



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 05:38 pm BST

PDB ID : 5D0T
Title : Yeast 20S proteasome beta5-D166N mutant in complex with MG132
Authors : Huber, E.M.; Groll, M.
Deposited on : 2015-08-03
Resolution : 2.60 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

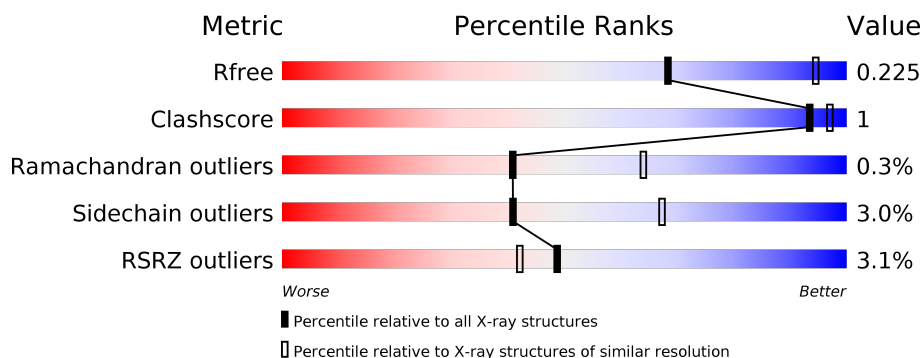
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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>3%</div> <div>98%</div> <div>•</div> </div>
1	O	250	<div> <div>4%</div> <div>98%</div> <div>•</div> </div>
2	B	258	<div> <div>4%</div> <div>91%</div> <div>• • 5%</div> </div>
2	P	258	<div> <div>4%</div> <div>91%</div> <div>• • 5%</div> </div>
3	C	254	<div> <div>7%</div> <div>87%</div> <div>6% • 6%</div> </div>
3	Q	254	<div> <div>9%</div> <div>88%</div> <div>6% • 6%</div> </div>

Continued on next page...

Continued from previous page...

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	232	
8	V	232	
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	196	
14	b	196	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 50090 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			

Continued on next page...

Continued from previous page...

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	0	0
			1644	1045	281	311	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1644	1045	281	311	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	168	ASN	ASP	engineered mutation	UNP P30656
Y	168	ASN	ASP	engineered mutation	UNP P30656

- 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	231	Total	C	N	O	S	0	0	0
			1806	1142	309	348	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			

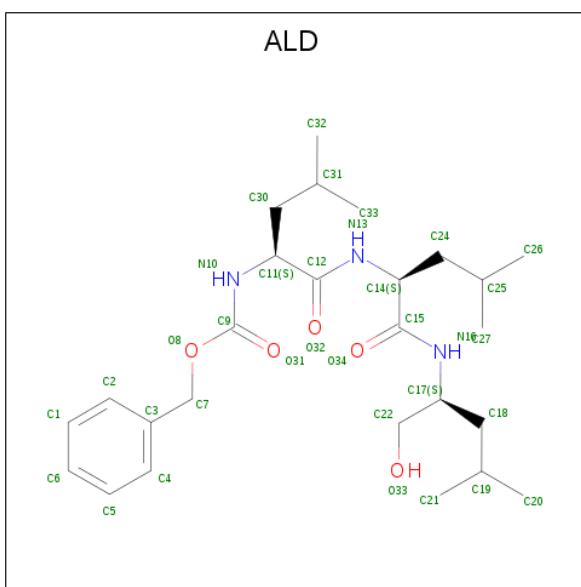
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	G	1	Total Mg 1 1	0	0
15	J	1	Total Mg 1 1	0	0
15	K	1	Total Mg 1 1	0	0
15	b	1	Total Mg 1 1	0	0
15	I	2	Total Mg 2 2	0	0
15	Z	1	Total Mg 1 1	0	0
15	N	1	Total Mg 1 1	0	0
15	X	1	Total Mg 1 1	0	0
15	L	1	Total Mg 1 1	0	0
15	M	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-[(benzyloxy)carbonyl]-L-leucyl-N-[(2S)-1-hydroxy-4-methylpentan-2-yl]-L-leucinamide (three-letter code: ALD) (formula: C₂₆H₄₃N₃O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	K	1	Total	C	N	O	0	0
			34	26	3	5		
17	N	1	Total	C	N	O	0	0
			34	26	3	5		
17	Y	1	Total	C	N	O	0	0
			34	26	3	5		
17	b	1	Total	C	N	O	0	0
			34	26	3	5		

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	16	Total	O	0	0
			16	16		
18	B	21	Total	O	0	0
			21	21		
18	C	20	Total	O	0	0
			20	20		
18	D	10	Total	O	0	0
			10	10		
18	E	10	Total	O	0	0
			10	10		
18	F	17	Total	O	0	0
			17	17		
18	G	33	Total	O	0	0
			33	33		
18	H	25	Total	O	0	0
			25	25		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	I	18	Total 18	O 18	0	0
18	J	23	Total 23	O 23	0	0
18	K	37	Total 37	O 37	0	0
18	L	25	Total 25	O 25	0	0
18	M	27	Total 27	O 27	0	0
18	N	22	Total 22	O 22	0	0
18	O	18	Total 18	O 18	0	0
18	P	13	Total 13	O 13	0	0
18	Q	11	Total 11	O 11	0	0
18	R	13	Total 13	O 13	0	0
18	S	5	Total 5	O 5	0	0
18	T	18	Total 18	O 18	0	0
18	U	22	Total 22	O 22	0	0
18	V	24	Total 24	O 24	0	0
18	W	20	Total 20	O 20	0	0
18	X	19	Total 19	O 19	0	0
18	Y	36	Total 36	O 36	0	0
18	Z	28	Total 28	O 28	0	0
18	a	36	Total 36	O 36	0	0
18	b	24	Total 24	O 24	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

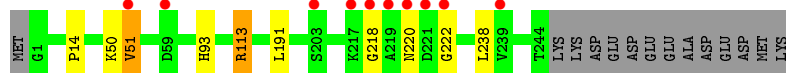
- Molecule 1: Proteasome subunit alpha type-2



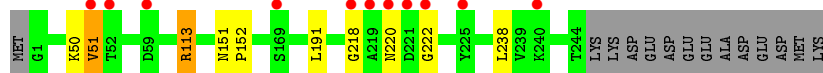
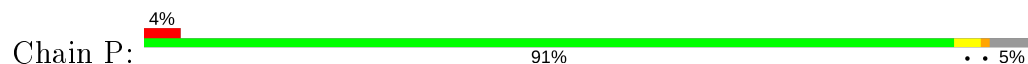
- Molecule 1: Proteasome subunit alpha type-2



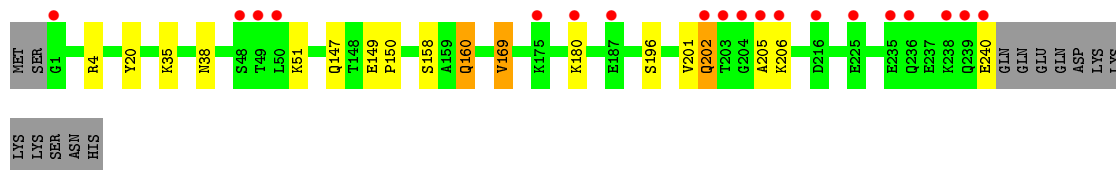
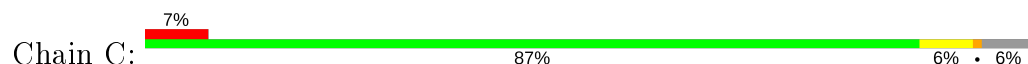
- Molecule 2: Proteasome subunit alpha type-3



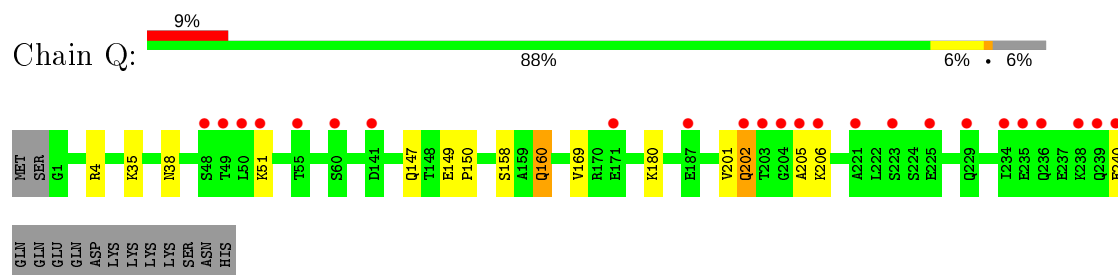
- Molecule 2: Proteasome subunit alpha type-3



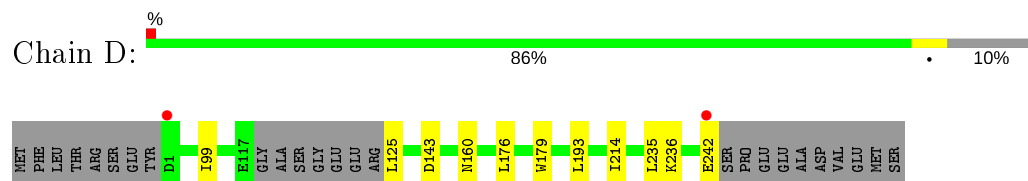
- Molecule 3: Proteasome subunit alpha type-4



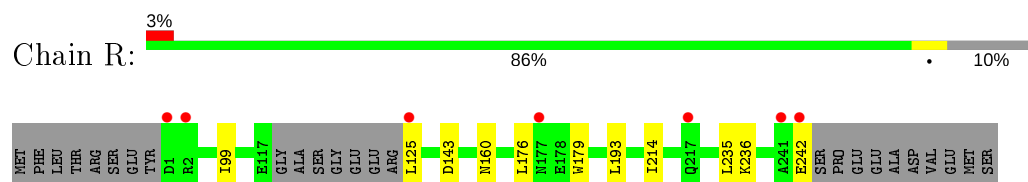
- Molecule 3: Proteasome subunit alpha type-4



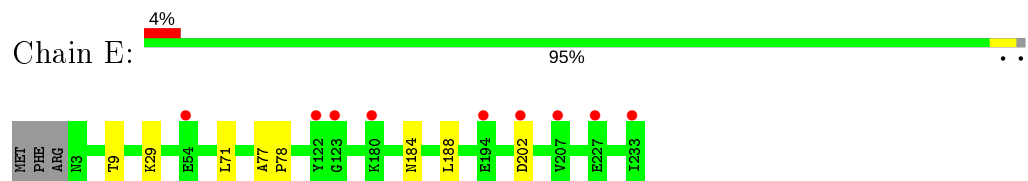
- Molecule 4: Proteasome subunit alpha type-5



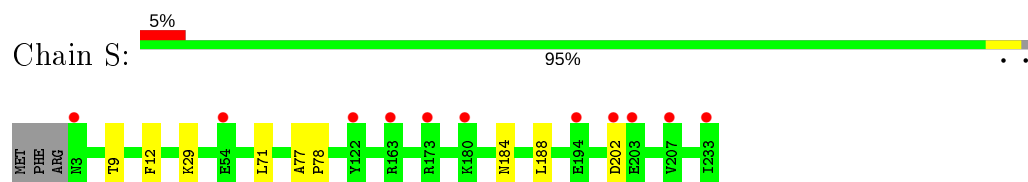
- Molecule 4: Proteasome subunit alpha type-5



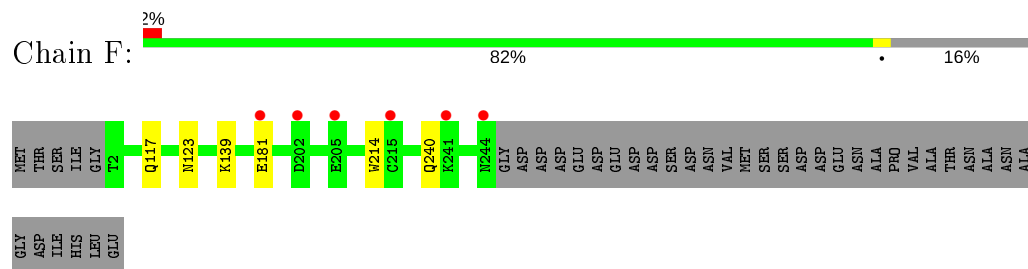
- Molecule 5: Proteasome subunit alpha type-6



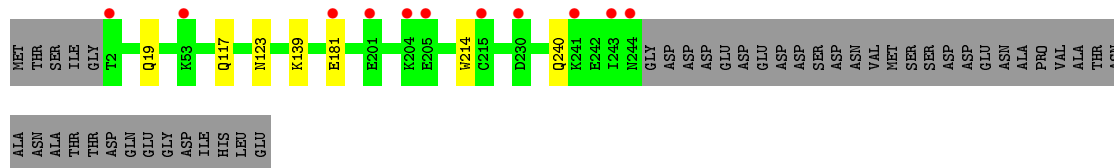
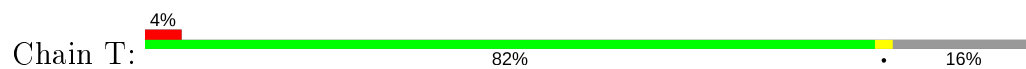
- Molecule 5: Proteasome subunit alpha type-6



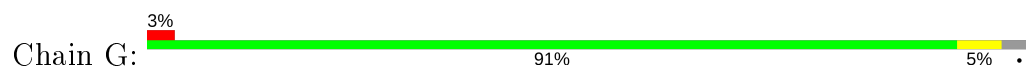
- Molecule 6: Probable proteasome subunit alpha type-7



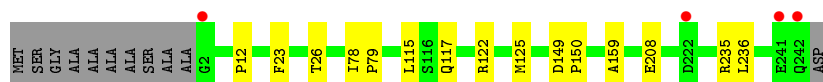
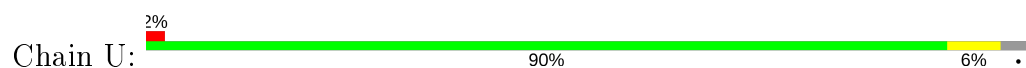
- Molecule 6: Probable proteasome subunit alpha type-7



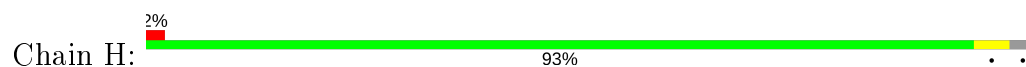
- Molecule 7: Proteasome subunit alpha type-1



- Molecule 7: Proteasome subunit alpha type-1



- Molecule 8: Proteasome subunit beta type-2



- Molecule 8: Proteasome subunit beta type-2

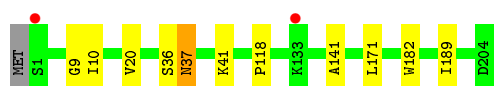


- Molecule 9: Proteasome subunit beta type-3

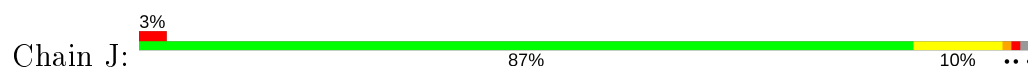


- Molecule 9: Proteasome subunit beta type-3

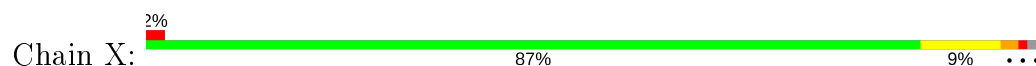




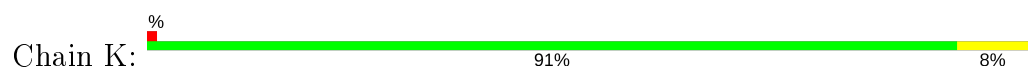
- Molecule 10: Proteasome subunit beta type-4



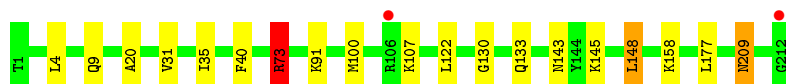
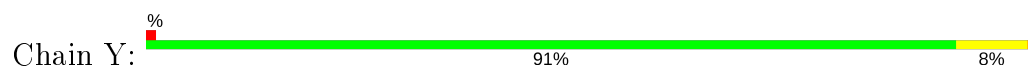
- Molecule 10: Proteasome subunit beta type-4



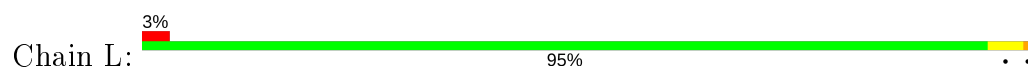
- Molecule 11: Proteasome subunit beta type-5



- Molecule 11: Proteasome subunit beta type-5



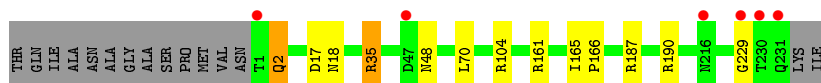
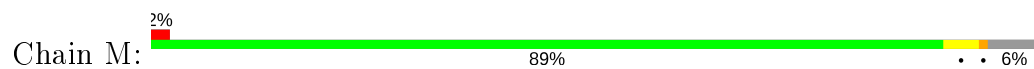
- Molecule 12: Proteasome subunit beta type-6



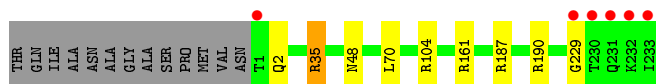
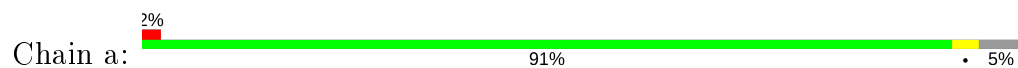
- Molecule 12: Proteasome subunit beta type-6



- Molecule 13: Proteasome subunit beta type-7



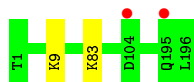
- Molecule 13: Proteasome subunit beta type-7



- 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	136.86Å 300.14Å 145.06Å 90.00° 113.26° 90.00°	Depositor
Resolution (Å)	15.00 – 2.60 15.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.2 (15.00-2.60) 98.2 (15.00-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.195 , 0.218 0.202 , 0.225	Depositor DCC
R_{free} test set	16029 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	54.9	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 34.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	50090	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ALD, MG, 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	0/1952	0.46	0/2642
1	O	0.27	0/1952	0.46	0/2642
2	B	0.27	0/1934	0.49	0/2618
2	P	0.27	0/1934	0.48	0/2618
3	C	0.27	0/1910	0.49	0/2586
3	Q	0.27	0/1910	0.49	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	0.27	0/1932	0.44	0/2609
6	T	0.27	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	0.25	0/1750	0.50	1/2373 (0.0%)
8	V	0.25	0/1750	0.49	0/2373
9	I	0.26	0/1611	0.49	0/2174
9	W	0.26	0/1611	0.49	0/2174
10	J	0.27	0/1589	0.56	2/2142 (0.1%)
10	X	0.27	0/1589	0.56	1/2142 (0.0%)
11	K	0.38	1/1681 (0.1%)	0.60	3/2274 (0.1%)
11	Y	0.39	1/1681 (0.1%)	0.61	2/2274 (0.1%)
12	L	0.27	0/1795	0.49	0/2420
12	Z	0.27	0/1795	0.49	0/2420
13	M	0.29	0/1837	0.66	3/2492 (0.1%)
13	a	0.28	0/1855	0.77	4/2514 (0.2%)
14	N	0.25	0/1541	0.47	0/2087
14	b	0.25	0/1541	0.48	0/2087
All	All	0.28	2/50246 (0.0%)	0.51	16/67940 (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
11	K	0	1
11	Y	0	1
13	a	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	73	ARG	CD-NE	-9.13	1.30	1.46
11	Y	73	ARG	CD-NE	-8.31	1.32	1.46

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	35	ARG	NE-CZ-NH2	22.26	131.43	120.30
13	M	35	ARG	NE-CZ-NH1	16.06	128.33	120.30
13	a	35	ARG	NE-CZ-NH1	-12.79	113.91	120.30
11	Y	73	ARG	NE-CZ-NH2	-10.59	115.01	120.30
11	K	73	ARG	NE-CZ-NH1	-10.21	115.19	120.30
13	M	35	ARG	NE-CZ-NH2	-9.71	115.45	120.30
11	Y	73	ARG	NE-CZ-NH1	9.48	125.04	120.30
13	a	35	ARG	CD-NE-CZ	9.40	136.76	123.60
13	M	35	ARG	CD-NE-CZ	7.29	133.81	123.60
11	K	73	ARG	CB-CG-CD	-6.24	95.37	111.60
13	a	35	ARG	NH1-CZ-NH2	-6.09	112.70	119.40
10	X	143	LEU	CD1-CG-CD2	-5.76	93.22	110.50
10	J	143	LEU	CD1-CG-CD2	-5.74	93.29	110.50
11	K	73	ARG	NE-CZ-NH2	5.73	123.17	120.30
10	J	143	LEU	CB-CG-CD2	5.34	120.07	111.00
8	H	22	GLN	CA-CB-CG	5.09	124.60	113.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	K	73	ARG	Sidechain
11	Y	73	ARG	Sidechain
13	a	35	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	0	0
1	O	1915	0	1929	2	0
2	B	1904	0	1904	4	0
2	P	1904	0	1904	4	0
3	C	1881	0	1895	7	0
3	Q	1881	0	1895	5	0
4	D	1813	0	1797	1	0
4	R	1813	0	1797	1	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	5	0
8	H	1719	0	1719	5	0
8	V	1719	0	1719	4	0
9	I	1581	0	1574	5	0
9	W	1581	0	1574	6	0
10	J	1561	0	1569	28	0
10	X	1561	0	1569	28	0
11	K	1644	0	1596	10	0
11	Y	1644	0	1596	11	0
12	L	1757	0	1711	6	0
12	Z	1757	0	1711	6	0
13	M	1806	0	1808	5	0
13	a	1824	0	1832	0	0
14	N	1512	0	1480	4	0
14	b	1512	0	1480	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	1	0	0	0	0
15	L	1	0	0	0	0
15	M	1	0	0	0	0
15	N	1	0	0	0	0
15	X	1	0	0	0	0
15	Z	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	b	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	34	0	42	0	0
17	N	34	0	42	0	0
17	Y	34	0	42	0	0
17	b	34	0	42	0	0
18	A	16	0	0	0	0
18	B	21	0	0	2	0
18	C	20	0	0	0	0
18	D	10	0	0	0	0
18	E	10	0	0	0	0
18	F	17	0	0	0	0
18	G	33	0	0	0	0
18	H	25	0	0	0	0
18	I	18	0	0	0	0
18	J	23	0	0	1	0
18	K	37	0	0	0	0
18	L	25	0	0	0	0
18	M	27	0	0	3	0
18	N	22	0	0	0	0
18	O	18	0	0	0	0
18	P	13	0	0	1	0
18	Q	11	0	0	0	0
18	R	13	0	0	0	0
18	S	5	0	0	0	0
18	T	18	0	0	0	0
18	U	22	0	0	0	0
18	V	24	0	0	0	0
18	W	20	0	0	0	0
18	X	19	0	0	0	0
18	Y	36	0	0	0	0
18	Z	28	0	0	0	0
18	a	36	0	0	0	0
18	b	24	0	0	0	0
All	All	50090	0	49274	129	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 (129) 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)
11:Y:40:PHE:CD2	11:Y:73:ARG:NH2	2.29	1.00
11:K:209:ASN:O	9:W:37:ASN:ND2	2.20	0.73
9:I:37:ASN:ND2	11:Y:209:ASN:O	2.24	0.71
11:K:40:PHE:CD2	11:K:73:ARG:NH2	2.60	0.70
10:J:135:TYR:CG	10:X:25:ILE:HD11	2.28	0.67
10:J:25:ILE:HD11	10:X:135:TYR:CG	2.30	0.66
11:Y:145:LYS:HB2	11:Y:148:LEU:CD1	2.28	0.64
10:J:174:MET:HA	10:X:174:MET:HA	1.79	0.63
10:J:1:MET:HG2	10:J:135:TYR:HD2	1.64	0.63
11:K:145:LYS:HB2	11:K:148:LEU:CD1	2.29	0.63
10:X:143:LEU:HD23	10:X:164:CYS:SG	2.39	0.63
11:Y:40:PHE:CG	11:Y:73:ARG:NH2	2.68	0.62
10:X:1:MET:HG2	10:X:135:TYR:HD2	1.64	0.61
10:J:135:TYR:CD1	10:X:25:ILE:HD11	2.35	0.61
10:J:143:LEU:HD23	10:J:164:CYS:SG	2.42	0.60
10:J:25:ILE:HD11	10:X:135:TYR:CD1	2.37	0.60
10:J:135:TYR:HB3	10:X:25:ILE:HD11	1.84	0.59
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	1.86	0.58
10:J:25:ILE:HD11	10:X:135:TYR:HB3	1.84	0.58
8:H:22:GLN:HE21	8:H:22:GLN:HA	1.69	0.58
11:K:145:LYS:HB2	11:K:148:LEU:HD13	1.86	0.58
14:N:152:VAL:HA	14:N:175:MET:HE1	1.86	0.57
10:J:135:TYR:CD1	10:X:25:ILE:CD1	2.89	0.55
10:X:1:MET:HG2	10:X:135:TYR:CD2	2.42	0.55
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.72	0.55
8:V:22:GLN:HG3	8:V:27:ALA:HB2	1.89	0.54
10:J:1:MET:HG2	10:J:135:TYR:CD2	2.41	0.54
10:J:25:ILE:CD1	10:X:135:TYR:CD1	2.91	0.54
10:X:174:MET:CE	10:X:174:MET:N	2.72	0.53
13:M:35:ARG:NH2	18:M:401:HOH:O	2.40	0.53
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.72	0.52
10:X:173:PRO:HB2	10:X:174:MET:CE	2.39	0.52
10:J:173:PRO:HB2	10:J:174:MET:CE	2.40	0.51
10:J:147:HIS:HB2	10:J:160:LEU:HD11	1.93	0.51
3:C:201:VAL:O	3:C:202:GLN:CB	2.58	0.51
7:U:23:PHE:O	7:U:26:THR:HB	2.10	0.51
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.59	0.51
7:G:23:PHE:O	7:G:26:THR:HB	2.11	0.51
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.93	0.50
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.93	0.50
10:X:147:HIS:HB2	10:X:160:LEU:HD11	1.93	0.50
10:J:1:MET:HA	18:J:303:HOH:O	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:174:MET:CE	10:J:174:MET:N	2.75	0.49
10:J:25:ILE:HD11	10:X:135:TYR:CB	2.44	0.48
13:M:2:GLN:NE2	18:M:402:HOH:O	2.46	0.48
10:J:135:TYR:CB	10:X:25:ILE:HD11	2.43	0.48
10:J:21:VAL:HG11	11:K:122:LEU:HD11	1.96	0.48
10:X:23:ARG:HA	10:X:23:ARG:HD3	1.76	0.47
10:J:50:ALA:O	11:K:91:LYS:NZ	2.47	0.47
10:X:50:ALA:O	11:Y:91:LYS:NZ	2.47	0.47
10:X:173:PRO:HB2	10:X:174:MET:HE3	1.95	0.47
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.95	0.47
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.97	0.47
8:H:80:LEU:HD12	8:H:113:ILE:HD11	1.97	0.46
8:H:22:GLN:CA	8:H:22:GLN:HE21	2.27	0.46
3:Q:201:VAL:O	3:Q:202:GLN:HB3	2.16	0.46
3:C:201:VAL:O	3:C:202:GLN:HB3	2.16	0.46
3:C:35:LYS:HG2	3:C:158:SER:O	2.15	0.45
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.46	0.45
2:B:93:HIS:HB3	18:B:301:HOH:O	2.16	0.45
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.16	0.45
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.99	0.45
10:X:173:PRO:CB	10:X:174:MET:HE3	2.46	0.45
10:J:169:GLU:O	10:X:177:LYS:NZ	2.50	0.45
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.53	0.44
11:K:158:LYS:HB2	11:K:177:LEU:HD11	2.00	0.44
10:J:177:LYS:NZ	10:X:169:GLU:O	2.50	0.44
12:Z:13:LEU:HD11	12:Z:150:LEU:HD21	2.00	0.44
9:W:36:SER:HB2	10:X:126:VAL:HG11	2.00	0.44
10:X:173:PRO:HD2	10:X:174:MET:HE3	1.99	0.44
9:I:20:VAL:HG13	9:I:118:PRO:HB3	2.00	0.44
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.48	0.44
8:V:104:ASP:HB2	8:V:105:PRO:HD2	2.00	0.44
2:B:50:LYS:O	2:B:51:VAL:C	2.56	0.43
12:L:13:LEU:HD11	12:L:150:LEU:HD21	1.99	0.43
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.83	0.43
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.48	0.43
9:I:9:GLY:HA3	9:I:41:LYS:HE2	2.00	0.43
13:M:35:ARG:NE	18:M:401:HOH:O	2.52	0.43
1:O:55:LEU:HB3	7:U:159:ALA:O	2.18	0.43
2:P:50:LYS:O	2:P:51:VAL:C	2.56	0.43
9:W:20:VAL:HG13	9:W:118:PRO:HB3	2.00	0.43
11:Y:158:LYS:HB2	11:Y:177:LEU:HD11	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:78:ILE:N	7:G:79:PRO:CD	2.82	0.43
9:W:9:GLY:HA3	9:W:41:LYS:HE2	2.01	0.43
2:P:113:ARG:NE	18:P:301:HOH:O	2.49	0.42
12:Z:23:LEU:HD13	12:Z:43:VAL:HG13	2.01	0.42
8:H:104:ASP:HB2	8:H:105:PRO:HD2	2.00	0.42
10:J:2:ASP:O	10:J:3:ILE:C	2.58	0.42
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.53	0.42
5:S:12:PHE:H	6:T:19:GLN:HE22	1.66	0.42
3:C:160:GLN:HA	3:C:160:GLN:HE21	1.84	0.42
11:K:130:GLY:O	11:K:133:GLN:HG2	2.20	0.42
10:J:174:MET:HE3	10:J:174:MET:N	2.34	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.42
10:J:173:PRO:HD2	10:J:174:MET:HE3	2.01	0.42
12:L:23:LEU:HD13	12:L:43:VAL:HG13	2.01	0.42
10:X:143:LEU:CD2	10:X:164:CYS:SG	3.06	0.42
11:Y:209:ASN:H	11:Y:209:ASN:HD22	1.67	0.42
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	2.01	0.41
8:V:35:HIS:HB3	8:V:56:THR:HG21	2.02	0.41
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.51	0.41
10:J:173:PRO:HB2	10:J:174:MET:HE3	2.02	0.41
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.03	0.41
5:S:77:ALA:N	5:S:78:PRO:CD	2.84	0.41
11:Y:130:GLY:O	11:Y:133:GLN:HG2	2.20	0.41
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.56	0.41
8:H:35:HIS:HB3	8:H:56:THR:HG21	2.02	0.41
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.03	0.41
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.03	0.41
9:I:10:ILE:HG21	9:I:141:ALA:HB3	2.03	0.41
9:W:20:VAL:HG23	9:W:189:ILE:HB	2.03	0.41
2:B:113:ARG:NE	18:B:301:HOH:O	2.43	0.41
3:C:169:VAL:HG23	3:C:196:SER:HB2	2.03	0.41
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.51	0.41
2:P:50:LYS:HD3	2:P:50:LYS:HA	1.92	0.41
2:B:14:PRO:HA	3:C:20:TYR:CE1	2.55	0.41
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.51	0.41
5:E:77:ALA:N	5:E:78:PRO:CD	2.84	0.40
11:K:20:ALA:HB2	11:K:31:VAL:HG11	2.03	0.40
12:L:8:ASN:HA	12:L:30:ILE:O	2.21	0.40
11:Y:20:ALA:HB2	11:Y:31:VAL:HG11	2.03	0.40
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.56	0.40
13:M:17:ASP:OD1	13:M:18:ASN:N	2.55	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.56	0.40
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.20	0.40
12:L:100:LYS:HD3	12:L:105:TYR:CE2	2.56	0.40
11:K:209:ASN:HD22	11:K:209:ASN:H	1.67	0.40
9:W:10:ILE:HG21	9:W:141:ALA:HB3	2.03	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	248/250 (99%)	241 (97%)	6 (2%)	1 (0%)	34	57
1	O	248/250 (99%)	240 (97%)	7 (3%)	1 (0%)	34	57
2	B	242/258 (94%)	234 (97%)	4 (2%)	4 (2%)	9	18
2	P	242/258 (94%)	233 (96%)	5 (2%)	4 (2%)	9	18
3	C	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	19	39
3	Q	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	19	39
4	D	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
4	R	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
5	E	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
5	S	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	188 (97%)	4 (2%)	1 (0%)	29	52
10	X	193/198 (98%)	190 (98%)	2 (1%)	1 (0%)	29	52
11	K	210/212 (99%)	204 (97%)	6 (3%)	0	100	100
11	Y	210/212 (99%)	204 (97%)	6 (3%)	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	229/246 (93%)	221 (96%)	7 (3%)	1 (0%)	34	57
13	a	231/246 (94%)	222 (96%)	8 (4%)	1 (0%)	34	57
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	b	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
All	All	6282/6614 (95%)	6126 (98%)	138 (2%)	18 (0%)	41	64

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN
10	J	3	ILE
2	P	51	VAL
3	Q	202	GLN
10	X	3	ILE
2	B	218	GLY
2	B	222	GLY
2	P	218	GLY
2	P	222	GLY
1	A	2	THR
1	O	2	THR
2	B	220	ASN
2	P	220	ASN
3	C	205	ALA
3	Q	205	ALA
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	209/209 (100%)	206 (99%)	3 (1%)	67	85
1	O	209/209 (100%)	206 (99%)	3 (1%)	67	85
2	B	203/216 (94%)	200 (98%)	3 (2%)	65	83
2	P	203/216 (94%)	200 (98%)	3 (2%)	65	83
3	C	212/226 (94%)	203 (96%)	9 (4%)	30	55
3	Q	212/226 (94%)	203 (96%)	9 (4%)	30	55
4	D	194/215 (90%)	185 (95%)	9 (5%)	27	51
4	R	194/215 (90%)	185 (95%)	9 (5%)	27	51
5	E	190/193 (98%)	184 (97%)	6 (3%)	39	65
5	S	190/193 (98%)	184 (97%)	6 (3%)	39	65
6	F	201/239 (84%)	195 (97%)	6 (3%)	41	67
6	T	201/239 (84%)	195 (97%)	6 (3%)	41	67
7	G	206/210 (98%)	200 (97%)	6 (3%)	42	68
7	U	206/210 (98%)	199 (97%)	7 (3%)	37	63
8	H	185/190 (97%)	180 (97%)	5 (3%)	44	71
8	V	185/190 (97%)	181 (98%)	4 (2%)	52	76
9	I	172/173 (99%)	169 (98%)	3 (2%)	60	81
9	W	172/173 (99%)	169 (98%)	3 (2%)	60	81
10	J	173/175 (99%)	164 (95%)	9 (5%)	23	46
10	X	173/175 (99%)	164 (95%)	9 (5%)	23	46
11	K	169/169 (100%)	160 (95%)	9 (5%)	22	45
11	Y	169/169 (100%)	160 (95%)	9 (5%)	22	45
12	L	185/185 (100%)	183 (99%)	2 (1%)	73	88
12	Z	185/185 (100%)	183 (99%)	2 (1%)	73	88
13	M	197/208 (95%)	190 (96%)	7 (4%)	35	61
13	a	199/208 (96%)	192 (96%)	7 (4%)	36	62

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	162/162 (100%)	160 (99%)	2 (1%)	71	87
14	b	162/162 (100%)	160 (99%)	2 (1%)	71	87
All	All	5318/5540 (96%)	5160 (97%)	158 (3%)	41	67

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
2	B	113	ARG
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	206	LYS
3	C	240	GLU
4	D	99	ILE
4	D	125	LEU
4	D	143	ASP
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	71	LEU
5	E	184	ASN
5	E	188	LEU
5	E	202	ASP
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	181	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	F	214	TRP
6	F	240	GLN
7	G	115	LEU
7	G	122	ARG
7	G	125	MET
7	G	208	GLU
7	G	235	ARG
7	G	236	LEU
8	H	22	GLN
8	H	30	ASN
8	H	34	LEU
8	H	68	LEU
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
9	I	182	TRP
10	J	1	MET
10	J	3	ILE
10	J	23	ARG
10	J	90	LYS
10	J	99	GLN
10	J	136	SER
10	J	143	LEU
10	J	149	ARG
10	J	174	MET
11	K	4	LEU
11	K	9	GLN
11	K	35	ILE
11	K	73	ARG
11	K	100	MET
11	K	107	LYS
11	K	143	ASN
11	K	148	LEU
11	K	209	ASN
12	L	23	LEU
12	L	150	LEU
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	M	190	ARG
14	N	9	LYS
14	N	83	LYS
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	113	ARG
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	206	LYS
3	Q	240	GLU
4	R	99	ILE
4	R	125	LEU
4	R	143	ASP
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	71	LEU
5	S	184	ASN
5	S	188	LEU
5	S	202	ASP
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	181	GLU
6	T	214	TRP
6	T	240	GLN
7	U	115	LEU
7	U	117	GLN
7	U	122	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	U	125	MET
7	U	208	GLU
7	U	235	ARG
7	U	236	LEU
8	V	30	ASN
8	V	34	LEU
8	V	68	LEU
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
9	W	182	TRP
10	X	1	MET
10	X	3	ILE
10	X	23	ARG
10	X	90	LYS
10	X	99	GLN
10	X	136	SER
10	X	143	LEU
10	X	149	ARG
10	X	174	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	35	ILE
11	Y	73	ARG
11	Y	100	MET
11	Y	107	LYS
11	Y	143	ASN
11	Y	148	LEU
11	Y	209	ASN
12	Z	23	LEU
12	Z	150	LEU
13	a	2	GLN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
13	a	190	ARG
14	b	9	LYS
14	b	83	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	20	GLN
2	B	58	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
3	C	147	GLN
3	C	160	GLN
4	D	91	HIS
4	D	146	GLN
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	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
8	H	22	GLN
10	J	55	GLN
11	K	85	ASN
11	K	143	ASN
11	K	176	ASN
11	K	209	ASN
12	L	3	ASN
12	L	70	ASN
12	L	79	HIS
13	M	48	ASN
13	M	102	GLN
13	M	108	ASN
13	M	179	ASN
14	N	161	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	20	GLN
2	P	58	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	91	HIS
4	R	146	GLN
4	R	225	ASN
5	S	68	HIS
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
10	X	55	GLN
11	Y	85	ASN
11	Y	143	ASN
11	Y	176	ASN
11	Y	209	ASN
12	Z	3	ASN
12	Z	79	HIS
13	a	48	ASN
13	a	102	GLN
13	a	179	ASN
14	b	161	GLN

5.3.3 RNA ⓘ

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 19 ligands modelled in this entry, 15 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	ALD	Y	301	11	34,34,34	1.06	1 (2%)	44,44,44	0.93	3 (6%)
17	ALD	K	301	11	34,34,34	1.06	1 (2%)	44,44,44	0.93	3 (6%)
17	ALD	b	201	15,14	34,34,34	1.09	1 (2%)	44,44,44	0.89	3 (6%)
17	ALD	N	201	14	34,34,34	1.10	1 (2%)	44,44,44	0.91	3 (6%)

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	ALD	Y	301	11	-	4/39/39/39	0/1/1/1
17	ALD	K	301	11	-	4/39/39/39	0/1/1/1
17	ALD	b	201	15,14	-	2/39/39/39	0/1/1/1
17	ALD	N	201	14	-	2/39/39/39	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	N	201	ALD	O8-C9	5.71	1.46	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	201	ALD	O8-C9	5.68	1.46	1.35
17	Y	301	ALD	O8-C9	5.29	1.45	1.35
17	K	301	ALD	O8-C9	5.28	1.45	1.35

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Y	301	ALD	C7-O8-C9	3.01	122.64	115.93
17	N	201	ALD	O8-C9-N10	3.00	116.61	110.50
17	K	301	ALD	C7-O8-C9	2.99	122.61	115.93
17	b	201	ALD	O8-C9-N10	2.91	116.42	110.50
17	N	201	ALD	C7-O8-C9	2.68	121.92	115.93
17	b	201	ALD	C7-O8-C9	2.64	121.82	115.93
17	N	201	ALD	O8-C9-O31	-2.56	119.34	124.25
17	b	201	ALD	O8-C9-O31	-2.47	119.51	124.25
17	K	301	ALD	O8-C9-N10	2.46	115.51	110.50
17	Y	301	ALD	O8-C9-N10	2.40	115.37	110.50
17	K	301	ALD	O8-C9-O31	-2.26	119.91	124.25
17	Y	301	ALD	O8-C9-O31	-2.24	119.95	124.25

There are no chirality outliers.

All (12) torsion outliers are listed below:

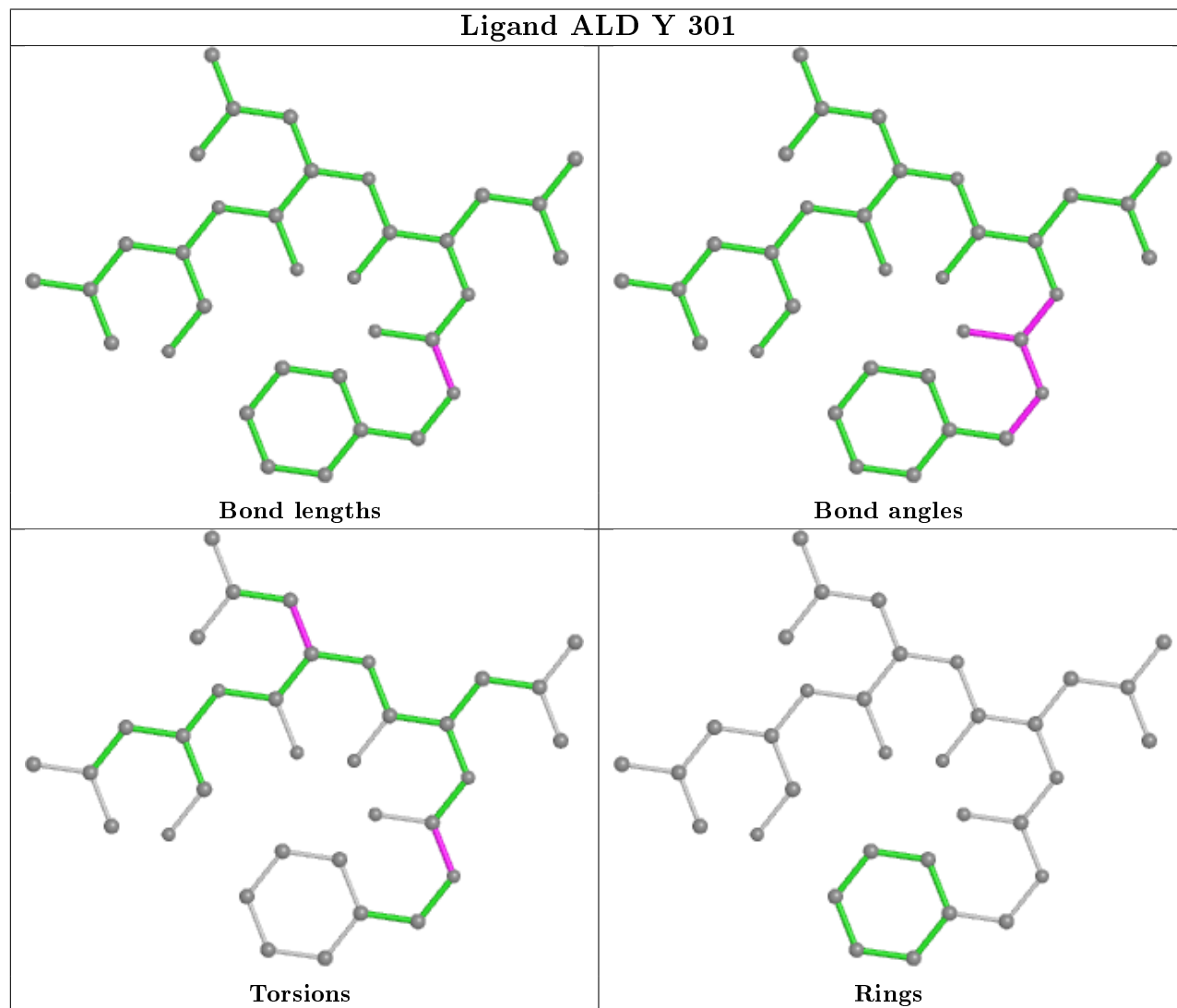
Mol	Chain	Res	Type	Atoms
17	K	301	ALD	O31-C9-O8-C7
17	Y	301	ALD	O31-C9-O8-C7
17	K	301	ALD	N10-C9-O8-C7
17	Y	301	ALD	N10-C9-O8-C7
17	N	201	ALD	N10-C9-O8-C7
17	N	201	ALD	O31-C9-O8-C7
17	b	201	ALD	N10-C9-O8-C7
17	b	201	ALD	O31-C9-O8-C7
17	K	301	ALD	C15-C14-C24-C25
17	Y	301	ALD	C15-C14-C24-C25
17	K	301	ALD	N13-C14-C24-C25
17	Y	301	ALD	N13-C14-C24-C25

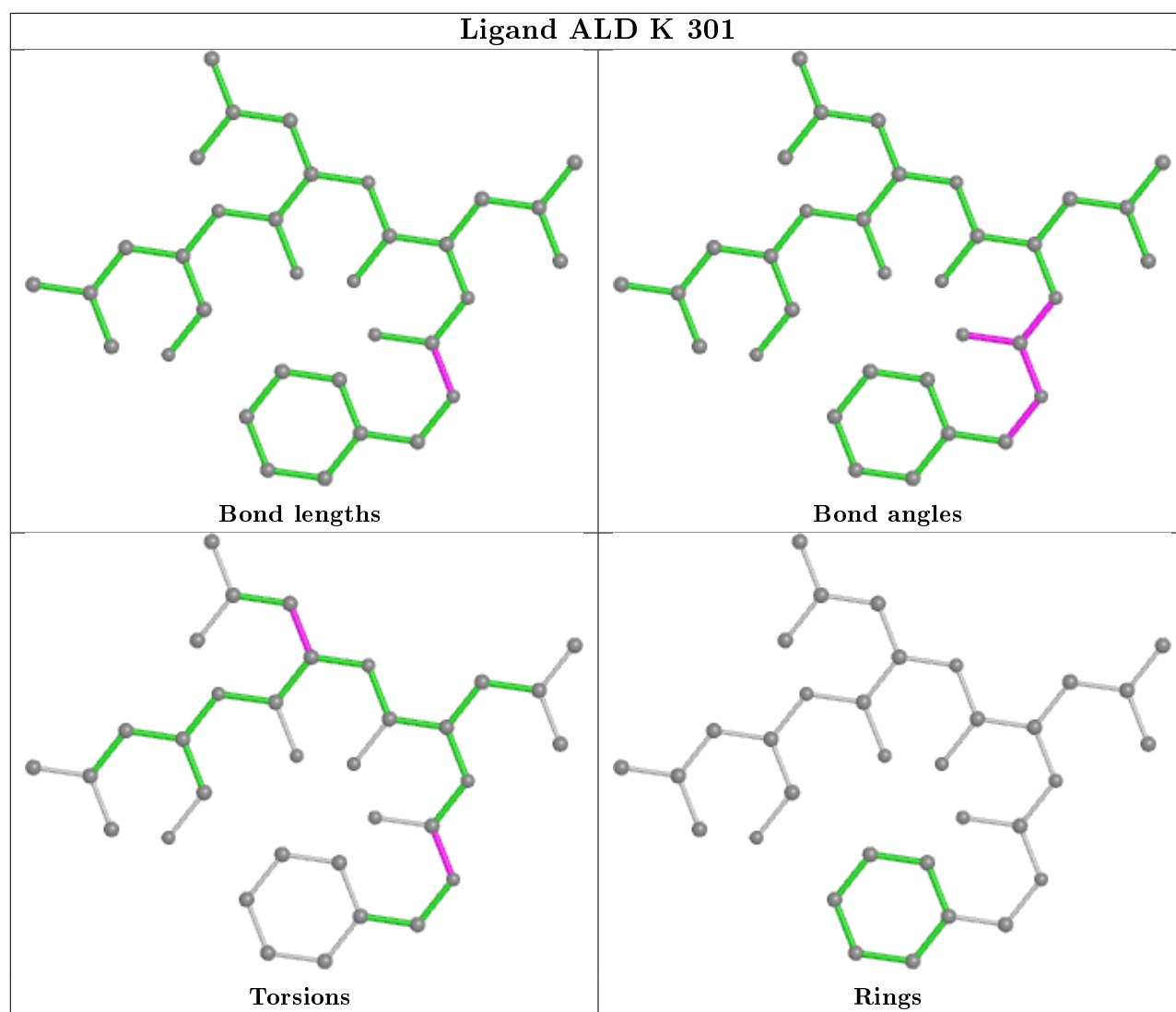
There are no ring outliers.

No monomer is involved in short contacts.

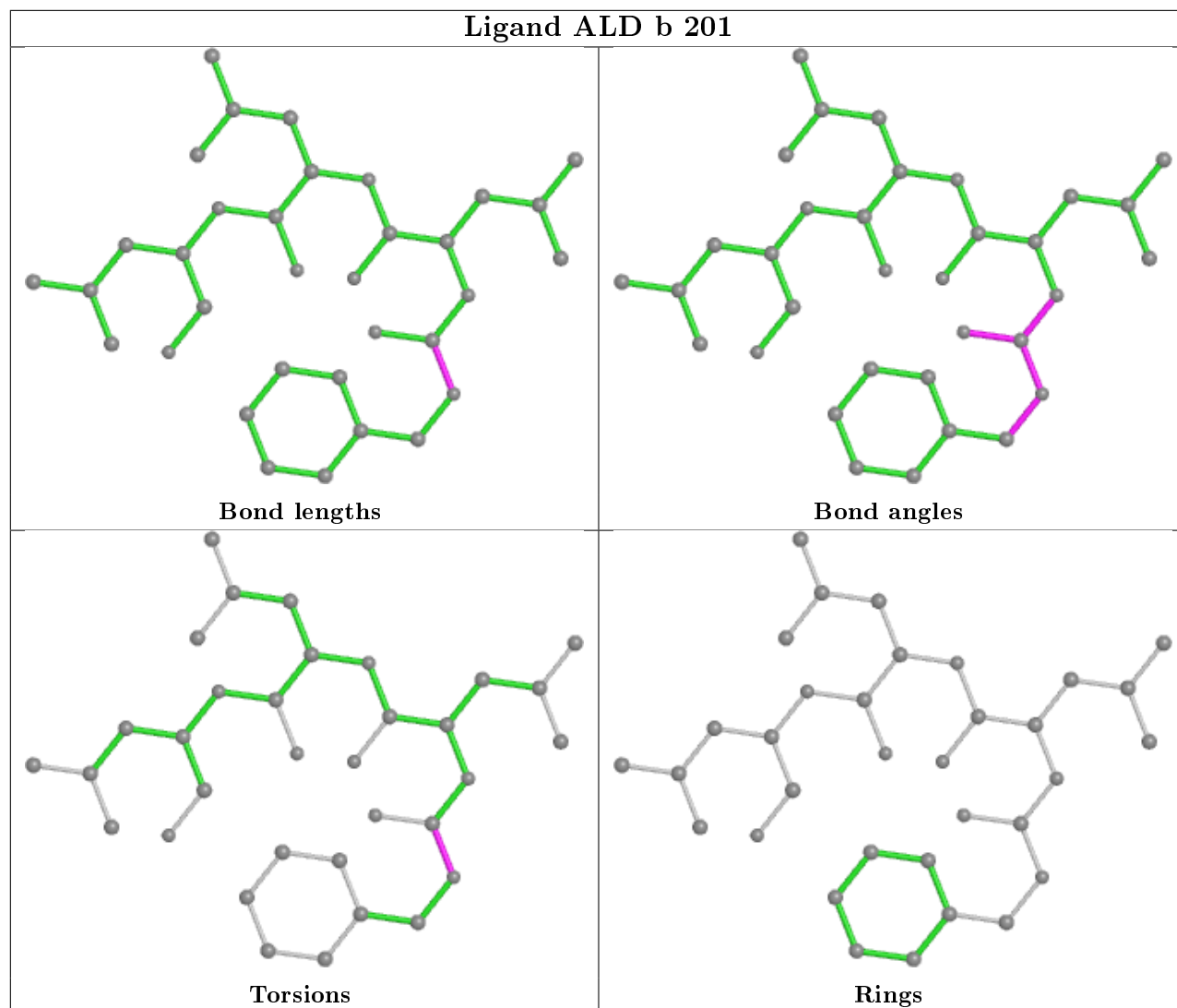
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

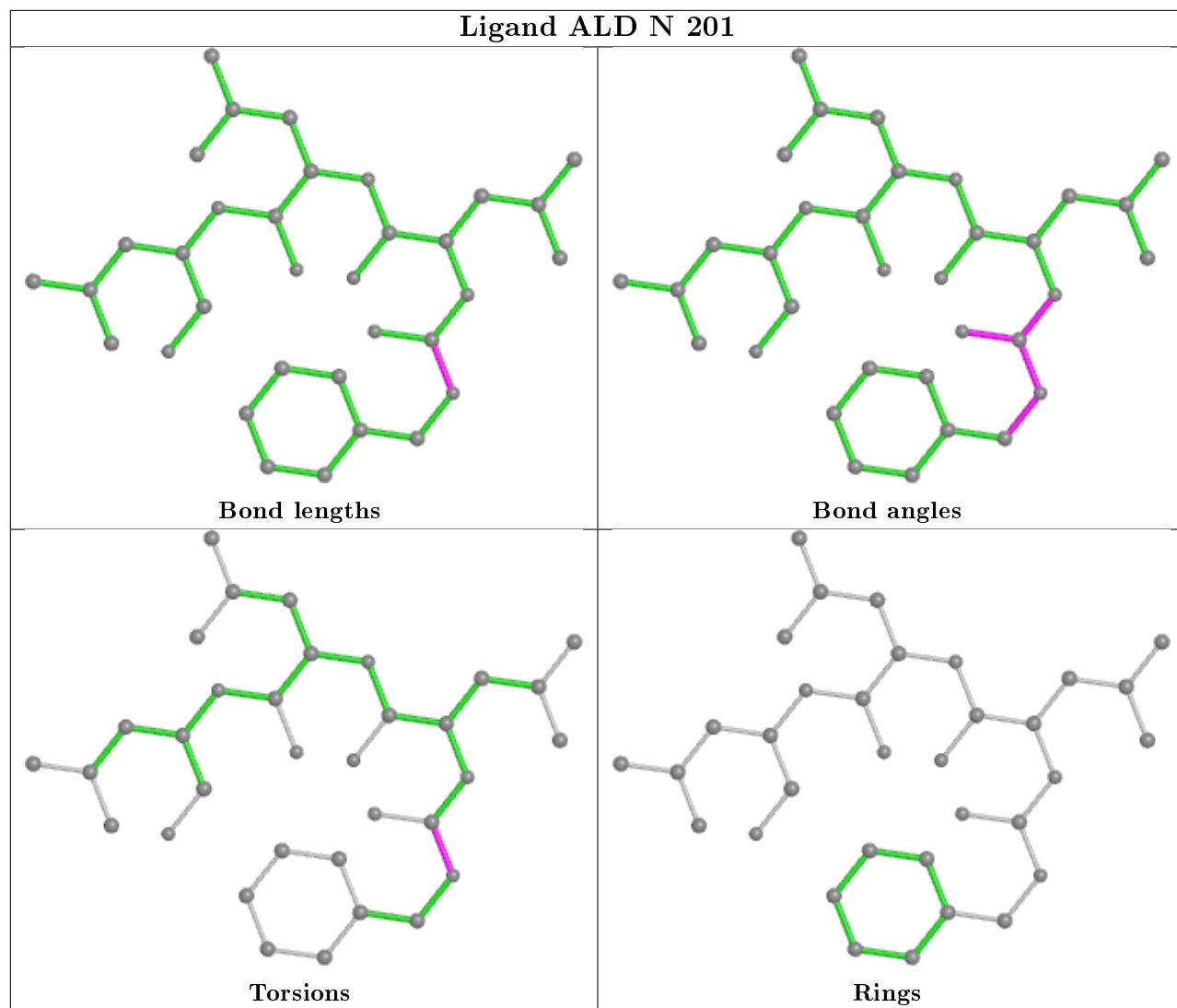
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.





Ligand ALD b 201





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%)	-0.36	7 (2%) 53 46	37, 53, 90, 128	0
1	O	250/250 (100%)	-0.31	9 (3%) 42 35	42, 62, 106, 140	0
2	B	244/258 (94%)	-0.20	10 (4%) 37 30	39, 60, 105, 165	0
2	P	244/258 (94%)	-0.12	11 (4%) 33 26	43, 65, 107, 162	0
3	C	240/254 (94%)	-0.10	19 (7%) 12 9	40, 65, 128, 160	0
3	Q	240/254 (94%)	0.16	24 (10%) 7 4	50, 79, 163, 186	0
4	D	235/260 (90%)	-0.34	2 (0%) 84 82	43, 65, 101, 145	0
4	R	235/260 (90%)	-0.25	7 (2%) 50 43	48, 68, 111, 147	0
5	E	231/234 (98%)	-0.17	9 (3%) 39 32	46, 68, 105, 149	0
5	S	231/234 (98%)	-0.08	11 (4%) 30 24	47, 73, 120, 152	0
6	F	243/288 (84%)	-0.38	6 (2%) 57 51	34, 59, 110, 138	0
6	T	243/288 (84%)	-0.24	11 (4%) 33 26	33, 68, 128, 156	0
7	G	241/252 (95%)	-0.43	8 (3%) 46 39	37, 56, 95, 152	0
7	U	241/252 (95%)	-0.38	4 (1%) 70 66	42, 57, 94, 138	0
8	H	226/232 (97%)	-0.31	5 (2%) 62 56	38, 54, 91, 150	0
8	V	226/232 (97%)	-0.24	7 (3%) 49 42	39, 57, 93, 185	0
9	I	204/205 (99%)	-0.57	3 (1%) 73 70	35, 50, 86, 110	0
9	W	204/205 (99%)	-0.53	2 (0%) 82 80	37, 54, 87, 107	0
10	J	195/198 (98%)	-0.36	6 (3%) 49 42	33, 56, 84, 121	0
10	X	195/198 (98%)	-0.37	4 (2%) 63 58	33, 59, 86, 136	0
11	K	212/212 (100%)	-0.42	2 (0%) 84 82	36, 54, 88, 106	0
11	Y	212/212 (100%)	-0.42	2 (0%) 84 82	38, 54, 90, 108	0
12	L	222/222 (100%)	-0.40	7 (3%) 47 40	35, 55, 105, 134	0
12	Z	222/222 (100%)	-0.41	6 (2%) 54 48	38, 53, 103, 135	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	M	231/246 (93%)	-0.48	6 (2%)	56	50	33, 53, 83, 99	0
13	a	233/246 (94%)	-0.47	6 (2%)	56	50	34, 52, 79, 108	0
14	N	196/196 (100%)	-0.64	2 (1%)	82	80	34, 47, 80, 105	0
14	b	196/196 (100%)	-0.60	2 (1%)	82	80	34, 49, 83, 110	0
All	All	6342/6614 (95%)	-0.33	198 (3%)	49	42	33, 59, 106, 186	0

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	V	226	GLU	8.6
8	V	222	ASP	8.2
3	Q	49	THR	7.6
3	Q	206	LYS	7.1
3	Q	50	LEU	6.9
13	a	233	ILE	6.9
8	V	224	GLN	6.9
12	Z	174	TYR	6.6
2	P	220	ASN	6.3
13	M	230	THR	6.3
2	B	220	ASN	6.3
2	P	221	ASP	6.1
2	P	219	ALA	6.0
12	L	174	TYR	5.9
5	S	202	ASP	5.9
8	H	224	GLN	5.9
8	H	222	ASP	5.8
8	V	223	ILE	5.8
1	O	1	MET	5.7
2	P	51	VAL	5.7
8	H	223	ILE	5.5
2	B	221	ASP	5.5
8	V	225	GLU	5.3
8	H	221	CYS	5.3
9	W	1	SER	5.3
3	Q	239	GLN	5.2
2	B	51	VAL	5.2
13	M	229	GLY	5.1
5	E	202	ASP	5.1
3	C	50	LEU	5.1
3	Q	48	SER	4.9
8	H	226	GLU	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	O	249	ALA	4.8
1	A	1	MET	4.8
13	M	231	GLN	4.7
3	Q	236	GLN	4.5
3	C	238	LYS	4.5
10	X	194	ASP	4.5
2	B	219	ALA	4.5
12	L	165	ASN	4.4
2	P	222	GLY	4.4
12	Z	173	LYS	4.4
12	Z	163	GLY	4.2
10	X	1	MET	4.2
3	C	49	THR	4.2
13	a	232	LYS	4.2
3	Q	238	LYS	4.2
2	B	218	GLY	4.1
8	V	221	CYS	4.1
1	A	2	THR	4.1
2	P	218	GLY	4.1
7	U	242	GLN	4.1
3	Q	205	ALA	4.1
5	S	180	LYS	3.9
2	P	59	ASP	3.9
5	E	123	GLY	3.9
1	O	2	THR	3.9
3	C	202	GLN	3.8
10	J	194	ASP	3.7
6	T	244	ASN	3.7
3	Q	55	THR	3.6
14	b	195	GLN	3.6
5	S	173	ARG	3.6
11	K	212	GLY	3.6
3	Q	240	GLU	3.5
7	U	222	ASP	3.5
13	a	230	THR	3.5
5	S	54	GLU	3.5
3	C	225	GLU	3.5
4	R	241	ALA	3.5
3	Q	223	SER	3.4
6	T	241	LYS	3.4
12	Z	165	ASN	3.4
3	C	206	LYS	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
12	L	163	GLY	3.4
3	Q	202	GLN	3.4
6	T	243	ILE	3.3
3	C	239	GLN	3.3
2	B	217	LYS	3.3
10	J	1	MET	3.3
1	A	250	LEU	3.2
6	F	202	ASP	3.2
1	A	249	ALA	3.2
6	T	230	ASP	3.1
11	Y	212	GLY	3.1
5	E	54	GLU	3.1
13	M	216	ASN	3.0
4	D	242	GLU	3.0
10	J	174	MET	3.0
7	G	2	GLY	3.0
6	F	215	CYS	3.0
12	Z	168	VAL	2.9
3	C	180	LYS	2.9
3	C	205	ALA	2.9
1	A	248	GLU	2.9
5	S	207	VAL	2.9
9	W	133	LYS	2.9
5	S	122	TYR	2.9
3	C	236	GLN	2.8
3	Q	225	GLU	2.8
4	R	242	GLU	2.8
4	R	125	LEU	2.8
3	Q	234	ILE	2.8
3	Q	51	LYS	2.8
4	R	1	ASP	2.7
5	E	122	TYR	2.7
2	B	222	GLY	2.7
13	a	1	THR	2.7
13	a	231	GLN	2.7
5	S	233	ILE	2.7
3	C	216	ASP	2.6
2	B	203	SER	2.6
6	T	53	LYS	2.6
6	T	181	GLU	2.6
13	a	229	GLY	2.6
6	F	244	ASN	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	N	195	GLN	2.5
3	C	240	GLU	2.5
5	S	203	GLU	2.5
7	G	222	ASP	2.5
7	G	179	LYS	2.5
9	I	1	SER	2.5
7	G	241	GLU	2.5
3	Q	203	THR	2.5
10	J	149	ARG	2.5
5	E	233	ILE	2.5
7	G	3	TYR	2.5
7	G	188	GLU	2.5
7	G	242	GLN	2.5
12	L	1	GLN	2.5
2	B	59	ASP	2.5
12	L	168	VAL	2.5
3	Q	141	ASP	2.5
1	O	250	LEU	2.5
3	C	175	LYS	2.5
3	C	204	GLY	2.4
6	T	2	THR	2.4
6	T	204	LYS	2.4
4	R	2	ARG	2.4
6	F	205	GLU	2.4
1	O	201	GLU	2.4
6	T	201	GLU	2.4
2	P	169	SER	2.4
1	A	201	GLU	2.4
11	Y	106	ARG	2.4
12	Z	1	GLN	2.3
9	I	133	LYS	2.3
6	T	205	GLU	2.3
3	Q	187	GLU	2.3
8	V	145	ASP	2.3
1	O	231	LYS	2.3
2	P	225	TYR	2.3
1	O	248	GLU	2.3
3	C	235	GLU	2.3
10	J	193	ASP	2.3
3	C	48	SER	2.3
3	Q	235	GLU	2.3
2	P	52	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	E	180	LYS	2.2
4	D	1	ASP	2.2
4	R	217	GLN	2.2
3	Q	204	GLY	2.2
7	U	2	GLY	2.2
6	T	215	CYS	2.2
13	M	47	ASP	2.2
3	Q	60	SER	2.2
12	L	173	LYS	2.2
3	C	1	GLY	2.2
3	C	203	THR	2.2
3	Q	171	GLU	2.2
10	X	149	ARG	2.1
5	E	194	GLU	2.1
11	K	147	ASP	2.1
10	X	174	MET	2.1
5	E	207	VAL	2.1
10	J	150	PRO	2.1
3	Q	221	ALA	2.1
13	M	1	THR	2.1
5	S	163	ARG	2.1
4	R	177	ASN	2.1
3	Q	229	GLN	2.1
2	P	240	LYS	2.1
1	A	182	GLU	2.1
1	O	178	ARG	2.1
1	O	52	SER	2.1
6	F	241	LYS	2.0
12	L	162	PRO	2.0
5	E	227	GLU	2.0
5	S	194	GLU	2.0
6	F	181	GLU	2.0
14	N	105	LYS	2.0
9	I	131	GLU	2.0
5	S	3	ASN	2.0
7	G	68	ARG	2.0
7	U	241	GLU	2.0
14	b	104	ASP	2.0
3	C	187	GLU	2.0
2	B	239	VAL	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 carbohydrates in this entry.

6.4 Ligands [i](#)

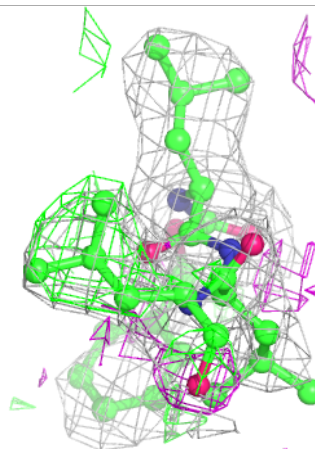
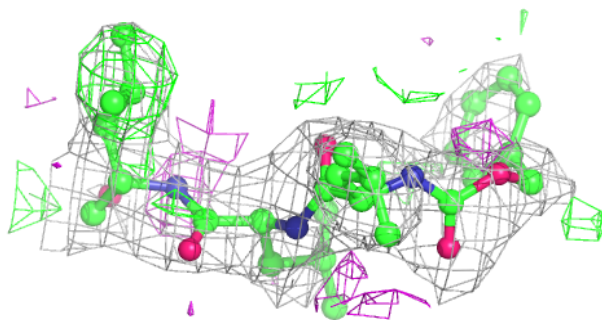
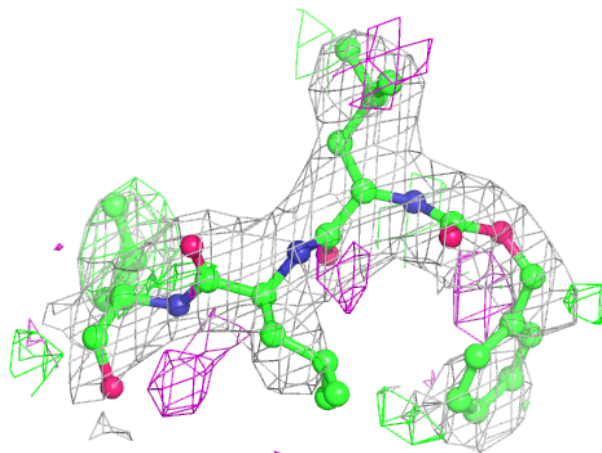
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
17	ALD	N	201	34/34	0.80	0.29	63,100,136,138	0
17	ALD	Y	301	34/34	0.81	0.25	68,104,128,136	0
17	ALD	b	201	34/34	0.82	0.28	68,91,126,132	0
17	ALD	K	301	34/34	0.85	0.25	64,96,115,116	0
15	MG	I	302	1/1	0.88	0.11	54,54,54,54	0
15	MG	G	301	1/1	0.92	0.12	58,58,58,58	0
16	CL	b	203	1/1	0.93	0.30	94,94,94,94	0
15	MG	I	301	1/1	0.93	0.17	67,67,67,67	0
15	MG	L	301	1/1	0.96	0.10	67,67,67,67	0
15	MG	X	201	1/1	0.96	0.18	38,38,38,38	0
15	MG	Z	301	1/1	0.96	0.15	59,59,59,59	0
15	MG	K	302	1/1	0.97	0.08	68,68,68,68	0
16	CL	N	203	1/1	0.98	0.17	73,73,73,73	0
15	MG	N	202	1/1	0.98	0.07	44,44,44,44	0
16	CL	U	301	1/1	0.99	0.20	44,44,44,44	0
15	MG	J	201	1/1	0.99	0.30	42,42,42,42	0
15	MG	M	301	1/1	0.99	0.28	46,46,46,46	0
16	CL	G	302	1/1	0.99	0.08	42,42,42,42	0
15	MG	b	202	1/1	1.00	0.07	34,34,34,34	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.

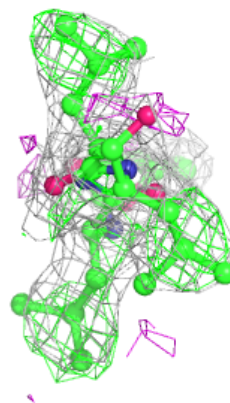
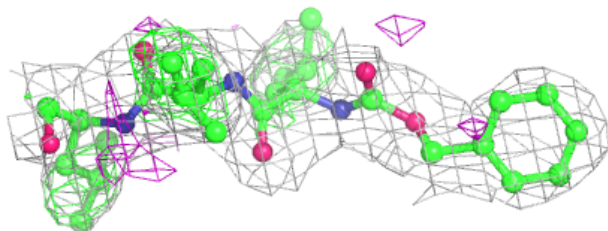
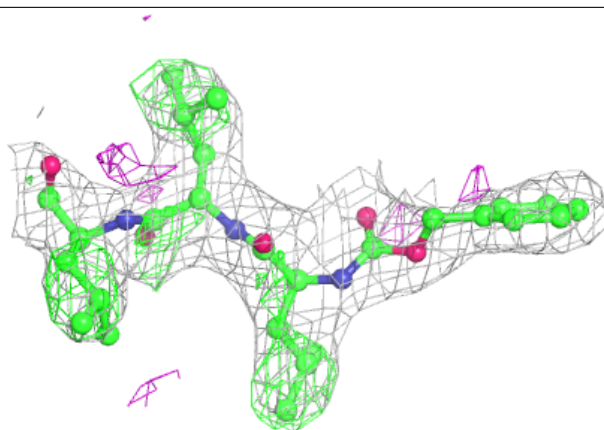
Electron density around ALD N 201:

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



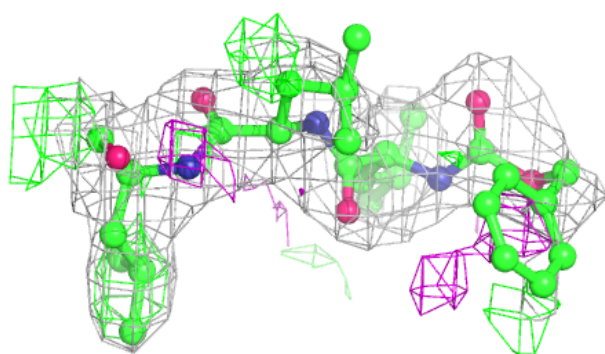
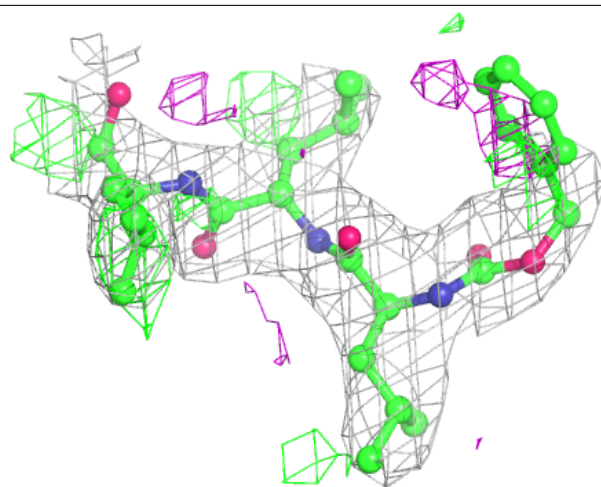
Electron density around ALD Y 301:

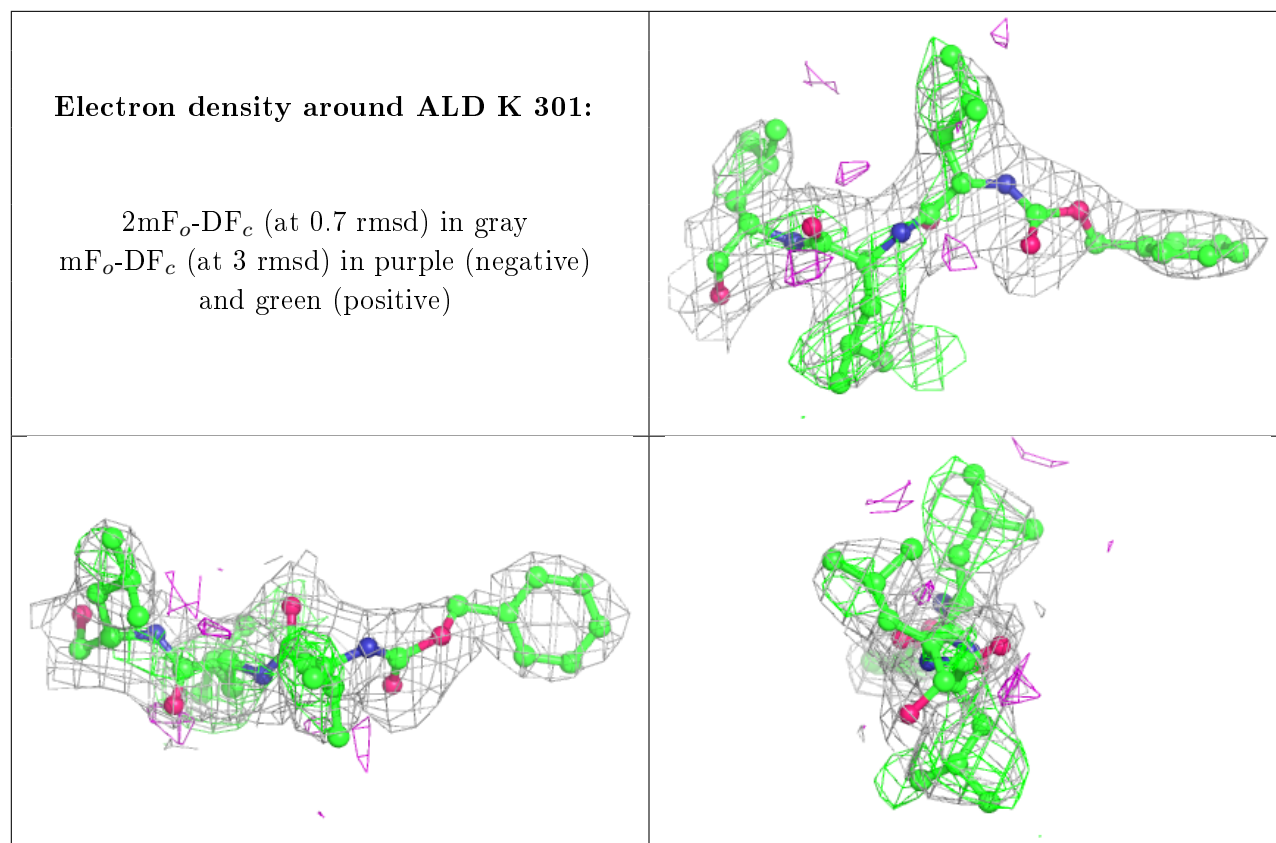
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ALD b 201:

$2mF_o-DF_c$ (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.