	Total	C	N	O	S	0	0	0
			1719	1082	298	332	7			
8	V	226	Total	C	N	O	S	0	0	0
			1719	1082	298	332	7			

- 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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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, Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	211	Total	C	N	O	S	0	0	0
			1632	1036	282	306	8			
11	Y	211	Total	C	N	O	S	0	0	0
			1632	1036	282	306	8			

- Molecule 12 is a protein called Proteasome subunit beta type-6, Proteasome subunit beta type-1, Proteasome subunit beta type-6, Proteasome subunit beta type-1, Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1764	1119	305	336	4			
12	Z	222	Total	C	N	O	S	0	0	0
			1764	1119	305	336	4			

- Molecule 13 is a protein called Proteasome subunit beta type-7.

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

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

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

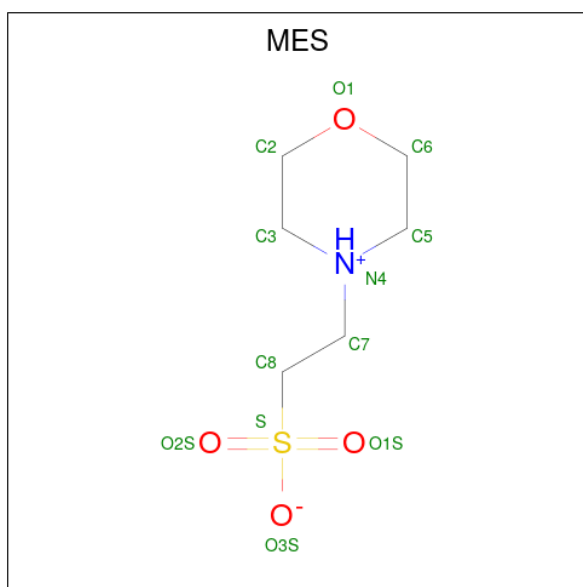
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

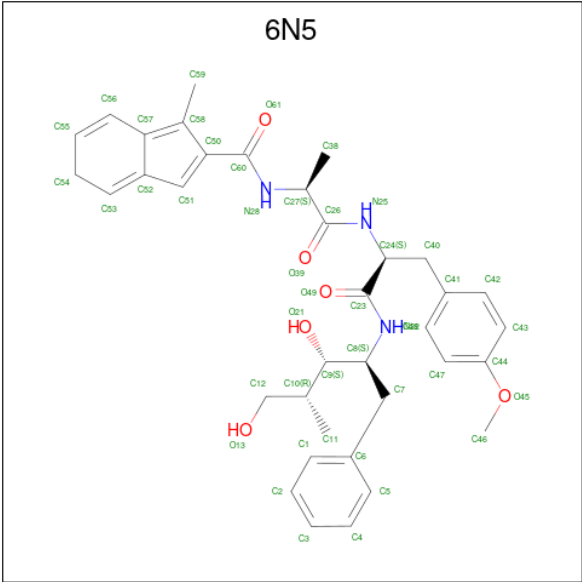
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total Cl 1 1	0	0
16	U	1	Total Cl 1 1	0	0

- Molecule 17 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
17	K	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
17	V	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
17	Y	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 18 is {N}-[(2 {S})-1-[[[(2 {S})-3-(4-methoxyphenyl)-1-[[[(2 {S}),3 {S}),4 {R})-4-methyl-3,5-bis(oxidanyl)-1-phenyl-pentan-2-yl]amino]-1-oxidanylidene-propan-2-yl]amino]-1-oxidanylidene-propan-2-yl]-1-methyl-5 {H}-indene-2-carboxamide (CCD ID: 6N5) (formula: C₃₆H₄₃N₃O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	K	1	Total	C	N	O	0	0
			45	36	3	6		
18	Y	1	Total	C	N	O	0	0
			45	36	3	6		

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	6	Total	O	0	0
			6	6		
19	B	7	Total	O	0	0
			7	7		
19	C	6	Total	O	0	0
			6	6		
19	D	4	Total	O	0	0
			4	4		
19	E	5	Total	O	0	0
			5	5		
19	F	12	Total	O	0	0
			12	12		
19	G	11	Total	O	0	0
			11	11		
19	H	15	Total	O	0	0
			15	15		
19	I	11	Total	O	0	0
			11	11		
19	J	9	Total	O	0	0
			9	9		

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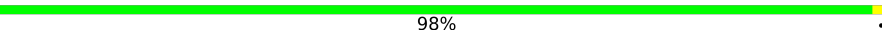
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	K	8	Total O 8 8	0	0
19	L	14	Total O 14 14	0	0
19	M	18	Total O 18 18	0	0
19	N	8	Total O 8 8	0	0
19	O	8	Total O 8 8	0	0
19	P	10	Total O 10 10	0	0
19	Q	6	Total O 6 6	0	0
19	R	8	Total O 8 8	0	0
19	S	4	Total O 4 4	0	0
19	T	8	Total O 8 8	0	0
19	U	20	Total O 20 20	0	0
19	V	11	Total O 11 11	0	0
19	W	12	Total O 12 12	0	0
19	X	10	Total O 10 10	0	0
19	Y	10	Total O 10 10	0	0
19	Z	7	Total O 7 7	0	0
19	a	12	Total O 12 12	0	0
19	b	9	Total O 9 9	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:  98% .



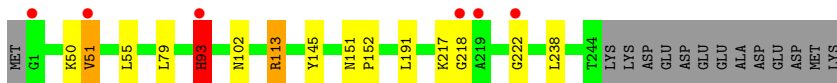
- Molecule 1: Proteasome subunit alpha type-2

Chain O:  98% .



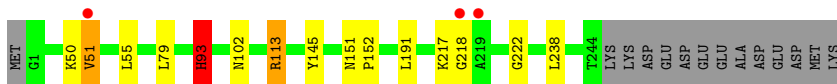
- Molecule 2: Proteasome subunit alpha type-3

Chain B:  89% 5% • 5%



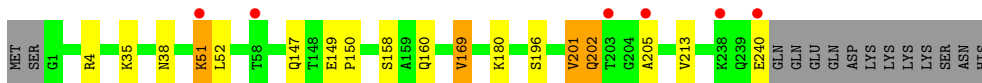
- Molecule 2: Proteasome subunit alpha type-3

Chain P:  89% 5% • 5%

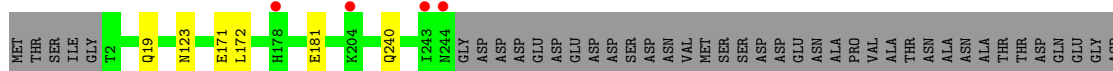
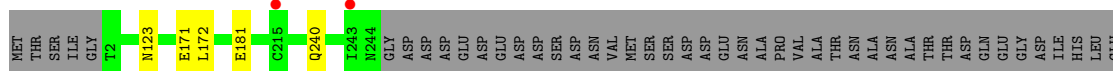
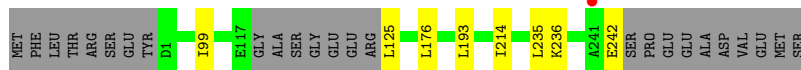
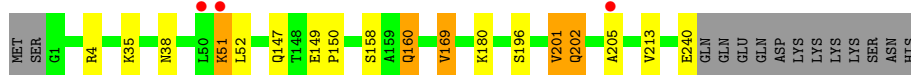


- Molecule 3: Proteasome subunit alpha type-4

Chain C:  87% 6% • 6%



- Molecule 3: Proteasome subunit alpha type-4



ILE
HIS
LEU
GLU

• Molecule 7: Proteasome subunit alpha type-1

Chain G:  91%

MET SER GLY ALA ALA ALA ALA ALA ALA ALA G2 F23 T26 I78 P79 L115 R122 M125 D149 P150 R235 L236 Q242 ASP

• Molecule 7: Proteasome subunit alpha type-1

Chain U:  91%

MET SER GLY ALA ALA ALA ALA ALA ALA ALA G2 P12 F23 T26 I78 P79 L115 R122 M125 D149 P150 R235 L236 Q242 ASP

• Molecule 8: Proteasome subunit beta type-2

Chain H:  94%

TH L34 H35 T56 L68 D104 P105 R196 I223 E226 GLN VAL ASP ILE THR ALA

• Molecule 8: Proteasome subunit beta type-2

Chain V:  94%

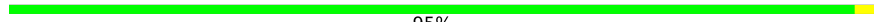
TH L34 H35 T56 L68 D104 P105 R196 I223 Q224 E226 GLN VAL ASP ILE THR ALA

• Molecule 9: Proteasome subunit beta type-3

Chain I:  94% 5%

MET S1 I10 V20 N37 K38 R98 I126 A141 E150 F163 L171 I189 R197 D204

• Molecule 9: Proteasome subunit beta type-3

Chain W:  95%

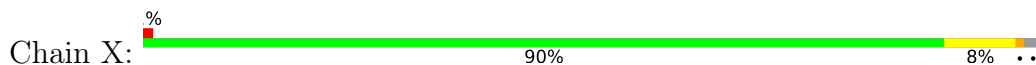
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• Molecule 10: Proteasome subunit beta type-4

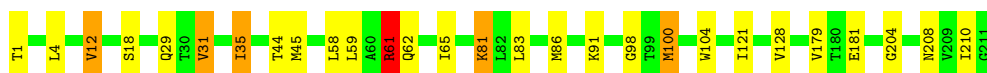
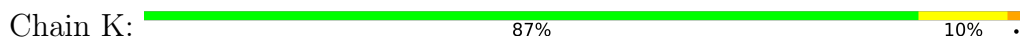
Chain J:  90% 8%



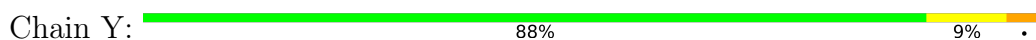
- Molecule 10: Proteasome subunit beta type-4



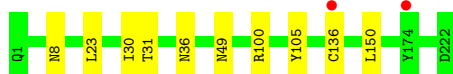
- Molecule 11: Proteasome subunit beta type-5, Proteasome subunit beta type-5



- Molecule 11: Proteasome subunit beta type-5, Proteasome subunit beta type-5



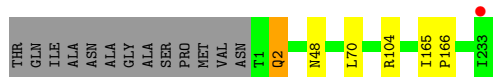
- Molecule 12: Proteasome subunit beta type-6, Proteasome subunit beta type-1, Proteasome subunit beta type-6, Proteasome subunit beta type-1, Proteasome subunit beta type-6



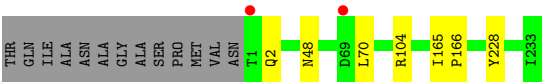
- Molecule 12: Proteasome subunit beta type-6, Proteasome subunit beta type-1, Proteasome subunit beta type-6, Proteasome subunit beta type-1, Proteasome subunit beta type-6



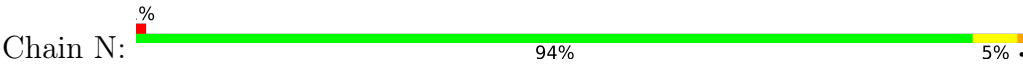
- Molecule 13: Proteasome subunit beta type-7



- 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	135.67Å 300.68Å 145.68Å 90.00° 112.84° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.5 (15.00-2.80) 96.8 (15.00-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.179 , 0.205 0.185 , 0.210	Depositor DCC
R_{free} test set	12740 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	57.6	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	49776	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% 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: 6N5, CL, MG, MES

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	0.39	0/1952	0.68	0/2642
1	O	0.39	0/1952	0.68	0/2642
2	B	0.45	0/1934	0.75	3/2618 (0.1%)
2	P	0.43	0/1934	0.76	3/2618 (0.1%)
3	C	0.39	0/1910	0.68	1/2586 (0.0%)
3	Q	0.39	0/1910	0.69	1/2586 (0.0%)
4	D	0.39	0/1837	0.65	0/2475
4	R	0.39	0/1837	0.65	0/2475
5	E	0.40	0/1800	0.65	0/2433
5	S	0.40	0/1800	0.65	0/2433
6	F	0.40	0/1932	0.68	0/2609
6	T	0.40	0/1932	0.68	0/2609
7	G	0.39	0/1945	0.67	0/2634
7	U	0.39	0/1945	0.67	0/2634
8	H	0.35	0/1750	0.65	0/2373
8	V	0.35	0/1750	0.65	0/2373
9	I	0.36	0/1611	0.80	4/2174 (0.2%)
9	W	0.35	0/1611	0.79	3/2174 (0.1%)
10	J	0.37	0/1589	0.65	0/2142
10	X	0.38	0/1589	0.65	0/2142
11	K	0.41	1/1668 (0.1%)	0.87	7/2253 (0.3%)
11	Y	0.42	1/1668 (0.1%)	0.87	9/2253 (0.4%)
12	L	0.39	0/1802	0.67	0/2430
12	Z	0.39	0/1802	0.67	0/2430
13	M	0.37	0/1855	0.67	0/2514
13	a	0.37	0/1855	0.67	0/2514
14	N	0.35	0/1541	0.67	0/2087
14	b	0.35	0/1541	0.67	0/2087
All	All	0.39	2/50252 (0.0%)	0.70	31/67940 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	Y	1	THR	CB-OG1	-6.22	1.33	1.43
11	K	1	THR	CB-OG1	-5.49	1.34	1.43

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	W	126	ILE	CG1-CB-CG2	-13.96	68.83	110.70
9	I	126	ILE	CG1-CB-CG2	-11.72	75.54	110.70
11	Y	61	ARG	NE-CZ-NH2	-11.62	108.75	119.20
11	K	61	ARG	NE-CZ-NH1	-11.36	110.14	121.50
11	K	61	ARG	NE-CZ-NH2	11.05	129.15	119.20
2	P	113	ARG	NE-CZ-NH2	10.90	129.01	119.20
9	I	126	ILE	CA-CB-CG1	10.72	128.63	110.40
9	W	126	ILE	CA-CB-CG1	10.29	127.90	110.40
11	Y	61	ARG	CD-NE-CZ	9.97	138.36	124.40
11	Y	59	LEU	CD1-CG-CD2	-9.75	89.35	110.80
11	K	59	LEU	CD1-CG-CD2	-9.27	90.40	110.80
11	K	61	ARG	CD-NE-CZ	8.59	136.42	124.40
2	B	113	ARG	NE-CZ-NH2	8.18	126.56	119.20
2	B	113	ARG	NH1-CZ-NH2	-7.98	108.93	119.30
11	Y	61	ARG	NE-CZ-NH1	7.92	129.42	121.50
2	P	113	ARG	NH1-CZ-NH2	-7.47	109.58	119.30
11	Y	61	ARG	CG-CD-NE	-7.32	95.90	112.00
9	I	126	ILE	N-CA-C	6.81	118.70	112.43
2	P	93	HIS	N-CA-C	5.64	117.11	111.07
3	Q	201	VAL	N-CA-C	5.51	116.24	110.62
9	W	126	ILE	CB-CA-C	5.48	120.28	111.29
9	I	126	ILE	CB-CG1-CD1	-5.45	102.35	113.80
3	C	201	VAL	N-CA-C	5.45	116.18	110.62
11	Y	31	VAL	N-CA-C	5.44	117.06	109.55
11	Y	1	THR	N-CA-C	5.31	125.86	111.00
11	Y	1	THR	CA-CB-CG2	5.30	119.51	110.50
11	K	31	VAL	N-CA-C	5.29	116.85	109.55
11	K	1	THR	CA-CB-CG2	5.26	119.44	110.50
11	K	1	THR	N-CA-C	5.21	125.58	111.00
11	Y	1	THR	CB-CA-C	-5.20	97.67	109.10
2	B	93	HIS	N-CA-C	5.06	116.48	111.07

There are no chirality outliers.

There are no planarity outliers.

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	1929	0	0
1	O	1915	0	1929	1	0
2	B	1904	0	1904	14	0
2	P	1904	0	1904	16	0
3	C	1881	0	1895	6	0
3	Q	1881	0	1895	7	0
4	D	1813	0	1797	0	0
4	R	1813	0	1797	0	0
5	E	1773	0	1775	1	0
5	S	1773	0	1775	2	0
6	F	1892	0	1883	0	0
6	T	1892	0	1883	1	0
7	G	1907	0	1901	3	0
7	U	1907	0	1901	4	0
8	H	1719	0	1719	4	0
8	V	1719	0	1719	3	0
9	I	1581	0	1574	7	0
9	W	1581	0	1574	9	0
10	J	1561	0	1569	10	0
10	X	1561	0	1569	10	0
11	K	1632	0	1590	13	0
11	Y	1632	0	1590	15	0
12	L	1764	0	1716	3	0
12	Z	1764	0	1716	4	0
13	M	1824	0	1832	2	0
13	a	1824	0	1832	2	0
14	N	1512	0	1481	6	0
14	b	1512	0	1481	5	0
15	A	1	0	0	0	0
15	G	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	K	2	0	0	0	0
15	L	1	0	0	0	0
15	N	1	0	0	0	0
15	Z	1	0	0	0	0
15	b	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	G	1	0	0	0	0
16	U	1	0	0	0	0
17	H	12	0	13	0	0
17	K	12	0	13	1	0
17	V	12	0	13	0	0
17	Y	12	0	13	0	0
18	K	45	0	0	2	0
18	Y	45	0	0	4	0
19	A	6	0	0	0	0
19	B	7	0	0	0	0
19	C	6	0	0	0	0
19	D	4	0	0	0	0
19	E	5	0	0	0	0
19	F	12	0	0	0	0
19	G	11	0	0	0	0
19	H	15	0	0	0	0
19	I	11	0	0	0	0
19	J	9	0	0	0	0
19	K	8	0	0	0	0
19	L	14	0	0	0	0
19	M	18	0	0	1	0
19	N	8	0	0	0	0
19	O	8	0	0	0	0
19	P	10	0	0	1	0
19	Q	6	0	0	0	0
19	R	8	0	0	0	0
19	S	4	0	0	0	0
19	T	8	0	0	0	0
19	U	20	0	0	0	0
19	V	11	0	0	0	0
19	W	12	0	0	0	0
19	X	10	0	0	0	0
19	Y	10	0	0	1	0
19	Z	7	0	0	0	0
19	a	12	0	0	0	0
19	b	9	0	0	0	0
All	All	49776	0	49182	137	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 1.

All (137) 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)
2:B:93:HIS:HE1	2:B:113:ARG:NH1	1.11	1.47
2:B:93:HIS:CE1	2:B:113:ARG:NH1	1.84	1.46
2:P:93:HIS:CE1	2:P:113:ARG:NH1	2.10	1.20
2:P:93:HIS:CE1	2:P:113:ARG:CZ	2.25	1.19
2:P:93:HIS:HE1	2:P:113:ARG:NH1	1.48	1.07
2:B:93:HIS:CE1	2:B:113:ARG:CZ	2.39	1.04
2:P:93:HIS:HE1	2:P:113:ARG:CZ	1.73	0.94
2:B:93:HIS:HE1	2:B:113:ARG:HH12	1.16	0.91
2:B:93:HIS:CE1	2:B:113:ARG:HH11	1.87	0.91
2:P:93:HIS:NE2	2:P:113:ARG:CZ	2.40	0.84
2:B:93:HIS:NE2	2:B:113:ARG:HD3	1.95	0.81
9:I:98:ARG:HD2	9:I:126:ILE:HD12	1.63	0.81
2:B:93:HIS:NE2	2:B:113:ARG:CZ	2.48	0.77
2:P:93:HIS:CE1	2:P:113:ARG:NH2	2.52	0.76
2:P:93:HIS:NE2	2:P:113:ARG:NE	2.37	0.73
2:P:93:HIS:HE1	2:P:113:ARG:NH2	1.86	0.72
2:B:93:HIS:NE2	2:B:113:ARG:CD	2.54	0.70
9:W:98:ARG:HD2	9:W:126:ILE:HD12	1.75	0.68
2:B:93:HIS:NE2	2:B:113:ARG:NH1	2.40	0.68
9:W:98:ARG:HD2	9:W:126:ILE:CD1	2.25	0.66
2:B:93:HIS:NE2	2:B:113:ARG:NE	2.47	0.63
10:J:139:TYR:OH	10:X:25:ILE:O	2.17	0.63
10:J:25:ILE:O	10:X:139:TYR:OH	2.16	0.62
2:P:93:HIS:NE2	2:P:113:ARG:CD	2.64	0.60
2:P:93:HIS:CE1	19:P:301:HOH:O	2.56	0.58
9:I:38:LYS:NZ	11:Y:208:ASN:O	2.38	0.56
2:P:93:HIS:NE2	2:P:113:ARG:HD3	2.21	0.56
11:K:208:ASN:O	9:W:38:LYS:NZ	2.39	0.56
11:Y:59:LEU:HD23	11:Y:63:CYS:SG	2.46	0.55
11:Y:44:THR:HG21	11:Y:100:MET:HE2	1.87	0.55
11:K:44:THR:HG21	11:K:100:MET:HE2	1.87	0.55
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.90	0.54
11:K:61:ARG:O	11:K:65:ILE:HG13	2.08	0.53
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.90	0.53
11:Y:61:ARG:O	11:Y:65:ILE:HG13	2.08	0.53
14:N:152:VAL:HA	14:N:175:MET:HE1	1.91	0.53
10:X:126:VAL:HG12	10:X:128:LEU:HG	1.90	0.53
14:b:152:VAL:HA	14:b:175:MET:HE1	1.90	0.53
11:Y:59:LEU:HD12	11:Y:83:LEU:HG	1.90	0.52
10:X:58:GLU:OE1	11:Y:81:LYS:NZ	2.43	0.52
10:J:126:VAL:HG12	10:J:128:LEU:HG	1.90	0.52
18:K:301:6N5:N28	18:K:301:6N5:C59	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Y:301:6N5:C46	18:Y:301:6N5:C59	2.87	0.52
10:J:58:GLU:OE1	11:K:81:LYS:NZ	2.43	0.52
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.76	0.51
18:Y:301:6N5:N25	18:Y:301:6N5:C48	2.73	0.51
3:C:201:VAL:O	3:C:202:GLN:CB	2.59	0.51
18:K:301:6N5:C48	18:K:301:6N5:N25	2.72	0.50
7:U:23:PHE:O	7:U:26:THR:HB	2.11	0.50
10:J:50:ALA:O	11:K:91:LYS:NZ	2.43	0.50
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.59	0.50
9:I:98:ARG:CD	9:I:126:ILE:HD12	2.38	0.50
10:J:1:MET:HG2	10:J:34:LYS:HE3	1.93	0.50
7:G:23:PHE:O	7:G:26:THR:HB	2.11	0.50
11:Y:59:LEU:HD12	11:Y:83:LEU:HB2	1.93	0.50
2:B:50:LYS:O	2:B:51:VAL:C	2.55	0.50
10:X:1:MET:HG2	10:X:34:LYS:HE3	1.93	0.50
2:P:50:LYS:O	2:P:51:VAL:C	2.54	0.50
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.75	0.50
3:C:201:VAL:O	3:C:202:GLN:HB3	2.13	0.49
11:Y:12:VAL:HG13	11:Y:179:VAL:HB	1.94	0.49
9:W:125:LEU:HD23	9:W:126:ILE:HG22	1.94	0.49
3:Q:201:VAL:O	3:Q:202:GLN:HB3	2.13	0.48
11:K:18:SER:O	11:K:31:VAL:HG22	2.14	0.48
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.44	0.48
11:K:12:VAL:HG13	11:K:179:VAL:HB	1.94	0.47
13:M:2:GLN:NE2	19:M:301:HOH:O	2.46	0.47
14:b:83:LYS:HG3	14:b:119:VAL:CG2	2.44	0.47
2:P:93:HIS:HE1	2:P:113:ARG:HH12	1.50	0.47
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.98	0.46
10:J:29:LYS:HD2	11:K:121:ILE:CG2	2.46	0.46
12:L:100:ARG:HD3	12:L:105:TYR:CE2	2.51	0.46
10:X:50:ALA:O	11:Y:91:LYS:NZ	2.49	0.46
12:Z:100:ARG:HD3	12:Z:105:TYR:CE2	2.51	0.45
3:C:51:LYS:O	3:C:52:LEU:HB2	2.16	0.45
11:Y:35:ILE:HB	11:Y:45:MET:HE3	1.98	0.45
14:b:176:VAL:HG12	14:b:178:LEU:HD13	1.99	0.45
11:Y:33:LYS:HG2	18:Y:301:6N5:C1	2.46	0.45
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.16	0.45
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.98	0.45
11:K:35:ILE:HB	11:K:45:MET:HE3	1.97	0.44
8:V:35:HIS:HB3	8:V:56:THR:HG21	2.00	0.44
9:I:20:VAL:HG23	9:I:189:ILE:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:33:LYS:HE2	18:Y:301:6N5:C6	2.48	0.44
3:C:35:LYS:HG2	3:C:158:SER:O	2.18	0.44
8:H:35:HIS:HB3	8:H:56:THR:HG21	2.00	0.44
11:K:98:GLY:HA3	17:K:304:MES:H62	1.98	0.44
10:X:3:ILE:HG23	10:X:18:SER:HB3	2.00	0.44
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.99	0.43
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.19	0.43
9:W:20:VAL:HG23	9:W:189:ILE:HB	2.00	0.43
10:J:3:ILE:HG23	10:J:18:SER:HB3	2.00	0.43
12:L:8:ASN:HA	12:L:30:ILE:O	2.19	0.43
9:W:10:ILE:HG21	9:W:141:ALA:HB3	2.01	0.43
9:I:10:ILE:HG21	9:I:141:ALA:HB3	2.01	0.42
2:P:145:TYR:OH	2:P:217:LYS:N	2.52	0.42
9:W:98:ARG:CD	9:W:126:ILE:CD1	2.95	0.42
2:B:50:LYS:HD3	2:B:50:LYS:HA	1.96	0.42
11:K:104:TRP:CE2	11:K:181:GLU:HB3	2.54	0.42
2:B:145:TYR:OH	2:B:217:LYS:N	2.53	0.42
3:C:169:VAL:HG23	3:C:196:SER:HB2	2.01	0.42
7:G:78:ILE:N	7:G:79:PRO:CD	2.83	0.42
11:Y:59:LEU:CD2	11:Y:63:CYS:SG	3.08	0.42
14:b:36:ARG:HG3	14:b:42:TRP:CE2	2.55	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.83	0.42
11:Y:208:ASN:ND2	19:Y:401:HOH:O	2.52	0.42
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	2.01	0.42
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.54	0.42
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.50	0.42
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.02	0.41
8:H:196:ARG:NH2	9:I:150:GLU:O	2.54	0.41
14:N:133:PHE:HA	14:b:132:THR:O	2.20	0.41
10:J:5:LEU:HD23	10:J:132:ALA:HB2	2.02	0.41
5:S:77:ALA:N	5:S:78:PRO:CD	2.84	0.41
8:V:35:HIS:CB	8:V:56:THR:HG21	2.51	0.41
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.55	0.41
5:E:77:ALA:N	5:E:78:PRO:CD	2.84	0.41
8:H:35:HIS:CB	8:H:56:THR:HG21	2.51	0.41
11:K:100:MET:HE2	11:K:100:MET:HB2	1.98	0.41
11:Y:104:TRP:CE2	11:Y:181:GLU:HB3	2.54	0.41
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.03	0.41
10:X:5:LEU:HD23	10:X:132:ALA:HB2	2.02	0.41
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.50	0.41
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:165:ILE:HB	13:a:166:PRO:HD3	2.03	0.41
9:I:163:PHE:CE1	9:I:197:ARG:HD2	2.56	0.41
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.20	0.41
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.56	0.41
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.52	0.40
14:N:35:THR:HG21	13:a:228:TYR:HE2	1.86	0.40
5:S:12:PHE:H	6:T:19:GLN:HE22	1.68	0.40
9:W:98:ARG:CD	9:W:126:ILE:HD11	2.50	0.40
9:W:98:ARG:CZ	9:W:126:ILE:HD11	2.52	0.40
2:P:93:HIS:NE2	2:P:113:ARG:NH1	2.59	0.40
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.52	0.40
11:K:204:GLY:C	10:X:149:ARG:HH22	2.28	0.40
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.86	0.40

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%)	240 (97%)	7 (3%)	1 (0%)	30	60
1	O	248/250 (99%)	240 (97%)	7 (3%)	1 (0%)	30	60
2	B	242/258 (94%)	232 (96%)	7 (3%)	3 (1%)	10	34
2	P	242/258 (94%)	232 (96%)	7 (3%)	3 (1%)	10	34
3	C	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	16	44
3	Q	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	16	44
4	D	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
4	R	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
5	E	229/234 (98%)	221 (96%)	8 (4%)	0	100	100
5	S	229/234 (98%)	222 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	241/288 (84%)	239 (99%)	2 (1%)	0	100	100
6	T	241/288 (84%)	239 (99%)	2 (1%)	0	100	100
7	G	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
7	U	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
8	H	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
8	V	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	194 (96%)	8 (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	209/211 (99%)	203 (97%)	6 (3%)	0	100	100
11	Y	209/211 (99%)	203 (97%)	6 (3%)	0	100	100
12	L	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
12	Z	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
13	M	231/246 (94%)	221 (96%)	10 (4%)	0	100	100
13	a	231/246 (94%)	221 (96%)	10 (4%)	0	100	100
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	b	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
All	All	6282/6612 (95%)	6117 (97%)	153 (2%)	12 (0%)	43	72

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN
2	P	51	VAL
3	Q	202	GLN
1	A	2	THR
2	B	218	GLY
2	B	222	GLY
1	O	2	THR
2	P	218	GLY
2	P	222	GLY
3	C	205	ALA
3	Q	205	ALA

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%)	205 (98%)	4 (2%)	50	81
1	O	209/209 (100%)	205 (98%)	4 (2%)	50	81
2	B	203/216 (94%)	197 (97%)	6 (3%)	36	72
2	P	203/216 (94%)	197 (97%)	6 (3%)	36	72
3	C	212/226 (94%)	203 (96%)	9 (4%)	26	61
3	Q	212/226 (94%)	203 (96%)	9 (4%)	26	61
4	D	194/215 (90%)	186 (96%)	8 (4%)	27	62
4	R	194/215 (90%)	186 (96%)	8 (4%)	27	62
5	E	190/193 (98%)	185 (97%)	5 (3%)	40	75
5	S	190/193 (98%)	185 (97%)	5 (3%)	40	75
6	F	201/239 (84%)	196 (98%)	5 (2%)	42	76
6	T	201/239 (84%)	196 (98%)	5 (2%)	42	76
7	G	206/210 (98%)	200 (97%)	6 (3%)	37	73
7	U	206/210 (98%)	200 (97%)	6 (3%)	37	73
8	H	185/190 (97%)	182 (98%)	3 (2%)	55	83
8	V	185/190 (97%)	182 (98%)	3 (2%)	55	83
9	I	172/173 (99%)	169 (98%)	3 (2%)	53	83
9	W	172/173 (99%)	169 (98%)	3 (2%)	53	83
10	J	173/175 (99%)	169 (98%)	4 (2%)	44	78
10	X	173/175 (99%)	169 (98%)	4 (2%)	44	78
11	K	165/165 (100%)	152 (92%)	13 (8%)	11	35
11	Y	165/165 (100%)	152 (92%)	13 (8%)	11	35
12	L	186/186 (100%)	182 (98%)	4 (2%)	45	78
12	Z	186/186 (100%)	181 (97%)	5 (3%)	39	74
13	M	199/208 (96%)	195 (98%)	4 (2%)	48	80
13	a	199/208 (96%)	195 (98%)	4 (2%)	48	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	162/162 (100%)	160 (99%)	2 (1%)	63	87
14	b	162/162 (100%)	160 (99%)	2 (1%)	63	87
All	All	5314/5534 (96%)	5161 (97%)	153 (3%)	37	73

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
2	B	55	LEU
2	B	79	LEU
2	B	93	HIS
2	B	102	ASN
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	51	LYS
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	213	VAL
3	C	240	GLU
4	D	99	ILE
4	D	125	LEU
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	29	LYS
5	E	55	LEU
5	E	71	LEU
5	E	188	LEU
6	F	123	ASN
6	F	171	GLU

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Mol	Chain	Res	Type
6	F	172	LEU
6	F	181	GLU
6	F	240	GLN
7	G	26	THR
7	G	115	LEU
7	G	122	ARG
7	G	125	MET
7	G	235	ARG
7	G	236	LEU
8	H	34	LEU
8	H	68	LEU
8	H	196	ARG
9	I	37	ASN
9	I	126	ILE
9	I	171	LEU
10	J	1	MET
10	J	3	ILE
10	J	23	ARG
10	J	99	GLN
11	K	4	LEU
11	K	12	VAL
11	K	29	GLN
11	K	35	ILE
11	K	58	LEU
11	K	61	ARG
11	K	62	GLN
11	K	81	LYS
11	K	83	LEU
11	K	86	MET
11	K	100	MET
11	K	128	VAL
11	K	210	ILE
12	L	23	LEU
12	L	49	ASN
12	L	136	CYS
12	L	150	LEU
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
14	N	9	LYS
14	N	178	LEU

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Mol	Chain	Res	Type
1	O	1	MET
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	55	LEU
2	P	79	LEU
2	P	93	HIS
2	P	102	ASN
2	P	191	LEU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	51	LYS
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	213	VAL
3	Q	240	GLU
4	R	99	ILE
4	R	125	LEU
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	55	LEU
5	S	71	LEU
5	S	188	LEU
6	T	123	ASN
6	T	171	GLU
6	T	172	LEU
6	T	181	GLU
6	T	240	GLN
7	U	26	THR
7	U	115	LEU
7	U	122	ARG
7	U	125	MET
7	U	235	ARG

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Mol	Chain	Res	Type
7	U	236	LEU
8	V	34	LEU
8	V	68	LEU
8	V	196	ARG
9	W	37	ASN
9	W	126	ILE
9	W	171	LEU
10	X	1	MET
10	X	3	ILE
10	X	23	ARG
10	X	99	GLN
11	Y	4	LEU
11	Y	12	VAL
11	Y	29	GLN
11	Y	31	VAL
11	Y	35	ILE
11	Y	58	LEU
11	Y	62	GLN
11	Y	81	LYS
11	Y	83	LEU
11	Y	86	MET
11	Y	100	MET
11	Y	128	VAL
11	Y	210	ILE
12	Z	18	GLU
12	Z	23	LEU
12	Z	49	ASN
12	Z	136	CYS
12	Z	150	LEU
13	a	2	GLN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
14	b	9	LYS
14	b	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	119	GLN
2	B	123	GLN
2	B	124	HIS

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Mol	Chain	Res	Type
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	91	HIS
4	D	100	ASN
4	D	106	GLN
4	D	180	HIS
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	151	ASN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	123	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	175	ASN
9	I	63	ASN
9	I	88	GLN
9	I	203	GLN
10	J	10	GLN
10	J	55	GLN
10	J	63	ASN
10	J	78	GLN
11	K	85	ASN
11	K	142	ASN
12	L	29	ASN
12	L	36	ASN
12	L	49	ASN
12	L	70	ASN
12	L	79	HIS
12	L	158	ASN
12	L	197	GLN
13	M	48	ASN

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Mol	Chain	Res	Type
13	M	62	HIS
13	M	108	ASN
13	M	149	HIS
14	N	38	HIS
14	N	141	ASN
2	P	124	HIS
2	P	220	ASN
3	Q	17	GLN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
4	R	180	HIS
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	120	GLN
5	S	151	ASN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	123	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
8	V	35	HIS
8	V	66	HIS
9	W	63	ASN
9	W	88	GLN
9	W	203	GLN
10	X	10	GLN
10	X	55	GLN
10	X	63	ASN
11	Y	85	ASN
11	Y	142	ASN
12	Z	3	ASN
12	Z	29	ASN
12	Z	36	ASN

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Mol	Chain	Res	Type
12	Z	49	ASN
12	Z	70	ASN
12	Z	158	ASN
12	Z	197	GLN
13	a	48	ASN
13	a	62	HIS
13	a	108	ASN
13	a	149	HIS
14	b	38	HIS
14	b	141	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 19 ligands modelled in this entry, 13 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
18	6N5	Y	301	11	47,48,48	2.11	11 (23%)	55,66,66	1.83	13 (23%)
17	MES	V	301	-	12,12,12	2.37	1 (8%)	15,16,16	1.01	1 (6%)
17	MES	H	301	-	12,12,12	2.21	1 (8%)	15,16,16	1.09	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	MES	Y	302	-	12,12,12	2.31	1 (8%)	15,16,16	1.04	0
17	MES	K	304	-	12,12,12	2.36	1 (8%)	15,16,16	1.05	0
18	6N5	K	301	11	47,48,48	2.14	12 (25%)	55,66,66	1.91	10 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	6N5	Y	301	11	-	12/44/67/67	0/4/4/4
17	MES	V	301	-	-	1/6/14/14	0/1/1/1
17	MES	H	301	-	-	1/6/14/14	0/1/1/1
17	MES	Y	302	-	-	0/6/14/14	0/1/1/1
17	MES	K	304	-	-	0/6/14/14	0/1/1/1
18	6N5	K	301	11	-	13/44/67/67	0/4/4/4

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	304	MES	C8-S	-7.91	1.66	1.77
17	V	301	MES	C8-S	-7.84	1.66	1.77
17	Y	302	MES	C8-S	-7.72	1.66	1.77
17	H	301	MES	C8-S	-7.31	1.67	1.77
18	K	301	6N5	C40-C41	-6.30	1.36	1.51
18	Y	301	6N5	C7-C6	-5.91	1.37	1.51
18	K	301	6N5	C50-C60	-5.66	1.33	1.49
18	Y	301	6N5	C40-C41	-5.48	1.38	1.51
18	K	301	6N5	C7-C6	-5.22	1.39	1.51
18	Y	301	6N5	C50-C60	-5.15	1.34	1.49
18	Y	301	6N5	C57-C52	-5.02	1.31	1.47
18	K	301	6N5	C57-C52	-4.93	1.32	1.47
18	Y	301	6N5	C10-C9	3.89	1.60	1.53
18	K	301	6N5	C56-C57	-3.55	1.32	1.40
18	Y	301	6N5	C56-C57	-3.51	1.32	1.40
18	K	301	6N5	C54-C53	-3.32	1.38	1.49
18	Y	301	6N5	C54-C53	-3.31	1.38	1.49
18	K	301	6N5	O21-C9	-3.05	1.35	1.43
18	Y	301	6N5	C57-C58	-2.80	1.31	1.37
18	K	301	6N5	C50-C58	-2.77	1.31	1.41
18	Y	301	6N5	C50-C58	-2.73	1.32	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	K	301	6N5	C57-C58	-2.70	1.31	1.37
18	K	301	6N5	C10-C9	2.44	1.57	1.53
18	K	301	6N5	C54-C55	-2.32	1.36	1.47
18	Y	301	6N5	O21-C9	-2.25	1.37	1.43
18	K	301	6N5	C27-C26	-2.24	1.47	1.52
18	Y	301	6N5	C54-C55	-2.17	1.37	1.47

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	K	301	6N5	C7-C8-N22	-8.22	98.41	110.08
18	Y	301	6N5	C7-C8-N22	-5.87	101.74	110.08
18	K	301	6N5	C50-C51-C52	-5.25	104.24	109.72
18	Y	301	6N5	C46-O45-C44	-4.92	106.95	117.50
18	K	301	6N5	C46-O45-C44	-4.15	108.60	117.50
18	Y	301	6N5	C50-C51-C52	-4.09	105.45	109.72
18	Y	301	6N5	C50-C58-C57	4.07	110.88	107.98
18	K	301	6N5	C50-C58-C57	3.65	110.58	107.98
18	Y	301	6N5	C50-C60-N28	3.52	120.83	116.25
18	K	301	6N5	C56-C57-C58	-2.62	130.72	134.07
18	Y	301	6N5	O21-C9-C10	2.59	114.74	109.79
18	Y	301	6N5	C56-C57-C58	-2.51	130.87	134.07
18	Y	301	6N5	C59-C58-C57	-2.49	122.40	128.43
18	K	301	6N5	C41-C40-C24	-2.47	106.78	113.36
18	Y	301	6N5	C7-C6-C1	-2.40	116.43	120.90
18	K	301	6N5	O21-C9-C8	-2.30	103.77	109.28
18	K	301	6N5	C59-C58-C57	-2.27	122.94	128.43
18	K	301	6N5	C50-C60-N28	2.24	119.16	116.25
18	Y	301	6N5	C38-C27-C26	-2.22	105.93	110.14
18	Y	301	6N5	C41-C40-C24	-2.20	107.50	113.36
18	K	301	6N5	C26-C27-N28	-2.17	106.22	111.59
17	H	301	MES	O3S-S-C8	2.13	110.17	106.00
18	Y	301	6N5	C6-C7-C8	2.10	116.96	113.40
18	Y	301	6N5	O21-C9-C8	-2.01	104.47	109.28
17	V	301	MES	O2S-S-C8	2.01	109.76	106.73

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	H	301	MES	N4-C7-C8-S
17	V	301	MES	C8-C7-N4-C5

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Mol	Chain	Res	Type	Atoms
18	K	301	6N5	C9-C10-C12-O13
18	K	301	6N5	C11-C10-C12-O13
18	Y	301	6N5	C11-C10-C9-C8
18	Y	301	6N5	C12-C10-C9-C8
18	Y	301	6N5	C9-C10-C12-O13
18	Y	301	6N5	C11-C10-C12-O13
18	K	301	6N5	C47-C44-O45-C46
18	K	301	6N5	C43-C44-O45-C46
18	Y	301	6N5	C47-C44-O45-C46
18	Y	301	6N5	C43-C44-O45-C46
18	Y	301	6N5	C5-C6-C7-C8
18	Y	301	6N5	C1-C6-C7-C8
18	K	301	6N5	C5-C6-C7-C8
18	K	301	6N5	C1-C6-C7-C8
18	K	301	6N5	C11-C10-C9-C8
18	K	301	6N5	C11-C10-C9-O21
18	Y	301	6N5	C11-C10-C9-O21
18	Y	301	6N5	C12-C10-C9-O21
18	K	301	6N5	C12-C10-C9-C8
18	K	301	6N5	O49-C23-C24-N25
18	Y	301	6N5	O49-C23-C24-N25
18	K	301	6N5	C12-C10-C9-O21
18	K	301	6N5	N22-C23-C24-N25
18	Y	301	6N5	N22-C23-C24-N25
18	K	301	6N5	C6-C7-C8-N22

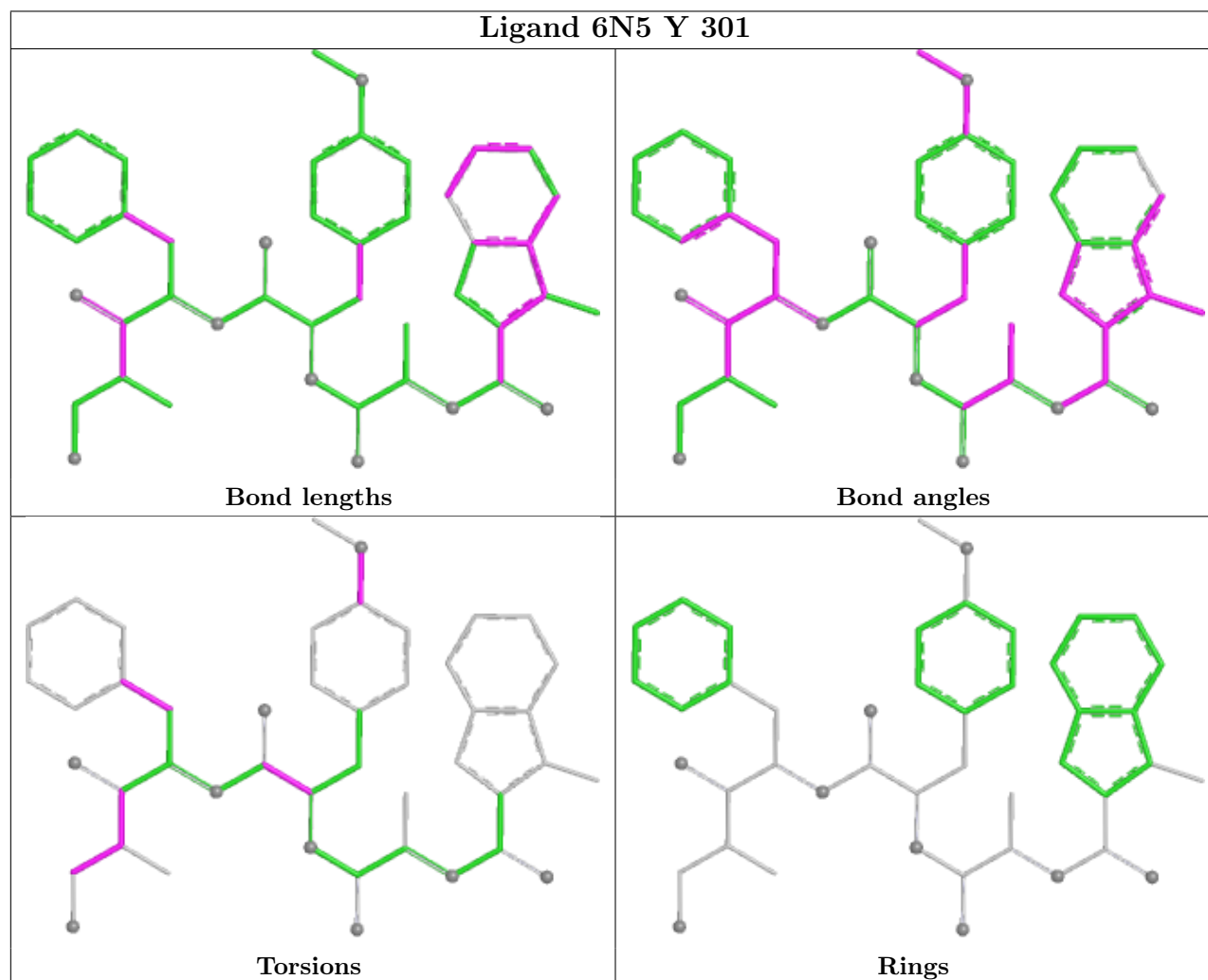
There are no ring outliers.

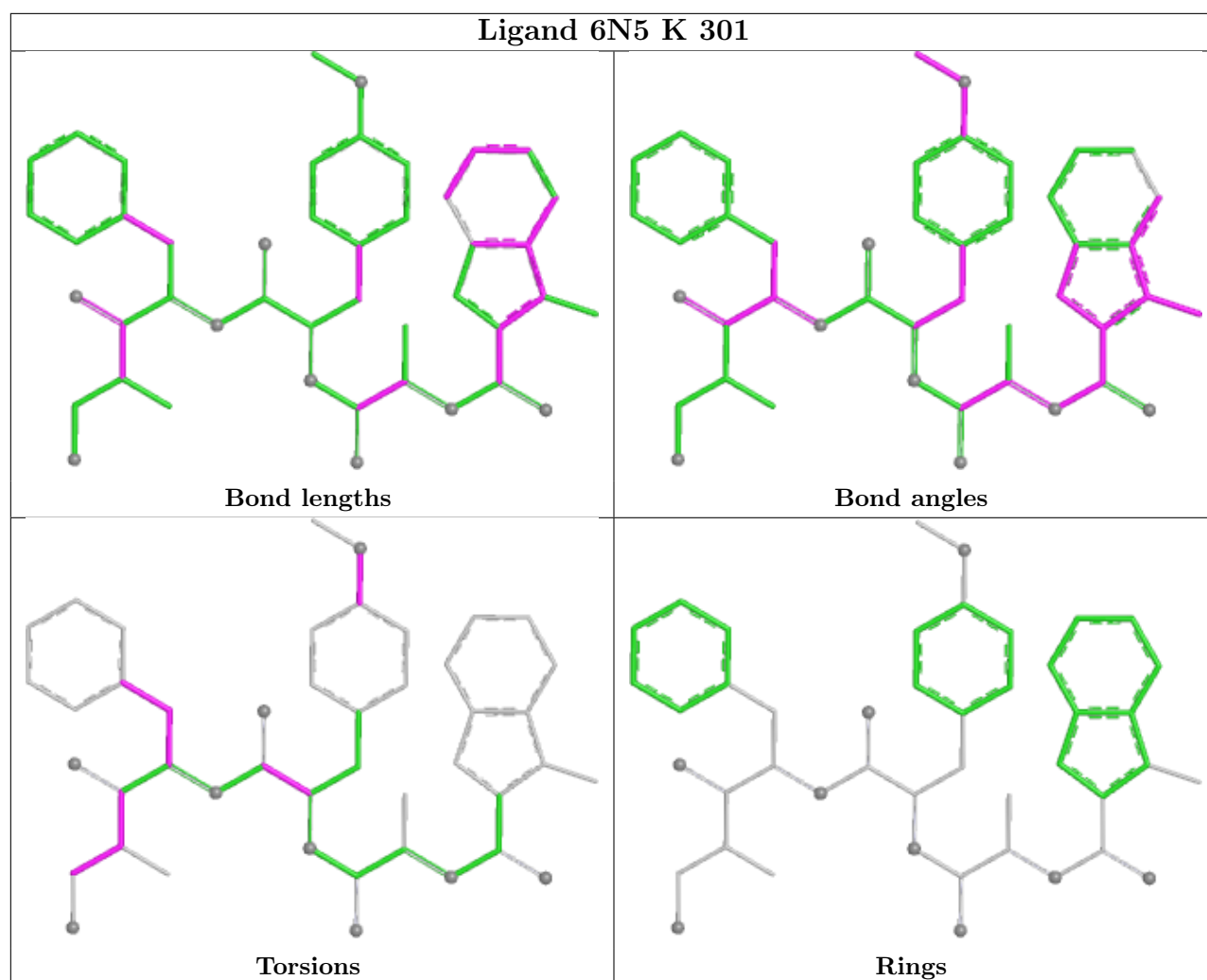
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	Y	301	6N5	4	0
17	K	304	MES	1	0
18	K	301	6N5	2	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](#)

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, 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	250/250 (100%)	-0.46	0 100 100	33, 53, 90, 127	0
1	O	250/250 (100%)	-0.39	3 (1%) 76 68	37, 55, 100, 139	0
2	B	244/258 (94%)	-0.29	6 (2%) 58 48	38, 58, 102, 156	0
2	P	244/258 (94%)	-0.34	3 (1%) 76 68	40, 58, 101, 154	0
3	C	240/254 (94%)	-0.17	6 (2%) 58 48	36, 65, 132, 168	0
3	Q	240/254 (94%)	-0.08	3 (1%) 75 66	42, 71, 150, 194	0
4	D	235/260 (90%)	-0.36	1 (0%) 88 84	40, 61, 93, 126	0
4	R	235/260 (90%)	-0.17	3 (1%) 75 66	51, 69, 110, 136	0
5	E	231/234 (98%)	-0.32	0 100 100	43, 65, 103, 150	0
5	S	231/234 (98%)	-0.21	2 (0%) 81 74	48, 70, 110, 146	0
6	F	243/288 (84%)	-0.38	2 (0%) 82 75	38, 60, 109, 137	0
6	T	243/288 (84%)	-0.31	4 (1%) 70 61	37, 65, 121, 157	0
7	G	241/252 (95%)	-0.41	0 100 100	37, 56, 98, 154	0
7	U	241/252 (95%)	-0.41	0 100 100	31, 54, 91, 130	0
8	H	226/232 (97%)	-0.40	1 (0%) 88 84	37, 53, 90, 147	0
8	V	226/232 (97%)	-0.41	2 (0%) 81 74	37, 53, 87, 155	0
9	I	204/205 (99%)	-0.56	1 (0%) 87 82	33, 50, 83, 105	0
9	W	204/205 (99%)	-0.60	1 (0%) 87 82	35, 51, 83, 106	0
10	J	195/198 (98%)	-0.49	1 (0%) 87 82	34, 55, 85, 125	0
10	X	195/198 (98%)	-0.45	1 (0%) 87 82	37, 56, 86, 133	0
11	K	211/211 (100%)	-0.36	0 100 100	35, 59, 91, 118	0
11	Y	211/211 (100%)	-0.31	0 100 100	26, 60, 90, 118	0
12	L	222/222 (100%)	-0.37	2 (0%) 81 74	42, 56, 98, 129	0
12	Z	222/222 (100%)	-0.32	2 (0%) 81 74	35, 59, 101, 131	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.45	1 (0%) 88 84	33, 54, 81, 100	0
13	a	233/246 (94%)	-0.48	2 (0%) 81 74	36, 55, 81, 108	0
14	N	196/196 (100%)	-0.55	1 (0%) 87 82	34, 50, 82, 106	0
14	b	196/196 (100%)	-0.63	0 100 100	33, 48, 81, 109	0
All	All	6342/6612 (95%)	-0.38	48 (0%) 82 75	26, 58, 102, 194	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	X	1	MET	5.9
10	J	1	MET	4.7
8	V	223	ILE	3.9
13	a	1	THR	3.7
13	a	69	ASP	3.5
8	V	224	GLN	3.2
2	B	51	VAL	3.2
6	T	243	ILE	3.2
12	Z	174	TYR	3.1
3	Q	205	ALA	3.0
3	Q	51	LYS	2.9
2	P	51	VAL	2.9
12	L	174	TYR	2.9
2	B	93	HIS	2.8
4	R	238	LYS	2.8
2	B	218	GLY	2.8
5	S	122	TYR	2.7
1	O	53	SER	2.7
3	C	51	LYS	2.7
3	Q	50	LEU	2.7
6	F	215	CYS	2.7
6	F	243	ILE	2.6
4	R	117	GLU	2.5
2	B	219	ALA	2.5
2	P	219	ALA	2.5
6	T	204	LYS	2.4
6	T	178	HIS	2.4
8	H	223	ILE	2.3
3	C	205	ALA	2.3
9	W	1	SER	2.3
1	O	249	ALA	2.3
3	C	240	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
5	S	3	ASN	2.2
12	Z	26	ASP	2.2
3	C	203	THR	2.2
9	I	1	SER	2.2
2	P	218	GLY	2.2
4	D	241	ALA	2.2
1	O	1	MET	2.2
2	B	1	GLY	2.2
4	R	241	ALA	2.2
14	N	181	ALA	2.2
13	M	233	ILE	2.1
3	C	238	LYS	2.1
12	L	136	CYS	2.0
6	T	244	ASN	2.0
3	C	58	THR	2.0
2	B	222	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
17	MES	V	301	12/12	0.80	0.21	66,73,100,101	0
17	MES	H	301	12/12	0.82	0.18	67,75,90,92	0
15	MG	A	301	1/1	0.89	0.23	52,52,52,52	0
18	6N5	K	301	45/45	0.90	0.10	33,50,66,71	0
17	MES	K	304	12/12	0.91	0.14	53,56,73,80	12
18	6N5	Y	301	45/45	0.91	0.10	24,51,65,70	0
15	MG	Z	301	1/1	0.93	0.08	71,71,71,71	0

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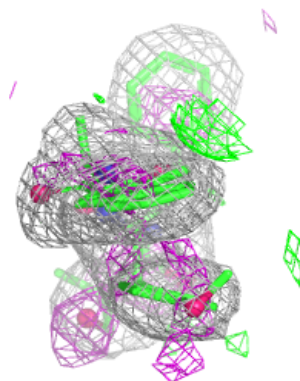
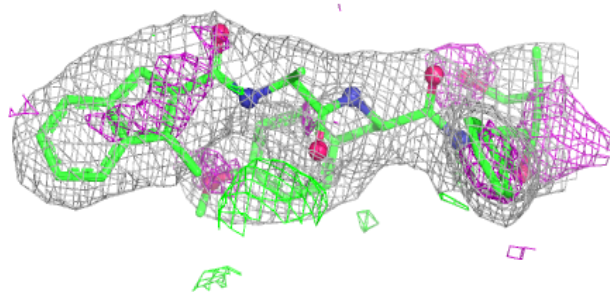
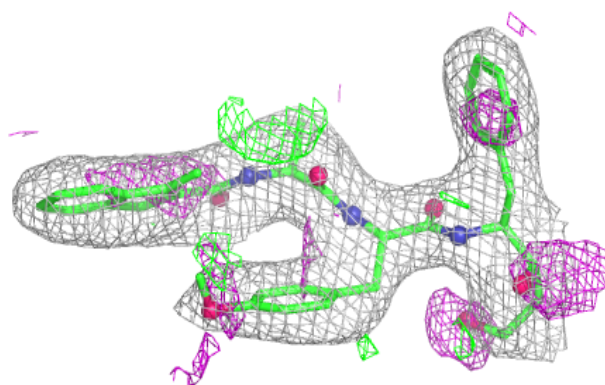
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
17	MES	Y	302	12/12	0.94	0.13	55,57,67,72	12
15	MG	K	303	1/1	0.96	0.10	57,57,57,57	0
15	MG	L	301	1/1	0.97	0.06	71,71,71,71	0
15	MG	J	201	1/1	0.98	0.09	56,56,56,56	0
16	CL	G	302	1/1	0.99	0.10	38,38,38,38	0
16	CL	U	301	1/1	0.99	0.10	40,40,40,40	0
15	MG	K	302	1/1	0.99	0.10	54,54,54,54	0
15	MG	I	301	1/1	0.99	0.05	46,46,46,46	0
15	MG	I	302	1/1	0.99	0.06	54,54,54,54	0
15	MG	N	201	1/1	0.99	0.04	55,55,55,55	0
15	MG	G	301	1/1	0.99	0.03	57,57,57,57	0
15	MG	b	201	1/1	0.99	0.02	43,43,43,43	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.

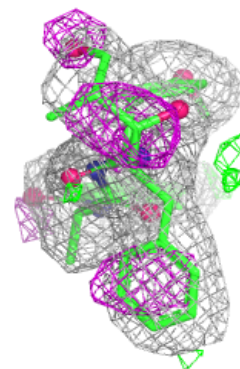
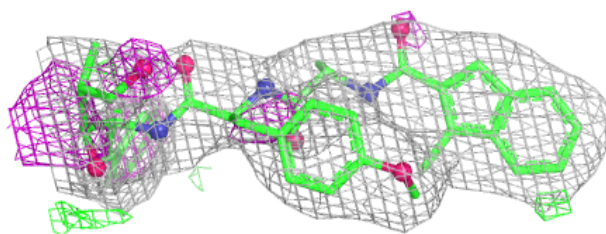
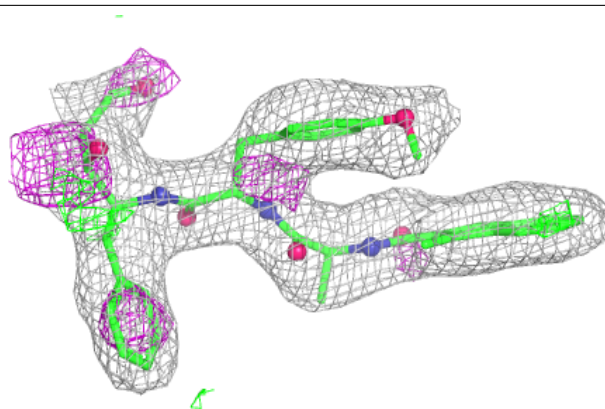
Electron density around 6N5 K 301:

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 6N5 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 [i](#)

There are no such residues in this entry.