



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:27 PM UTC

PDB ID : 5D0T / pdb_00005d0t
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 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

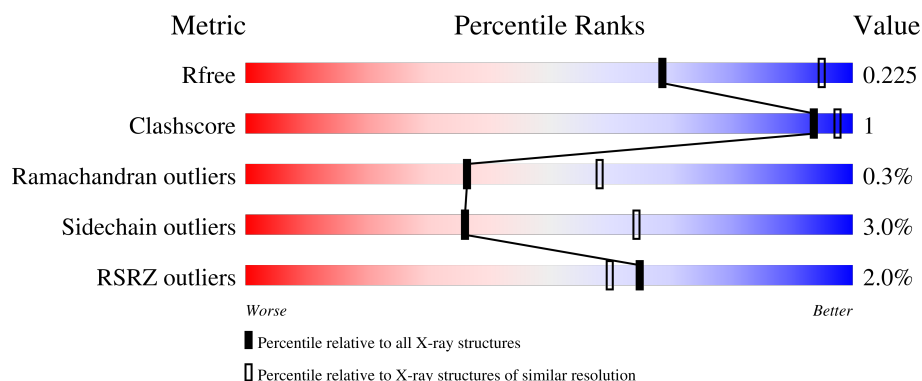
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

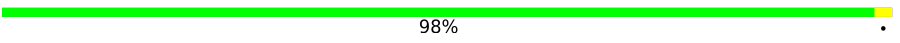
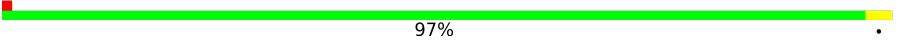
The reported resolution of this entry is 2.60 Å.

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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 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	 97%
2	B	258	 90%
2	P	258	 90%
3	C	254	 87%

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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	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			

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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.

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			

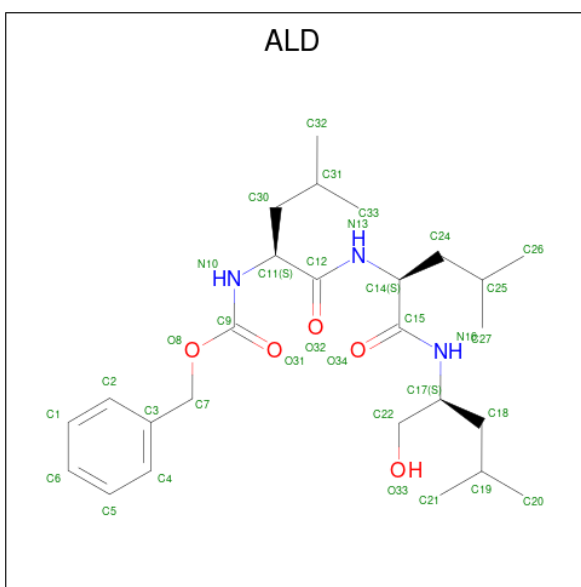
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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	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
15	N	1	Total Mg 1 1	0	0
15	X	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	N	1	Total Cl 1 1	0	0
16	U	1	Total Cl 1 1	0	0
16	b	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 (CCD ID: ALD) (formula: C₂₆H₄₃N₃O₅).



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

- Molecule 18 is water.

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

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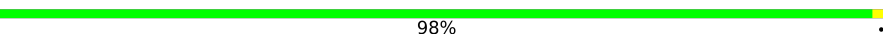
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	I	18	Total 18	O 18	0	0
18	J	23	Total 23	O 23	0	0
18	K	37	Total 37	O 37	0	0
18	L	25	Total 25	O 25	0	0
18	M	27	Total 27	O 27	0	0
18	N	22	Total 22	O 22	0	0
18	O	18	Total 18	O 18	0	0
18	P	13	Total 13	O 13	0	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](#)

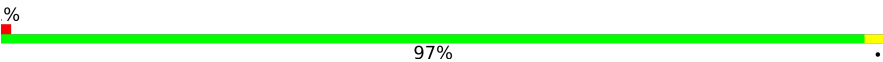
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

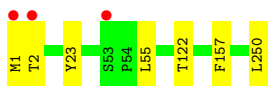
- Molecule 1: Proteasome subunit alpha type-2

Chain A:  98%

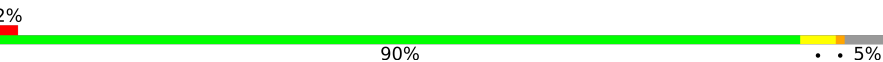


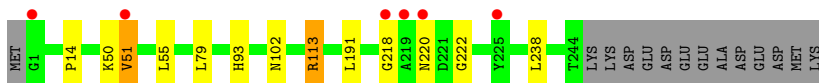
- Molecule 1: Proteasome subunit alpha type-2

Chain O:  97%

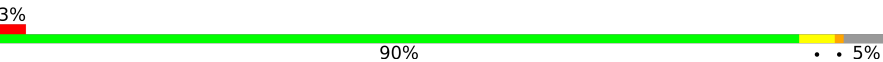


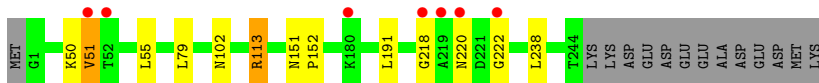
- Molecule 2: Proteasome subunit alpha type-3

Chain B:  90% 2% 5%



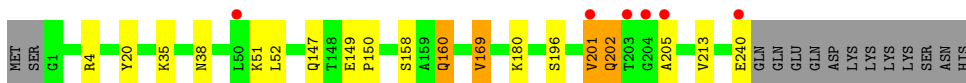
- Molecule 2: Proteasome subunit alpha type-3

Chain P:  90% 3% 5%

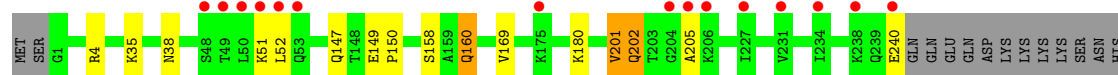
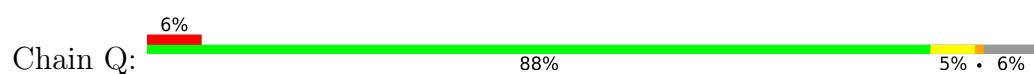


- Molecule 3: Proteasome subunit alpha type-4

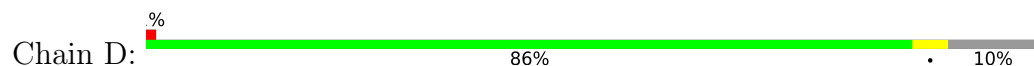
Chain C:  87% 2% 6% 6%



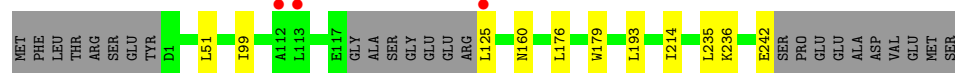
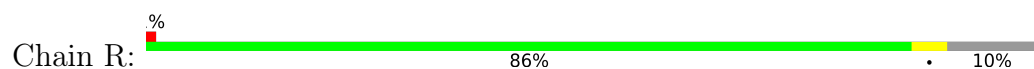
- Molecule 3: Proteasome subunit alpha type-4



- Molecule 4: Proteasome subunit alpha type-5



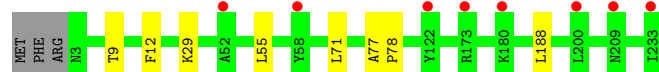
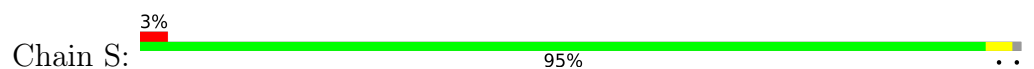
- Molecule 4: Proteasome subunit alpha type-5



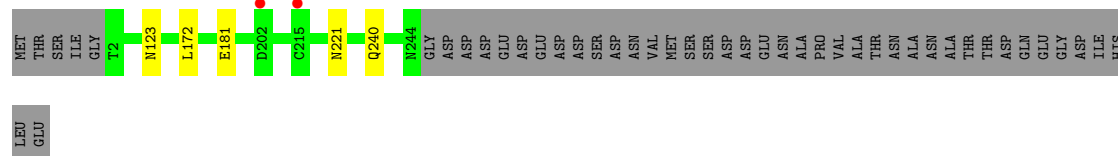
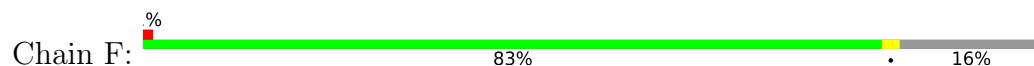
- Molecule 5: Proteasome subunit alpha type-6



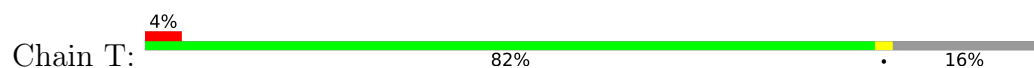
- Molecule 5: Proteasome subunit alpha type-6

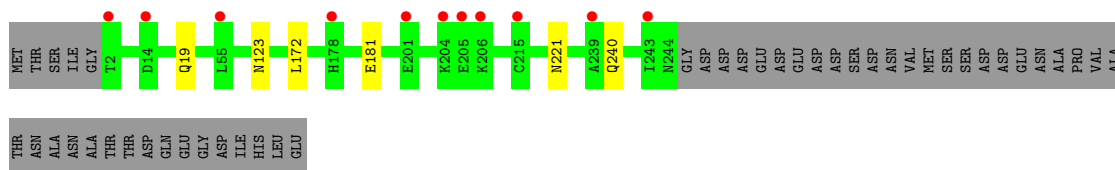


- Molecule 6: Probable proteasome subunit alpha type-7



- Molecule 6: Probable proteasome subunit alpha type-7





• Molecule 7: Proteasome subunit alpha type-1

Chain G: 91%



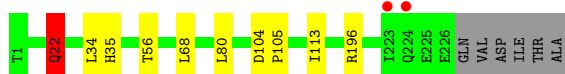
• Molecule 7: Proteasome subunit alpha type-1

Chain U: 90% 5%



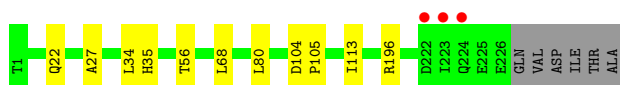
• Molecule 8: Proteasome subunit beta type-2

Chain H: 93% 5%



• Molecule 8: Proteasome subunit beta type-2

Chain V: 93% 5%



• Molecule 9: Proteasome subunit beta type-3

Chain I: 95%

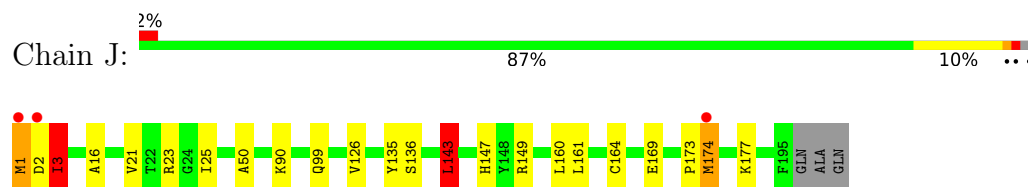


• Molecule 9: Proteasome subunit beta type-3

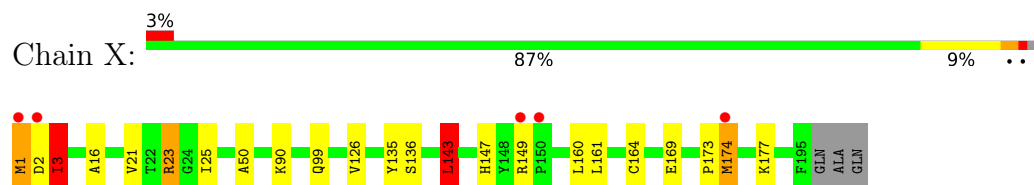
Chain W: 95%



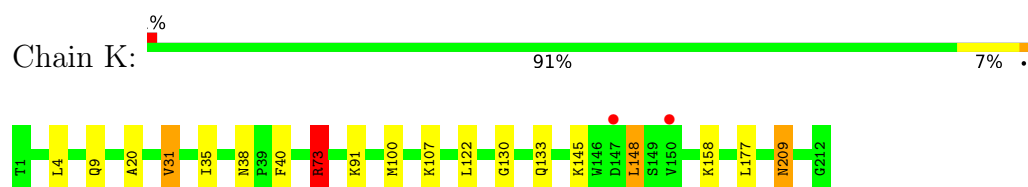
• Molecule 10: Proteasome subunit beta type-4



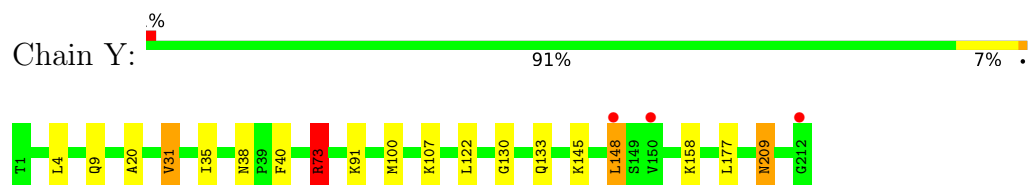
• Molecule 10: Proteasome subunit beta type-4



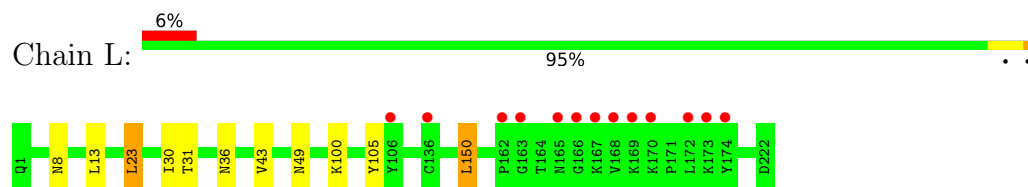
• Molecule 11: Proteasome subunit beta type-5



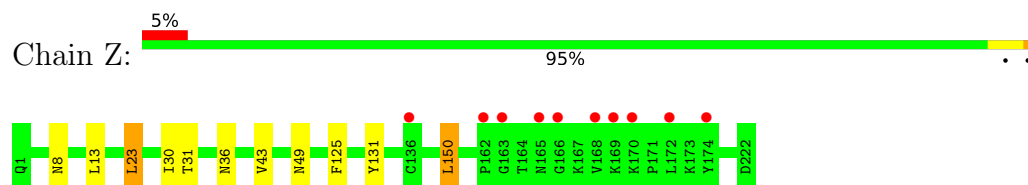
• Molecule 11: Proteasome subunit beta type-5



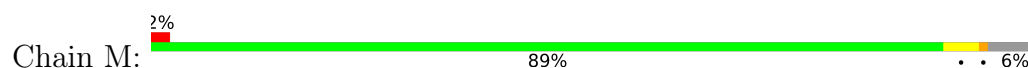
• Molecule 12: Proteasome subunit beta type-6



• Molecule 12: Proteasome subunit beta type-6

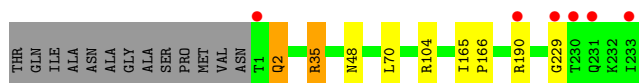


• Molecule 13: Proteasome subunit beta type-7





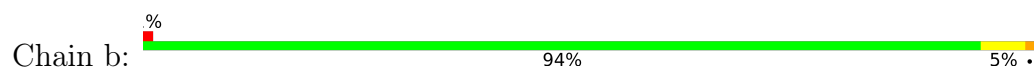
• Molecule 13: Proteasome subunit beta type-7



• 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) 97.6 (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)	0.30 , 51.4	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: MG, ALD, 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	0.40	0/1952	0.68	0/2642
1	O	0.40	0/1952	0.68	0/2642
2	B	0.40	0/1934	0.66	0/2618
2	P	0.39	0/1934	0.66	0/2618
3	C	0.39	0/1910	0.68	1/2586 (0.0%)
3	Q	0.39	0/1910	0.68	1/2586 (0.0%)
4	D	0.39	0/1837	0.66	0/2475
4	R	0.39	0/1837	0.66	0/2475
5	E	0.39	0/1800	0.65	0/2433
5	S	0.39	0/1800	0.65	0/2433
6	F	0.39	0/1932	0.68	0/2609
6	T	0.39	0/1932	0.69	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	0.67	2/2373 (0.1%)
8	V	0.36	0/1750	0.66	0/2373
9	I	0.35	0/1611	0.68	0/2174
9	W	0.35	0/1611	0.68	0/2174
10	J	0.40	0/1589	0.73	1/2142 (0.0%)
10	X	0.40	0/1589	0.73	1/2142 (0.0%)
11	K	0.48	1/1681 (0.1%)	0.73	2/2274 (0.1%)
11	Y	0.48	2/1681 (0.1%)	0.71	1/2274 (0.0%)
12	L	0.35	0/1795	0.67	0/2420
12	Z	0.36	0/1795	0.67	0/2420
13	M	0.38	0/1837	0.72	2/2492 (0.1%)
13	a	0.39	0/1855	0.79	4/2514 (0.2%)
14	N	0.35	0/1541	0.67	0/2087
14	b	0.35	0/1541	0.67	0/2087
All	All	0.39	3/50246 (0.0%)	0.68	15/67940 (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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	73	ARG	CD-NE	-10.95	1.30	1.46
11	Y	73	ARG	CD-NE	-9.95	1.32	1.46
11	Y	73	ARG	CZ-NH2	-5.07	1.26	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	35	ARG	NE-CZ-NH2	13.59	131.43	119.20
13	a	35	ARG	CD-NE-CZ	8.83	136.76	124.40
10	X	143	LEU	CD1-CG-CD2	-7.99	93.22	110.80
10	J	143	LEU	CD1-CG-CD2	-7.96	93.29	110.80
13	a	35	ARG	NE-CZ-NH1	-7.59	113.91	121.50
11	K	73	ARG	CB-CG-CD	-6.92	95.37	111.30
13	M	35	ARG	NE-CZ-NH1	6.83	128.33	121.50
13	M	35	ARG	CD-NE-CZ	6.72	133.81	124.40
8	H	22	GLN	CB-CG-CD	6.46	123.59	112.60
11	K	73	ARG	NE-CZ-NH1	-6.30	115.19	121.50
3	Q	201	VAL	N-CA-C	5.84	116.58	110.62
3	C	201	VAL	N-CA-C	5.76	116.49	110.62
11	Y	73	ARG	CD-NE-CZ	-5.26	117.04	124.40
8	H	22	GLN	CA-CB-CG	5.25	124.60	114.10
13	a	35	ARG	NH1-CZ-NH2	-5.08	112.70	119.30

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	29	0
11	K	1644	0	1596	11	0
11	Y	1644	0	1596	12	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	2	0
14	N	1512	0	1480	6	0
14	b	1512	0	1480	6	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

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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	1	0
All	All	50090	0	49274	140	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 (140) 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
10:J:174:MET:N	10:J:174:MET:HE3	1.84	0.93
10:X:174:MET:N	10:X:174:MET:HE3	1.88	0.87
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:J:135:TYR:CD1	10:X:25:ILE:HD11	2.35	0.61
10:X:1:MET:HG2	10:X:135:TYR:HD2	1.64	0.61
10:J:25:ILE:HD11	10:X:135:TYR:CD1	2.37	0.60
10:J:143:LEU:HD23	10:J:164:CYS:SG	2.42	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	1.89	0.55
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
14:b:152:VAL:HA	14:b:175:MET:HE1	1.88	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
13:a:2:GLN:HB3	18:b:311:HOH:O	2.08	0.54
13:M:35:ARG:NH2	18:M:401:HOH:O	2.40	0.53
10:J:174:MET:HE3	10:J:174:MET:H	1.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:173:PRO:C	10:J:174:MET:HE3	2.36	0.51
10:X:173:PRO:C	10:X:174:MET:HE3	2.34	0.50
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
2:B:50:LYS:O	2:B:51:VAL:C	2.56	0.48
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
2:P:50:LYS:O	2:P:51:VAL:C	2.56	0.48
10:X:23:ARG:HD3	10:X:23:ARG:HA	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	1.96	0.47
10:J:2:ASP:O	10:J:3:ILE:C	2.58	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:HE21	8:H:22:GLN:CA	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
10:X:174:MET:N	10:X:174:MET:CE	2.72	0.45
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.99	0.45
10:J:169:GLU:O	10:X:177:LYS:NZ	2.50	0.45
14:b:83:LYS:HG3	14:b:119:VAL:CG2	2.46	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
11:Y:38:ASN:OD1	11:Y:38:ASN:C	2.61	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
14:b:176:VAL:HG12	14:b:178:LEU:HD13	1.99	0.44
9:W:36:SER:HB2	10:X:126:VAL:HG11	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
10:X:2:ASP:O	10:X:3:ILE:C	2.61	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
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
7:G:78:ILE:N	7:G:79:PRO:CD	2.82	0.43
11:K:38:ASN:OD1	11:K:38:ASN:C	2.61	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
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
14:b:36:ARG:HG3	14:b:42:TRP:CE2	2.54	0.42
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.84	0.42
11:K:130:GLY:O	11:K:133:GLN:HG2	2.20	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	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:HD22	11:Y:209:ASN:H	1.67	0.42
14:N:133:PHE:HA	14:b:132:THR:O	2.19	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	2.03	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
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:50:LYS:HD3	2:P:50:LYS:HA	1.92	0.41
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:20:VAL:HG23	9:W:189:ILE:HB	2.03	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
14:N:132:THR:O	14:b:133:PHE:HA	2.20	0.40
11:Y:20:ALA:HB2	11:Y:31:VAL:HG11	2.03	0.40
13:a:165:ILE:HB	13:a:166:PRO:HD3	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
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:H	11:K:209:ASN:HD22	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 ⓘ

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%)	241 (97%)	6 (2%)	1 (0%)	30	51
1	O	248/250 (99%)	240 (97%)	7 (3%)	1 (0%)	30	51
2	B	242/258 (94%)	234 (97%)	4 (2%)	4 (2%)	7	15
2	P	242/258 (94%)	233 (96%)	5 (2%)	4 (2%)	7	15
3	C	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	16	34
3	Q	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	16	34
4	D	231/260 (89%)	227 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	24	46
10	X	193/198 (98%)	190 (98%)	2 (1%)	1 (0%)	24	46
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%)	30	51
13	a	231/246 (94%)	222 (96%)	8 (4%)	1 (0%)	30	51
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%)	36	58

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

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Mol	Chain	Res	Type
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%)	205 (98%)	4 (2%)	50	75
1	O	209/209 (100%)	205 (98%)	4 (2%)	50	75
2	B	203/216 (94%)	197 (97%)	6 (3%)	36	64
2	P	203/216 (94%)	197 (97%)	6 (3%)	36	64
3	C	212/226 (94%)	202 (95%)	10 (5%)	23	48
3	Q	212/226 (94%)	203 (96%)	9 (4%)	26	52
4	D	194/215 (90%)	185 (95%)	9 (5%)	24	49
4	R	194/215 (90%)	185 (95%)	9 (5%)	24	49
5	E	190/193 (98%)	185 (97%)	5 (3%)	40	68
5	S	190/193 (98%)	185 (97%)	5 (3%)	40	68
6	F	201/239 (84%)	196 (98%)	5 (2%)	42	69
6	T	201/239 (84%)	196 (98%)	5 (2%)	42	69
7	G	206/210 (98%)	199 (97%)	7 (3%)	32	60
7	U	206/210 (98%)	199 (97%)	7 (3%)	32	60
8	H	185/190 (97%)	181 (98%)	4 (2%)	45	72
8	V	185/190 (97%)	182 (98%)	3 (2%)	55	79
9	I	172/173 (99%)	170 (99%)	2 (1%)	63	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	W	172/173 (99%)	170 (99%)	2 (1%)	63	83
10	J	173/175 (99%)	164 (95%)	9 (5%)	21	44
10	X	173/175 (99%)	164 (95%)	9 (5%)	21	44
11	K	169/169 (100%)	161 (95%)	8 (5%)	23	48
11	Y	169/169 (100%)	160 (95%)	9 (5%)	20	43
12	L	185/185 (100%)	182 (98%)	3 (2%)	55	79
12	Z	185/185 (100%)	182 (98%)	3 (2%)	55	79
13	M	197/208 (95%)	192 (98%)	5 (2%)	42	69
13	a	199/208 (96%)	194 (98%)	5 (2%)	42	69
14	N	162/162 (100%)	159 (98%)	3 (2%)	50	75
14	b	162/162 (100%)	159 (98%)	3 (2%)	50	75
All	All	5318/5540 (96%)	5159 (97%)	159 (3%)	36	64

All (159) 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	102	ASN
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	52	LEU
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	51	LEU
4	D	99	ILE

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Mol	Chain	Res	Type
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	172	LEU
6	F	181	GLU
6	F	221	ASN
6	F	240	GLN
7	G	26	THR
7	G	75	ASN
7	G	115	LEU
7	G	122	ARG
7	G	125	MET
7	G	235	ARG
7	G	236	LEU
8	H	22	GLN
8	H	34	LEU
8	H	68	LEU
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
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	31	VAL

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Mol	Chain	Res	Type
11	K	35	ILE
11	K	100	MET
11	K	107	LYS
11	K	148	LEU
11	K	209	ASN
12	L	23	LEU
12	L	49	ASN
12	L	150	LEU
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	190	ARG
14	N	9	LYS
14	N	119	VAL
14	N	178	LEU
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	102	ASN
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	52	LEU
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	240	GLU
4	R	51	LEU
4	R	99	ILE
4	R	125	LEU
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	235	LEU

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Mol	Chain	Res	Type
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	172	LEU
6	T	181	GLU
6	T	221	ASN
6	T	240	GLN
7	U	26	THR
7	U	75	ASN
7	U	115	LEU
7	U	122	ARG
7	U	125	MET
7	U	235	ARG
7	U	236	LEU
8	V	34	LEU
8	V	68	LEU
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
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	31	VAL
11	Y	35	ILE
11	Y	73	ARG
11	Y	100	MET
11	Y	107	LYS
11	Y	148	LEU
11	Y	209	ASN

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Mol	Chain	Res	Type
12	Z	23	LEU
12	Z	49	ASN
12	Z	150	LEU
13	a	2	GLN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	190	ARG
14	b	9	LYS
14	b	119	VAL
14	b	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (111) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	119	GLN
2	B	123	GLN
2	B	124	HIS
2	B	220	ASN
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	106	GLN
4	D	225	ASN
5	E	68	HIS
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	123	ASN
7	G	6	HIS
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	175	ASN
8	H	22	GLN

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Mol	Chain	Res	Type
8	H	86	HIS
9	I	63	ASN
9	I	88	GLN
9	I	168	GLN
9	I	203	GLN
10	J	55	GLN
10	J	63	ASN
11	K	9	GLN
11	K	85	ASN
11	K	176	ASN
11	K	209	ASN
12	L	3	ASN
12	L	29	ASN
12	L	36	ASN
12	L	49	ASN
12	L	79	HIS
12	L	80	ASN
12	L	152	ASN
12	L	158	ASN
12	L	159	GLN
12	L	197	GLN
13	M	26	ASN
13	M	48	ASN
13	M	102	GLN
13	M	108	ASN
13	M	149	HIS
13	M	194	ASN
13	M	213	GLN
14	N	38	HIS
14	N	141	ASN
14	N	161	GLN
2	P	124	HIS
2	P	220	ASN
3	Q	38	ASN
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	106	GLN

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Mol	Chain	Res	Type
4	R	225	ASN
5	S	68	HIS
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
7	U	175	ASN
9	W	63	ASN
9	W	168	GLN
9	W	203	GLN
10	X	55	GLN
10	X	63	ASN
10	X	78	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	176	ASN
12	Z	3	ASN
12	Z	29	ASN
12	Z	36	ASN
12	Z	49	ASN
12	Z	79	HIS
12	Z	152	ASN
12	Z	158	ASN
12	Z	159	GLN
12	Z	197	GLN
13	a	26	ASN
13	a	48	ASN
13	a	62	HIS
13	a	102	GLN
13	a	108	ASN
13	a	194	ASN
13	a	213	GLN
14	b	38	HIS
14	b	141	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 ⓘ

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, 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	b	201	15,14	34,34,34	1.06	1 (2%)	44,44,44	0.88	3 (6%)
17	ALD	K	301	11	34,34,34	1.03	1 (2%)	44,44,44	0.93	3 (6%)
17	ALD	Y	301	11	34,34,34	1.04	1 (2%)	44,44,44	0.92	3 (6%)
17	ALD	N	201	14	34,34,34	1.07	1 (2%)	44,44,44	0.90	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	b	201	15,14	-	2/39/39/39	0/1/1/1
17	ALD	K	301	11	-	4/39/39/39	0/1/1/1
17	ALD	Y	301	11	-	4/39/39/39	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	5.49	1.46	1.35
17	b	201	ALD	O8-C9	5.45	1.46	1.35
17	Y	301	ALD	O8-C9	5.08	1.45	1.35
17	K	301	ALD	O8-C9	5.07	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	2.98	122.64	115.93
17	K	301	ALD	C7-O8-C9	2.97	122.61	115.93
17	N	201	ALD	O8-C9-N10	2.88	116.61	110.45
17	b	201	ALD	O8-C9-N10	2.79	116.42	110.45
17	N	201	ALD	C7-O8-C9	2.66	121.92	115.93
17	b	201	ALD	C7-O8-C9	2.62	121.82	115.93
17	N	201	ALD	O8-C9-O31	-2.56	119.34	124.26
17	b	201	ALD	O8-C9-O31	-2.48	119.51	124.26
17	K	301	ALD	O8-C9-N10	2.37	115.51	110.45
17	Y	301	ALD	O8-C9-N10	2.30	115.37	110.45
17	K	301	ALD	O8-C9-O31	-2.27	119.91	124.26
17	Y	301	ALD	O8-C9-O31	-2.25	119.95	124.26

There are no chirality outliers.

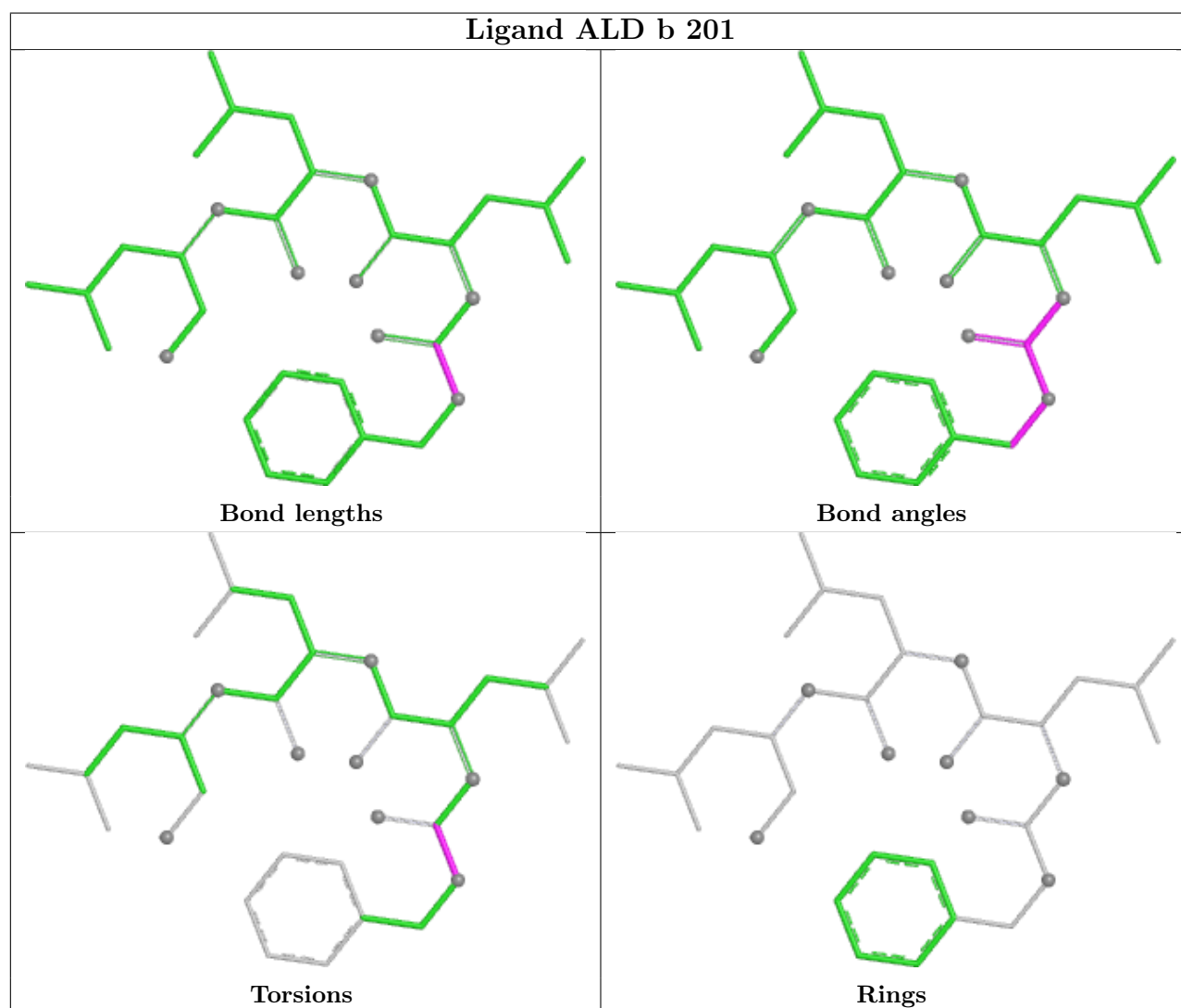
All (12) torsion outliers are listed below:

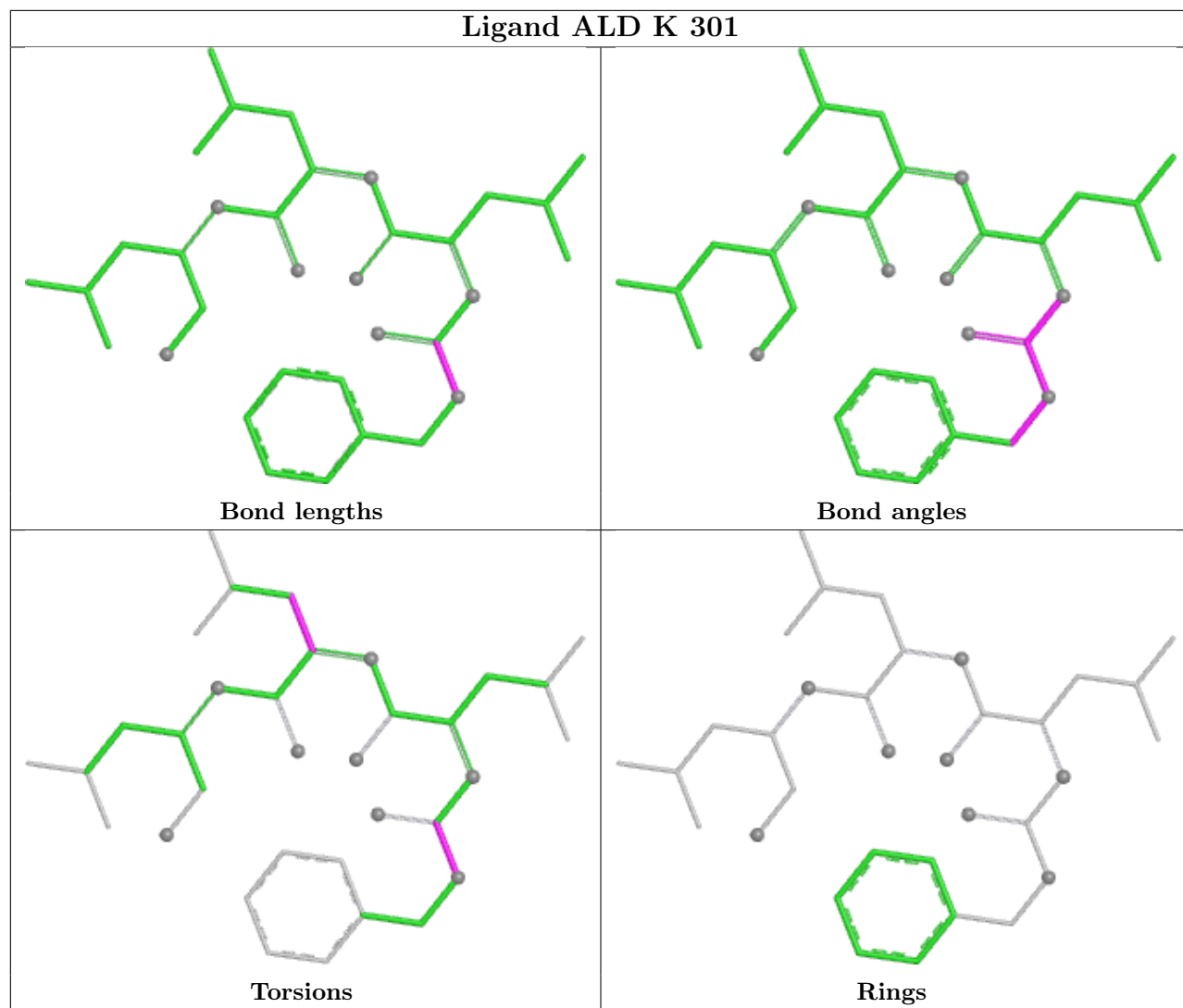
Mol	Chain	Res	Type	Atoms
17	K	301	ALD	O31-C9-O8-C7
17	Y	301	ALD	O31-C9-O8-C7
17	K	301	ALD	N10-C9-O8-C7
17	Y	301	ALD	N10-C9-O8-C7
17	N	201	ALD	N10-C9-O8-C7
17	N	201	ALD	O31-C9-O8-C7
17	b	201	ALD	N10-C9-O8-C7
17	b	201	ALD	O31-C9-O8-C7
17	Y	301	ALD	C15-C14-C24-C25
17	K	301	ALD	C15-C14-C24-C25
17	K	301	ALD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

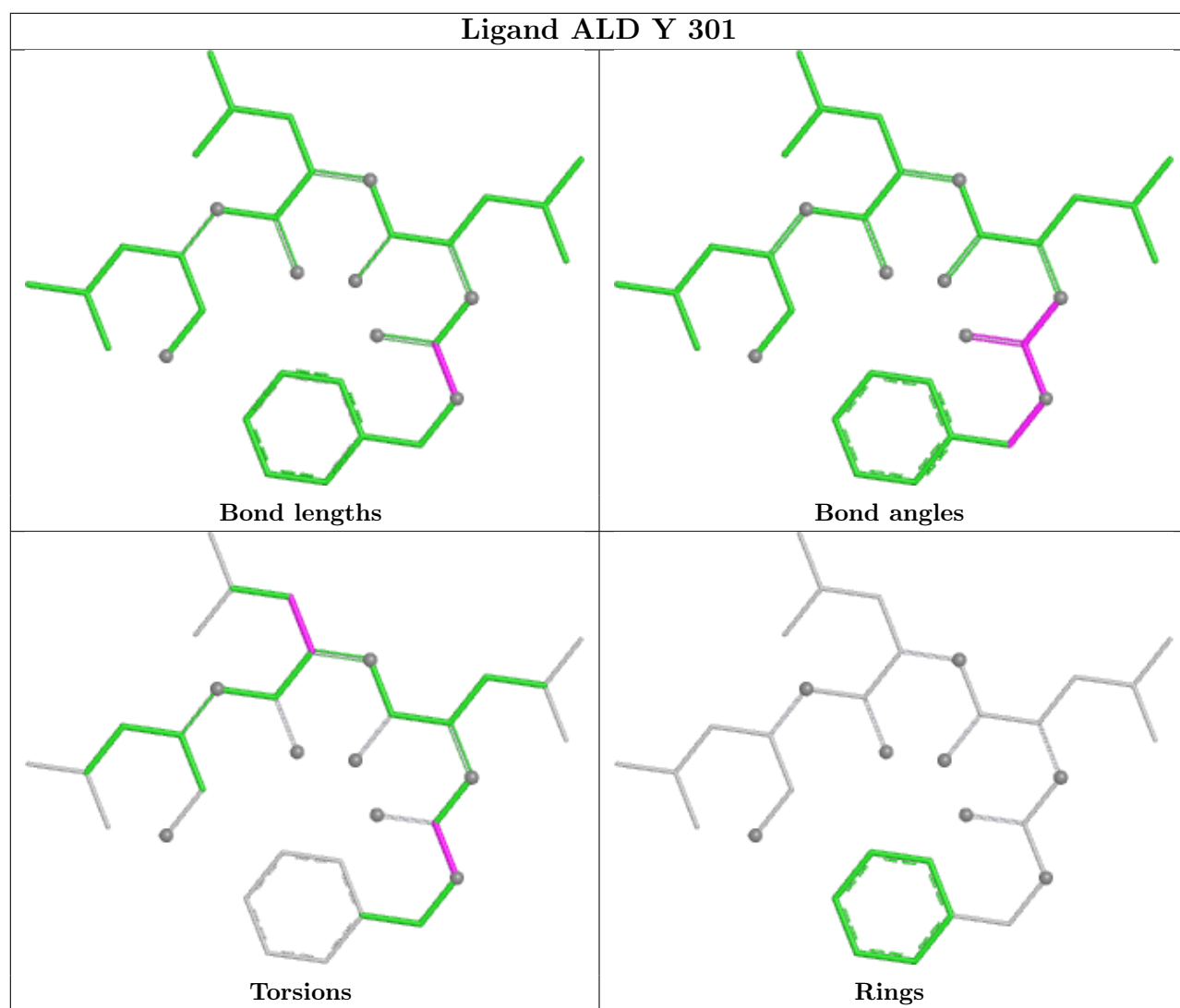
There are no ring outliers.

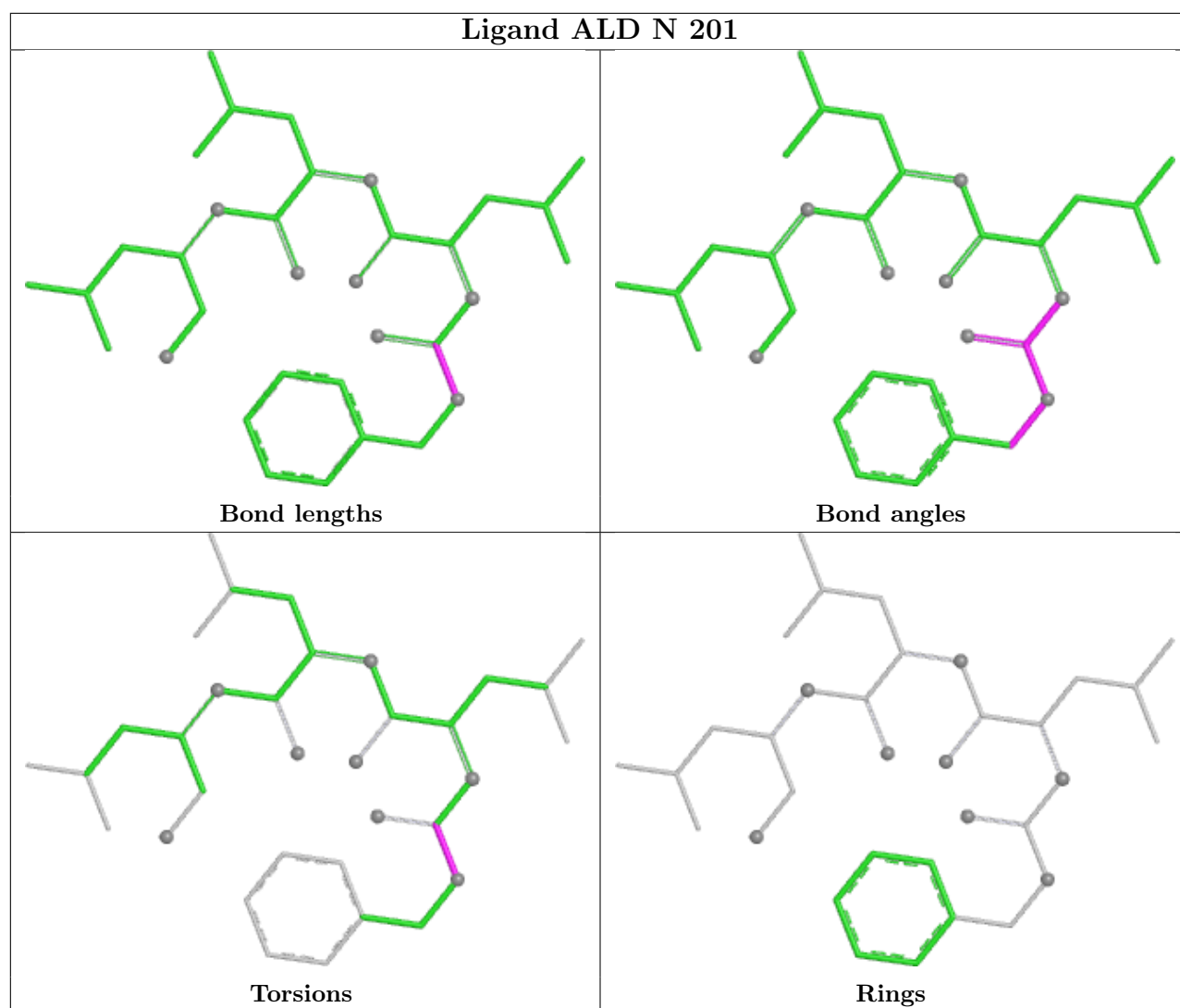
No monomer is involved in short contacts.

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.









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%)	-0.29	1 (0%) 88 86	37, 53, 90, 128	0
1	O	250/250 (100%)	-0.22	3 (1%) 76 73	42, 62, 106, 140	0
2	B	244/258 (94%)	-0.10	6 (2%) 58 52	39, 60, 105, 165	0
2	P	244/258 (94%)	0.00	7 (2%) 53 48	43, 65, 107, 162	0
3	C	240/254 (94%)	-0.06	6 (2%) 58 52	40, 65, 128, 160	0
3	Q	240/254 (94%)	0.22	15 (6%) 26 20	50, 79, 163, 186	0
4	D	235/260 (90%)	-0.14	3 (1%) 75 71	43, 65, 101, 145	0
4	R	235/260 (90%)	-0.08	3 (1%) 75 71	48, 68, 111, 147	0
5	E	231/234 (98%)	-0.03	2 (0%) 81 78	46, 68, 105, 149	0
5	S	231/234 (98%)	0.15	8 (3%) 47 41	47, 73, 120, 152	0
6	F	243/288 (84%)	-0.19	2 (0%) 82 80	34, 59, 110, 138	0
6	T	243/288 (84%)	0.01	11 (4%) 38 32	33, 68, 128, 156	0
7	G	241/252 (95%)	-0.31	1 (0%) 88 86	37, 56, 95, 152	0
7	U	241/252 (95%)	-0.23	4 (1%) 69 64	42, 57, 94, 138	0
8	H	226/232 (97%)	-0.20	2 (0%) 81 78	38, 54, 91, 150	0
8	V	226/232 (97%)	-0.17	3 (1%) 75 71	39, 57, 93, 185	0
9	I	204/205 (99%)	-0.43	0 100 100	35, 50, 86, 110	0
9	W	204/205 (99%)	-0.41	1 (0%) 87 85	37, 54, 87, 107	0
10	J	195/198 (98%)	-0.24	3 (1%) 72 68	33, 56, 84, 121	0
10	X	195/198 (98%)	-0.20	5 (2%) 57 51	33, 59, 86, 136	0
11	K	212/212 (100%)	-0.20	2 (0%) 81 78	36, 54, 88, 106	0
11	Y	212/212 (100%)	-0.14	3 (1%) 73 69	38, 54, 90, 108	0
12	L	222/222 (100%)	-0.16	13 (5%) 28 23	35, 55, 105, 134	0
12	Z	222/222 (100%)	-0.17	10 (4%) 38 32	38, 53, 103, 135	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	231/246 (93%)	-0.31	4 (1%) 69 64	33, 53, 83, 99	0
13	a	233/246 (94%)	-0.36	6 (2%) 57 51	34, 52, 79, 108	0
14	N	196/196 (100%)	-0.47	1 (0%) 87 85	34, 47, 80, 105	0
14	b	196/196 (100%)	-0.49	2 (1%) 79 76	34, 49, 83, 110	0
All	All	6342/6614 (95%)	-0.18	127 (2%) 65 60	33, 59, 106, 186	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	V	223	ILE	7.3
12	Z	174	TYR	6.8
3	Q	50	LEU	6.4
13	a	233	ILE	5.4
12	L	174	TYR	5.2
12	L	165	ASN	5.0
8	H	223	ILE	4.9
10	X	1	MET	4.5
3	Q	205	ALA	4.4
13	M	229	GLY	4.2
3	Q	51	LYS	4.2
12	Z	169	LYS	4.1
13	M	230	THR	4.1
6	T	204	LYS	4.1
3	Q	49	THR	4.0
4	D	240	ALA	3.9
3	C	50	LEU	3.9
6	F	215	CYS	3.8
12	Z	168	VAL	3.8
2	B	51	VAL	3.8
6	T	243	ILE	3.7
2	B	219	ALA	3.7
2	P	51	VAL	3.7
10	J	1	MET	3.7
2	B	218	GLY	3.7
3	Q	234	ILE	3.5
12	Z	165	ASN	3.4
3	C	205	ALA	3.4
13	a	1	THR	3.4
2	P	218	GLY	3.4
8	V	224	GLN	3.4
2	P	219	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
12	L	170	LYS	3.3
13	a	231	GLN	3.2
12	L	168	VAL	3.2
6	F	202	ASP	3.2
13	a	230	THR	3.1
3	Q	52	LEU	3.1
12	L	162	PRO	3.0
2	P	52	THR	3.0
12	L	169	LYS	3.0
7	U	222	ASP	3.0
10	J	2	ASP	3.0
12	L	167	LYS	3.0
14	b	103	ASP	3.0
12	L	172	LEU	2.9
3	C	204	GLY	2.9
12	Z	170	LYS	2.9
1	O	1	MET	2.9
14	b	1	THR	2.9
3	Q	204	GLY	2.9
12	Z	172	LEU	2.9
10	J	174	MET	2.8
1	A	249	ALA	2.8
1	O	2	THR	2.8
10	X	174	MET	2.8
5	S	52	ALA	2.7
5	S	122	TYR	2.7
3	C	240	GLU	2.7
6	T	215	CYS	2.7
1	O	53	SER	2.7
13	M	231	GLN	2.6
3	Q	240	GLU	2.6
4	R	113	LEU	2.6
2	B	1	GLY	2.6
3	Q	206	LYS	2.6
13	M	1	THR	2.6
4	R	125	LEU	2.6
3	Q	175	LYS	2.6
12	Z	166	GLY	2.6
12	L	136	CYS	2.6
3	C	203	THR	2.5
6	T	206	LYS	2.5
2	P	222	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
3	Q	48	SER	2.5
10	X	149	ARG	2.5
12	L	106	TYR	2.5
12	L	163	GLY	2.5
11	Y	148	LEU	2.5
10	X	2	ASP	2.5
11	K	147	ASP	2.5
12	Z	163	GLY	2.4
5	E	122	TYR	2.4
13	a	229	GLY	2.4
3	C	201	VAL	2.4
11	Y	212	GLY	2.4
3	Q	231	VAL	2.4
4	D	241	ALA	2.4
12	Z	162	PRO	2.3
5	E	123	GLY	2.3
6	T	55	LEU	2.3
5	S	58	TYR	2.3
3	Q	53	GLN	2.2
12	L	166	GLY	2.2
3	Q	238	LYS	2.2
6	T	205	GLU	2.2
10	X	150	PRO	2.2
2	P	220	ASN	2.2
8	V	222	ASP	2.2
9	W	130	ASP	2.2
14	N	103	ASP	2.2
3	Q	227	ILE	2.2
12	Z	136	CYS	2.1
7	U	179	LYS	2.1
12	L	173	LYS	2.1
5	S	233	ILE	2.1
4	D	242	GLU	2.1
2	B	220	ASN	2.1
5	S	209	ASN	2.1
7	U	242	GLN	2.1
11	K	150	VAL	2.1
11	Y	150	VAL	2.1
4	R	112	ALA	2.1
13	a	190	ARG	2.1
2	B	225	TYR	2.1
6	T	178	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
7	G	68	ARG	2.1
6	T	2	THR	2.1
5	S	200	LEU	2.1
7	U	2	GLY	2.0
5	S	173	ARG	2.0
6	T	14	ASP	2.0
6	T	201	GLU	2.0
2	P	180	LYS	2.0
5	S	180	LYS	2.0
6	T	239	ALA	2.0
8	H	224	GLN	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.

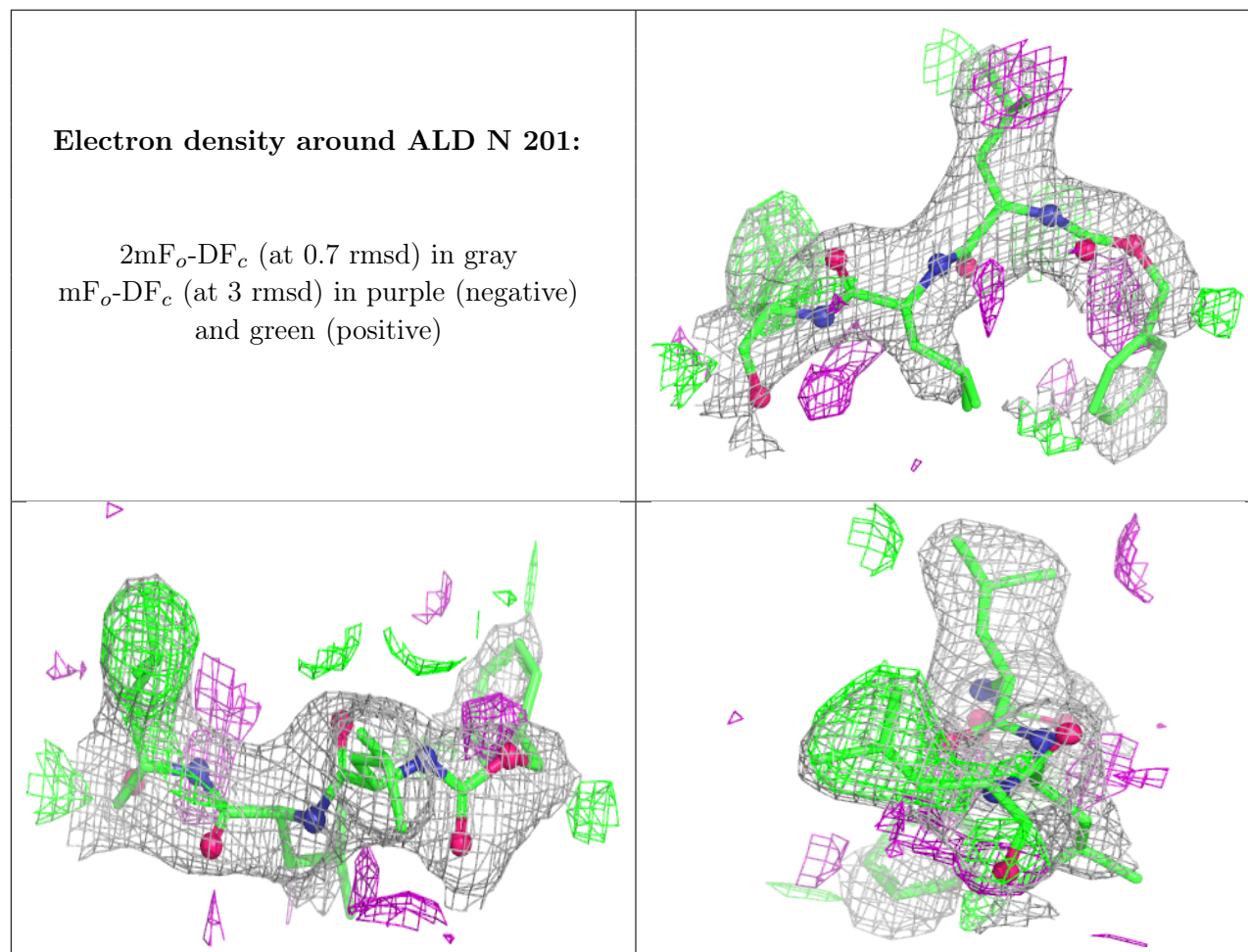
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
17	ALD	N	201	34/34	0.89	0.19	63,100,136,138	0
17	ALD	b	201	34/34	0.90	0.17	68,91,126,132	0
17	ALD	Y	301	34/34	0.91	0.20	68,104,128,136	0
17	ALD	K	301	34/34	0.92	0.19	64,96,115,116	0
16	CL	b	203	1/1	0.93	0.16	94,94,94,94	0
15	MG	I	302	1/1	0.94	0.10	54,54,54,54	0
15	MG	Z	301	1/1	0.95	0.05	59,59,59,59	0
15	MG	G	301	1/1	0.95	0.05	58,58,58,58	0
15	MG	X	201	1/1	0.96	0.07	38,38,38,38	0
15	MG	I	301	1/1	0.96	0.05	67,67,67,67	0
16	CL	N	203	1/1	0.96	0.13	73,73,73,73	0
15	MG	L	301	1/1	0.96	0.07	67,67,67,67	0

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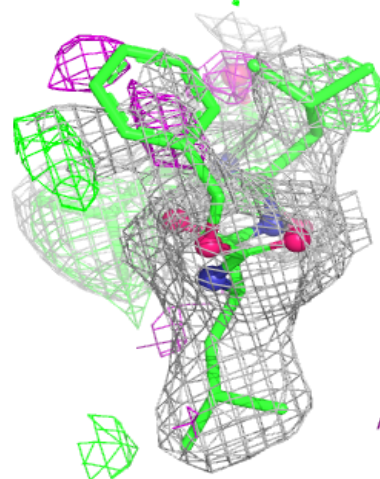
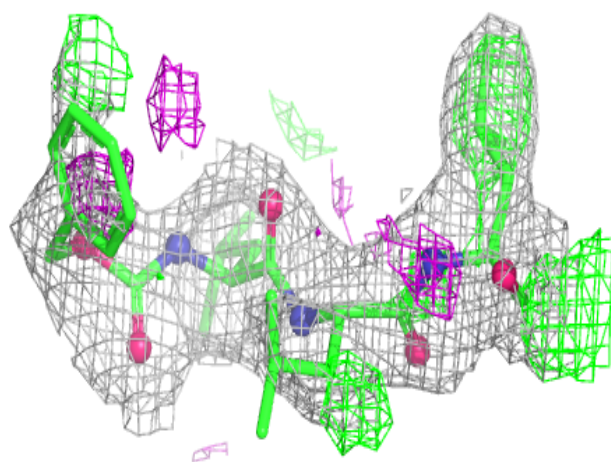
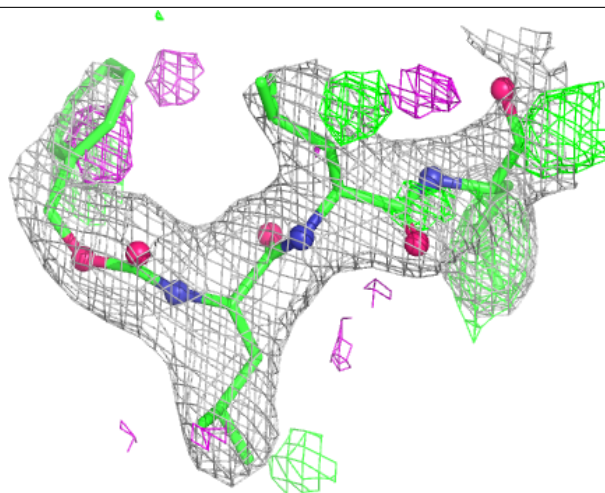
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	MG	K	302	1/1	0.97	0.06	68,68,68,68	0
15	MG	M	301	1/1	0.98	0.21	46,46,46,46	0
15	MG	N	202	1/1	0.99	0.04	44,44,44,44	0
15	MG	b	202	1/1	0.99	0.04	34,34,34,34	0
16	CL	G	302	1/1	0.99	0.06	42,42,42,42	0
15	MG	J	201	1/1	0.99	0.18	42,42,42,42	0
16	CL	U	301	1/1	0.99	0.10	44,44,44,44	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.



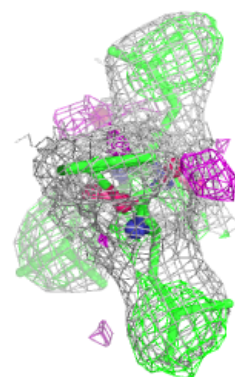
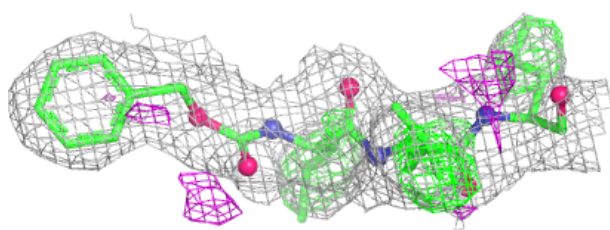
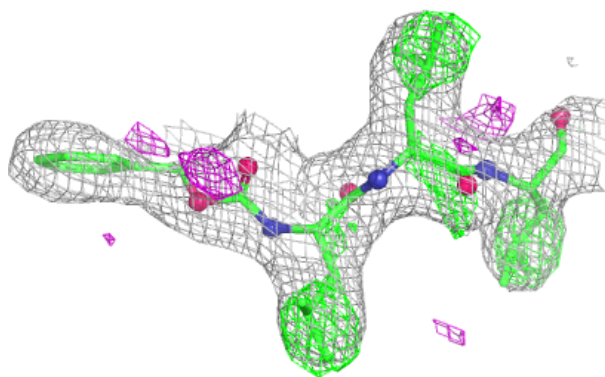
Electron density around ALD b 201:

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

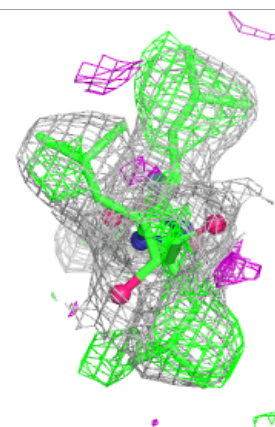
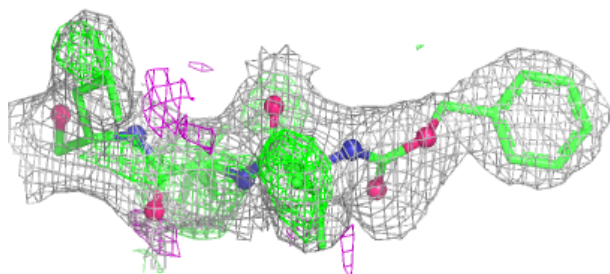
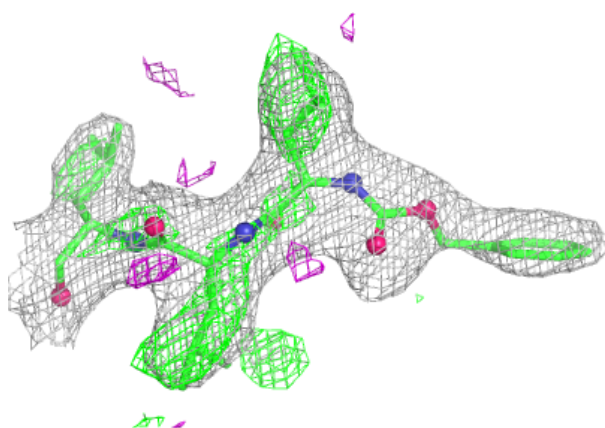


Electron density around ALD Y 301:

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

**Electron density around ALD 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.