



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 18, 2026 – 08:52 PM UTC

PDB ID : 9FSV / pdb_00009fsv
Title : Yeast 20S proteasome with human beta2i (1-53) in complex with epoxyketone inhibitor 16
Authors : Maurits, E.; Huber, E.M.; Dekker, P.M.; Wang, X.; Heinemeyer, W.; Florea, B.I.; Groll, M.; Overkleeft, H.S.
Deposited on : 2024-06-22
Resolution : 2.75 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

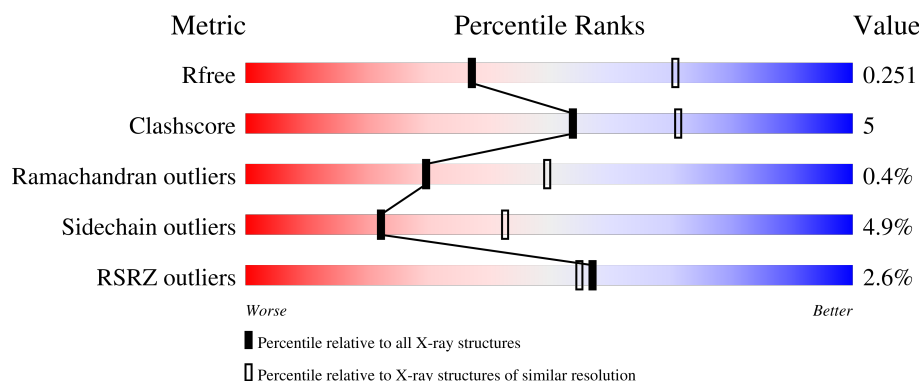
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	4% 91% 9%
1	O	250	4% 90% 9%
2	B	258	4% 79% 15% 5%
2	P	258	4% 79% 15% 5%

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Mol	Chain	Length	Quality of chain
3	C	254	5% 84% 9% • 6%
3	Q	254	9% 82% 10% • 6%
4	D	260	3% 77% 13% • 10%
4	R	260	4% 78% 11% • 10%
5	E	234	% 87% 10% ••
5	S	234	4% 83% 14% ••
6	F	288	% 74% 10% • 16%
6	T	288	3% 73% 11% • 16%
7	G	252	2% 81% 11% ••
7	U	252	2% 83% 12% ••
8	H	225	3% 88% 10% •
8	V	225	% 81% 16% ••
9	I	205	% 86% 13%
9	W	205	% 85% 13% •
10	J	198	2% 83% 13% •••
10	X	198	3% 84% 13% ••
11	K	211	% 84% 15% •
11	Y	211	% 83% 16% •
12	L	222	% 85% 13% •
12	Z	222	% 85% 13% •
13	M	246	2% 86% 8% • 5%
13	a	246	% 75% 17% • 5%
14	N	196	% 83% 15% •
14	b	196	% 83% 15% •

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 49917 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-10, Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	225	Total	C	N	O	S	0	0	0
			1709	1077	290	334	8			
8	V	222	Total	C	N	O	S	0	0	0
			1681	1062	286	325	8			

- 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	211	Total	C	N	O	S	0	0	0
			1637	1041	279	310	7			
11	Y	211	Total	C	N	O	S	0	0	0
			1637	1041	279	310	7			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	1	0
			1835	1160	316	352	7			
13	a	233	Total	C	N	O	S	0	1	0
			1835	1160	316	352	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	0	0
			1	1		
15	I	1	Total	Mg	0	0
			1	1		

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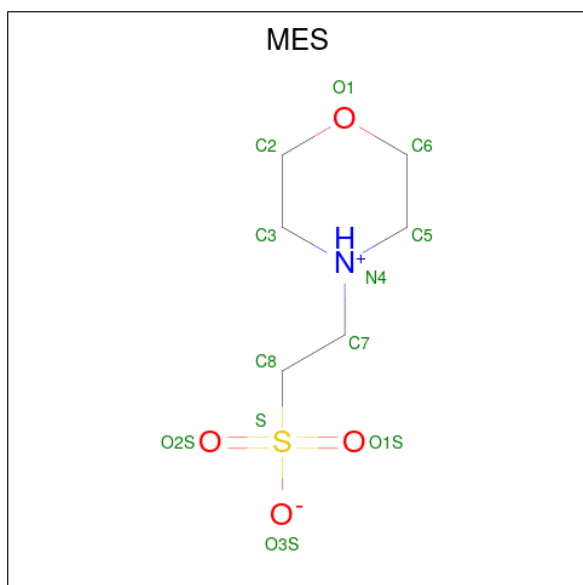
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	K	1	Total	Mg	0	0
			1	1		
15	N	1	Total	Mg	0	0
			1	1		
15	V	1	Total	Mg	0	0
			1	1		
15	W	1	Total	Mg	0	0
			1	1		
15	Y	1	Total	Mg	0	0
			1	1		
15	Z	1	Total	Mg	0	0
			1	1		

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

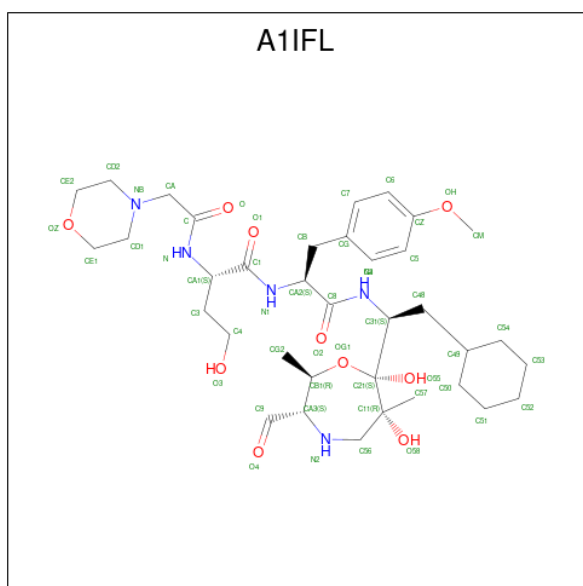
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	G	1	Total	Cl	0	0
			1	1		
16	N	1	Total	Cl	0	0
			1	1		
16	U	1	Total	Cl	0	0
			1	1		

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



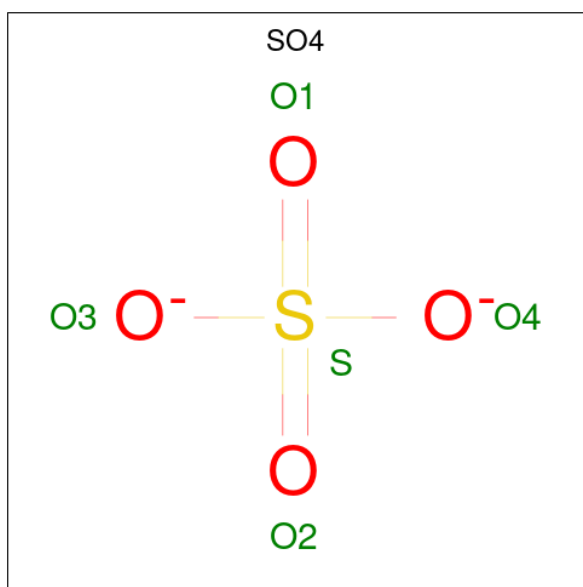
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
17	K	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
17	V	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
17	Y	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 18 is (2S)-N-[(2S)-1-[(1S)-2-cyclohexyl-1-[(2R,3S,6R,7S)-3-methanoyl-2,6-dimethyl-6,7-bis(oxidanyl)-1,4-oxazepan-7-yl]ethyl]amino]-3-(4-methoxyphenyl)-1-oxidanylidene-propan-2-yl]-2-(2-morpholin-4-ylethanoylamino)-4-oxidanyl-butanamide (CCD ID: A1IFL) (formula: C₃₆H₅₇N₅O₁₀) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	H	1	Total	C	N	O		0	0
			51	36	5	10			
18	K	1	Total	C	N	O		0	0
			51	36	5	10			
18	V	1	Total	C	N	O		0	0
			51	36	5	10			
18	Y	1	Total	C	N	O		0	0
			51	36	5	10			

- Molecule 19 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	K	1	Total	O	S	0	0
			5	4	1		
19	N	1	Total	O	S	0	0
			5	4	1		
19	Y	1	Total	O	S	0	0
			5	4	1		
19	b	1	Total	O	S	0	0
			5	4	1		

- Molecule 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	7	Total	O	0	0
			7	7		
20	B	14	Total	O	0	0
			14	14		
20	C	6	Total	O	0	0
			6	6		
20	D	9	Total	O	0	0
			9	9		
20	E	3	Total	O	0	0
			3	3		
20	F	13	Total	O	0	0
			13	13		
20	G	12	Total	O	0	0
			12	12		
20	H	14	Total	O	0	0
			14	14		

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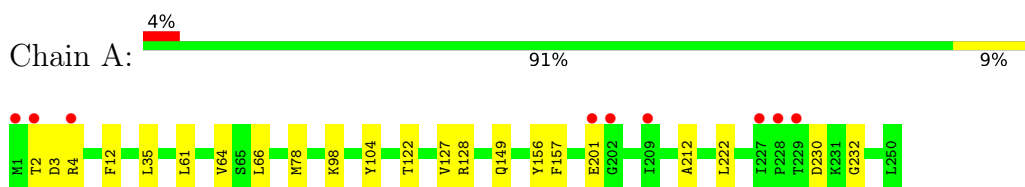
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	I	12	Total 12	O 12	0	0
20	J	10	Total 10	O 10	0	0
20	K	19	Total 19	O 19	0	0
20	L	25	Total 25	O 25	0	0
20	M	18	Total 18	O 18	0	0
20	N	10	Total 10	O 10	0	0
20	O	6	Total 6	O 6	0	0
20	P	3	Total 3	O 3	0	0
20	Q	7	Total 7	O 7	0	0
20	R	5	Total 5	O 5	0	0
20	S	3	Total 3	O 3	0	0
20	T	8	Total 8	O 8	0	0
20	U	16	Total 16	O 16	0	0
20	V	10	Total 10	O 10	0	0
20	W	10	Total 10	O 10	0	0
20	X	15	Total 15	O 15	0	0
20	Y	11	Total 11	O 11	0	0
20	Z	12	Total 12	O 12	0	0
20	a	17	Total 17	O 17	0	0
20	b	13	Total 13	O 13	0	0

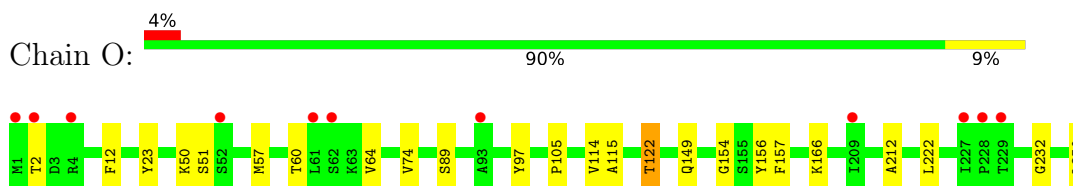
3 Residue-property plots [i](#)

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.

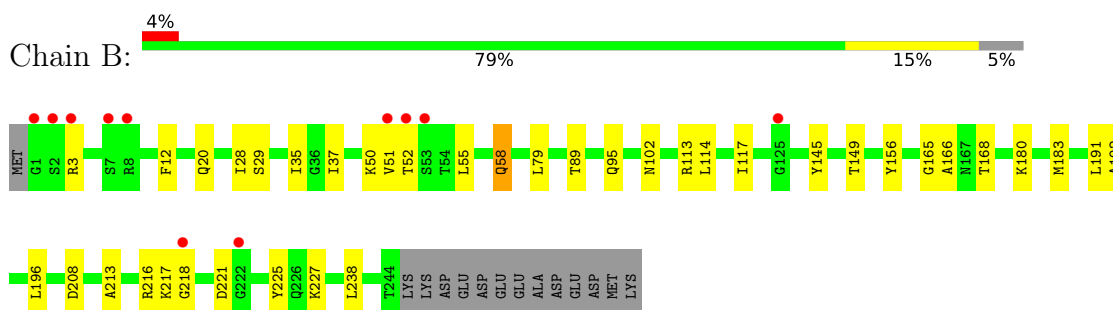
- Molecule 1: Proteasome subunit alpha type-2



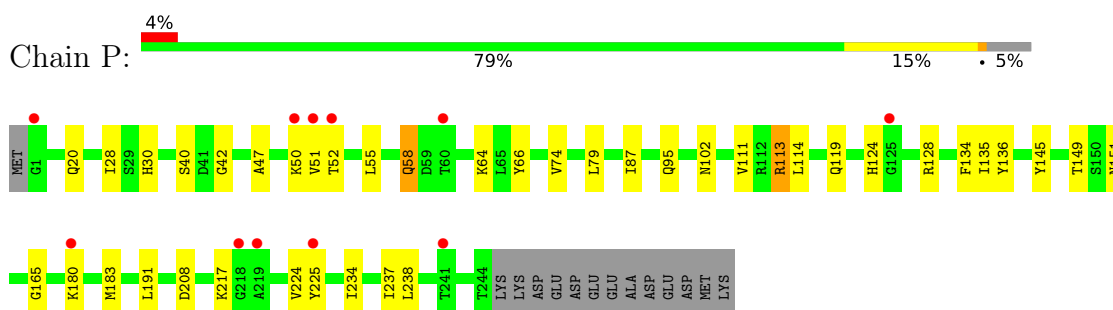
- Molecule 1: Proteasome subunit alpha type-2



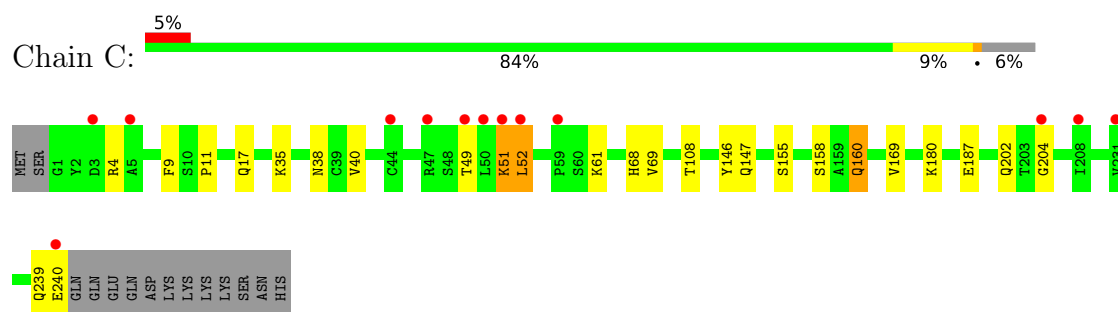
- Molecule 2: Proteasome subunit alpha type-3



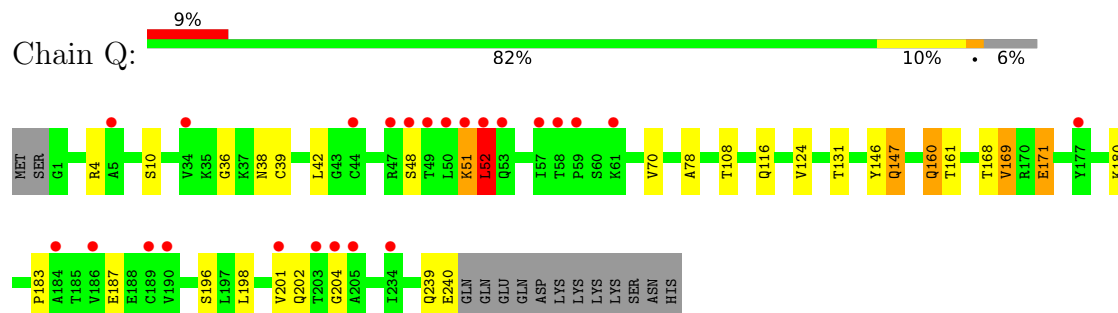
- Molecule 2: Proteasome subunit alpha type-3



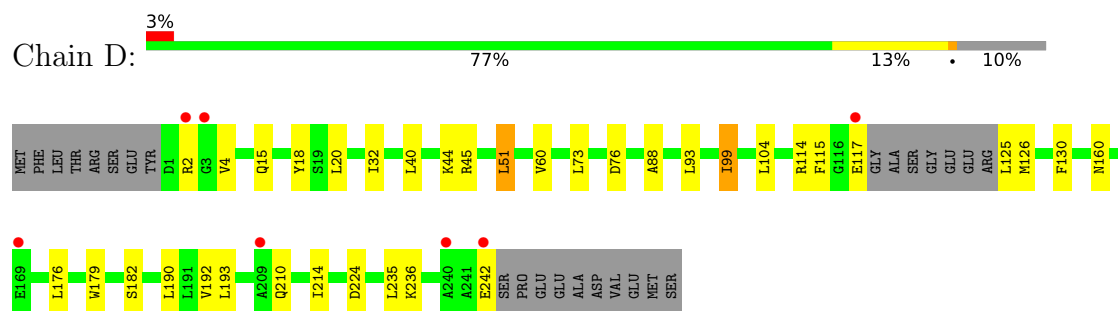
- Molecule 3: Proteasome subunit alpha type-4



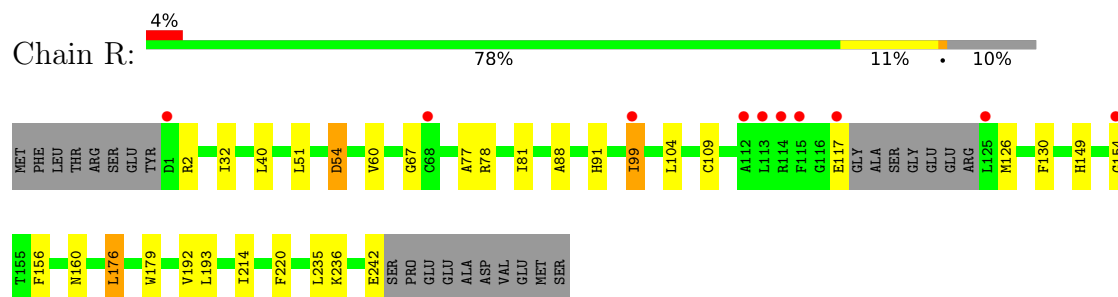
- Molecule 3: Proteasome subunit alpha type-4



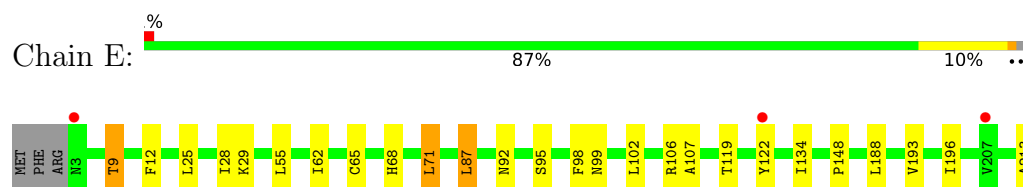
- Molecule 4: Proteasome subunit alpha type-5



- Molecule 4: Proteasome subunit alpha type-5



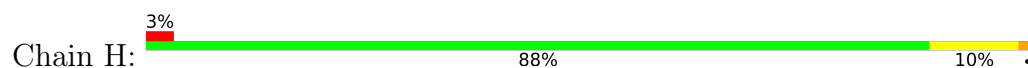
- Molecule 5: Proteasome subunit alpha type-6



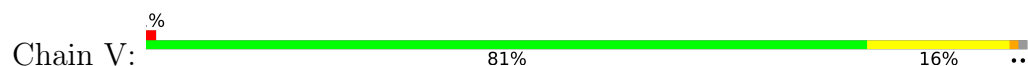
- Molecule 5: Proteasome subunit alpha type-6



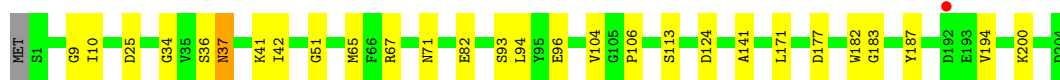
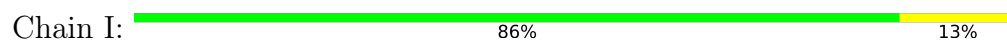
- Molecule 8: Proteasome subunit beta type-10, Proteasome subunit beta type-2



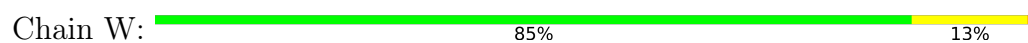
- Molecule 8: Proteasome subunit beta type-10, Proteasome subunit beta type-2



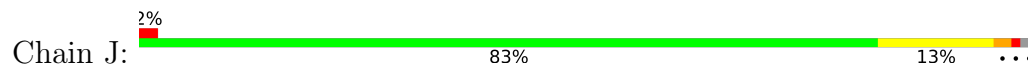
- Molecule 9: Proteasome subunit beta type-3



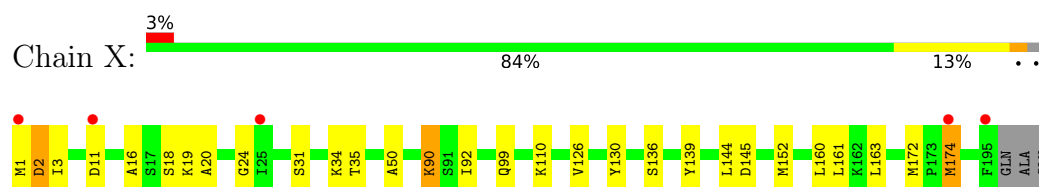
- Molecule 9: Proteasome subunit beta type-3



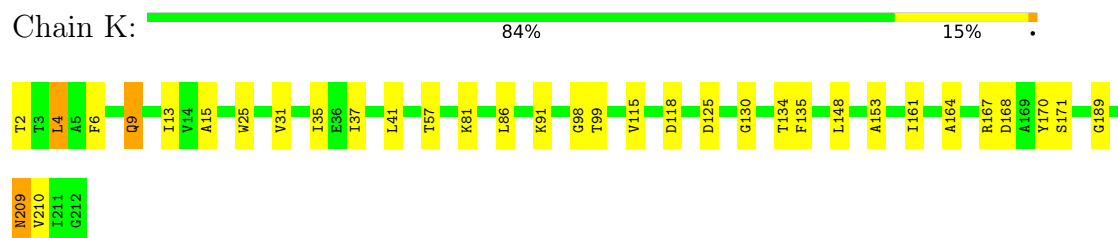
- Molecule 10: Proteasome subunit beta type-4



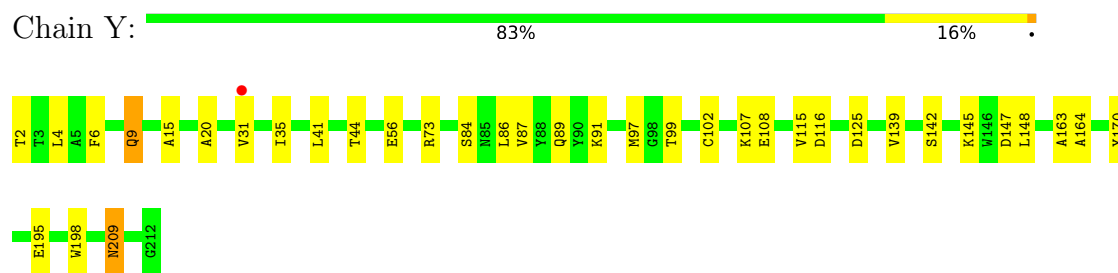
- Molecule 10: Proteasome subunit beta type-4



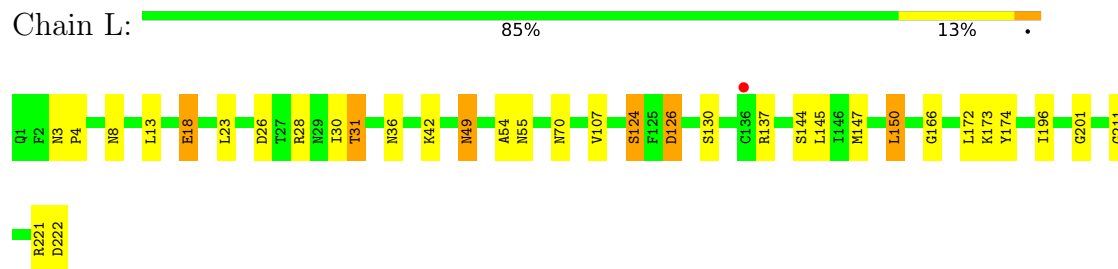
• Molecule 11: Proteasome subunit beta type-5



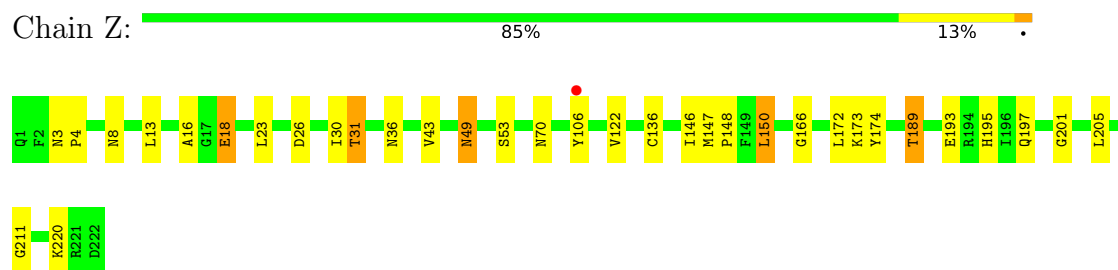
• Molecule 11: Proteasome subunit beta type-5



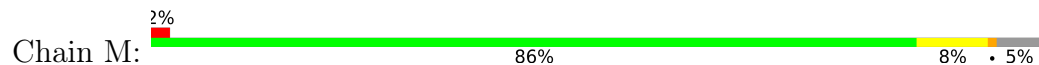
• Molecule 12: Proteasome subunit beta type-6



• Molecule 12: Proteasome subunit beta type-6

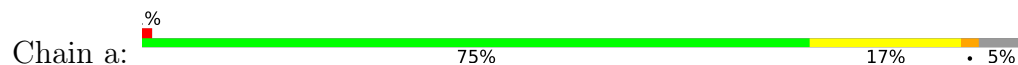


• Molecule 13: Proteasome subunit beta type-7

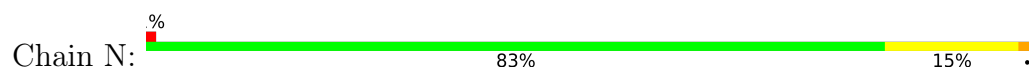




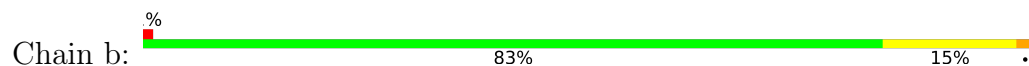
• Molecule 13: Proteasome subunit beta type-7



• 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	134.70Å 300.60Å 144.48Å 90.00° 112.83° 90.00°	Depositor
Resolution (Å)	30.00 – 2.75 30.00 – 2.75	Depositor EDS
% Data completeness (in resolution range)	94.9 (30.00-2.75) 94.9 (30.00-2.75)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.76Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.213 , 0.247 0.220 , 0.251	Depositor DCC
R_{free} test set	12976 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	58.7	Xtriage
Anisotropy	0.539	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	49917	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CL, SO4, A1IFL, MES

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.03	0/1952	1.40	0/2642
1	O	1.05	0/1952	1.45	1/2642 (0.0%)
2	B	1.00	0/1934	1.45	0/2618
2	P	1.03	0/1934	1.44	0/2618
3	C	1.04	0/1910	1.48	0/2586
3	Q	1.05	0/1910	1.47	0/2586
4	D	1.03	0/1837	1.48	2/2475 (0.1%)
4	R	1.04	0/1837	1.49	0/2475
5	E	1.02	0/1800	1.43	0/2433
5	S	1.04	0/1800	1.43	0/2433
6	F	1.03	0/1932	1.49	4/2609 (0.2%)
6	T	1.03	0/1932	1.46	1/2609 (0.0%)
7	G	1.04	2/1945 (0.1%)	1.44	0/2634
7	U	1.05	1/1945 (0.1%)	1.45	2/2634 (0.1%)
8	H	1.03	0/1739	1.46	0/2355
8	V	1.04	0/1711	1.45	2/2319 (0.1%)
9	I	1.04	0/1611	1.45	6/2174 (0.3%)
9	W	1.03	0/1611	1.44	2/2174 (0.1%)
10	J	0.99	0/1589	1.39	1/2142 (0.0%)
10	X	1.02	0/1589	1.39	3/2142 (0.1%)
11	K	1.02	0/1674	1.46	4/2264 (0.2%)
11	Y	1.03	0/1674	1.42	0/2264
12	L	1.02	0/1795	1.40	1/2420 (0.0%)
12	Z	1.00	0/1795	1.42	0/2420
13	M	1.01	0/1866	1.40	2/2528 (0.1%)
13	a	1.03	0/1866	1.44	1/2528 (0.0%)
14	N	1.02	0/1541	1.43	4/2087 (0.2%)
14	b	1.02	0/1541	1.41	2/2087 (0.1%)
All	All	1.03	3/50222 (0.0%)	1.44	38/67898 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	167	GLN	C-O	6.24	1.31	1.24
7	U	105	CYS	C-O	5.08	1.29	1.24
7	G	161	ALA	C-O	5.01	1.29	1.23

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	118	ASP	CA-CB-CG	7.44	120.04	112.60
9	W	9	GLY	CA-C-O	-6.80	117.41	122.37
6	F	104	PRO	CA-C-N	6.17	124.13	120.24
6	F	104	PRO	C-N-CA	6.17	124.13	120.24
10	X	145	ASP	CA-CB-CG	6.13	118.73	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	13	0
1	O	1915	0	1929	11	0
2	B	1904	0	1904	21	0
2	P	1904	0	1904	24	0
3	C	1881	0	1895	13	0
3	Q	1881	0	1895	15	0
4	D	1813	0	1797	21	0
4	R	1813	0	1797	17	0
5	E	1773	0	1775	21	0
5	S	1773	0	1775	24	0
6	F	1892	0	1883	16	0
6	T	1892	0	1883	17	0
7	G	1907	0	1901	26	0
7	U	1907	0	1901	15	0
8	H	1709	0	1693	16	0
8	V	1681	0	1673	23	0
9	I	1581	0	1574	18	0
9	W	1581	0	1574	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	1561	0	1569	26	0
10	X	1561	0	1569	16	0
11	K	1637	0	1585	23	0
11	Y	1637	0	1585	28	0
12	L	1757	0	1711	29	0
12	Z	1757	0	1711	24	0
13	M	1835	0	1844	10	0
13	a	1835	0	1844	29	0
14	N	1512	0	1481	23	0
14	b	1512	0	1481	22	0
15	G	1	0	0	0	0
15	I	1	0	0	0	0
15	K	1	0	0	0	0
15	N	1	0	0	0	0
15	V	1	0	0	0	0
15	W	1	0	0	0	0
15	Y	1	0	0	0	0
15	Z	1	0	0	0	0
16	G	1	0	0	0	0
16	N	1	0	0	0	0
16	U	1	0	0	0	0
17	H	12	0	13	0	0
17	K	12	0	13	1	0
17	V	12	0	13	0	0
17	Y	12	0	13	0	0
18	H	51	0	0	1	0
18	K	51	0	0	2	0
18	V	51	0	0	3	0
18	Y	51	0	0	2	0
19	K	5	0	0	0	0
19	N	5	0	0	0	0
19	Y	5	0	0	0	0
19	b	5	0	0	0	0
20	A	7	0	0	0	0
20	B	14	0	0	0	0
20	C	6	0	0	0	0
20	D	9	0	0	2	0
20	E	3	0	0	0	0
20	F	13	0	0	0	0
20	G	12	0	0	0	0
20	H	14	0	0	1	0
20	I	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	J	10	0	0	0	0
20	K	19	0	0	0	0
20	L	25	0	0	0	0
20	M	18	0	0	0	0
20	N	10	0	0	0	0
20	O	6	0	0	0	0
20	P	3	0	0	0	0
20	Q	7	0	0	1	0
20	R	5	0	0	0	0
20	S	3	0	0	0	0
20	T	8	0	0	0	0
20	U	16	0	0	0	0
20	V	10	0	0	0	0
20	W	10	0	0	0	0
20	X	15	0	0	0	0
20	Y	11	0	0	0	0
20	Z	12	0	0	0	0
20	a	17	0	0	0	0
20	b	13	0	0	0	0
All	All	49917	0	49114	481	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 5.

The worst 5 of 481 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)
10:X:1:MET:HA	10:X:34:LYS:HE2	1.21	1.14
10:J:3:ILE:CG2	10:J:18:SER:HB3	1.97	0.95
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.55	0.88
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.36	0.86
14:b:152:VAL:HA	14:b:175:MET:HE1	1.58	0.86

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%)	234 (94%)	13 (5%)	1 (0%)	30	50
1	O	248/250 (99%)	238 (96%)	8 (3%)	2 (1%)	16	30
2	B	242/258 (94%)	234 (97%)	7 (3%)	1 (0%)	30	50
2	P	242/258 (94%)	235 (97%)	7 (3%)	0	100	100
3	C	238/254 (94%)	227 (95%)	9 (4%)	2 (1%)	16	30
3	Q	238/254 (94%)	230 (97%)	4 (2%)	4 (2%)	7	14
4	D	231/260 (89%)	223 (96%)	7 (3%)	1 (0%)	30	50
4	R	231/260 (89%)	222 (96%)	8 (4%)	1 (0%)	30	50
5	E	229/234 (98%)	219 (96%)	10 (4%)	0	100	100
5	S	229/234 (98%)	220 (96%)	9 (4%)	0	100	100
6	F	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
6	T	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
7	G	239/252 (95%)	235 (98%)	3 (1%)	1 (0%)	30	50
7	U	239/252 (95%)	232 (97%)	7 (3%)	0	100	100
8	H	223/225 (99%)	215 (96%)	7 (3%)	1 (0%)	30	50
8	V	220/225 (98%)	211 (96%)	9 (4%)	0	100	100
9	I	202/205 (98%)	188 (93%)	14 (7%)	0	100	100
9	W	202/205 (98%)	190 (94%)	12 (6%)	0	100	100
10	J	193/198 (98%)	184 (95%)	6 (3%)	3 (2%)	7	14
10	X	193/198 (98%)	181 (94%)	11 (6%)	1 (0%)	24	43
11	K	209/211 (99%)	197 (94%)	12 (6%)	0	100	100
11	Y	209/211 (99%)	200 (96%)	8 (4%)	1 (0%)	24	43
12	L	220/222 (99%)	211 (96%)	8 (4%)	1 (0%)	24	43
12	Z	220/222 (99%)	212 (96%)	7 (3%)	1 (0%)	24	43
13	M	232/246 (94%)	224 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	232/246 (94%)	219 (94%)	11 (5%)	2 (1%)	14	28
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	b	194/196 (99%)	184 (95%)	10 (5%)	0	100	100
All	All	6279/6598 (95%)	6025 (96%)	231 (4%)	23 (0%)	30	50

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	3	ILE
1	A	3	ASP
3	C	204	GLY
3	C	239	GLN
1	O	50	LYS

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%)	203 (97%)	6 (3%)	37	61
1	O	209/209 (100%)	204 (98%)	5 (2%)	43	65
2	B	203/216 (94%)	193 (95%)	10 (5%)	22	43
2	P	203/216 (94%)	192 (95%)	11 (5%)	20	38
3	C	212/226 (94%)	200 (94%)	12 (6%)	18	35
3	Q	212/226 (94%)	199 (94%)	13 (6%)	17	31
4	D	194/215 (90%)	180 (93%)	14 (7%)	13	25
4	R	194/215 (90%)	182 (94%)	12 (6%)	16	31
5	E	190/193 (98%)	182 (96%)	8 (4%)	26	49
5	S	190/193 (98%)	182 (96%)	8 (4%)	26	49
6	F	201/239 (84%)	192 (96%)	9 (4%)	24	46
6	T	201/239 (84%)	192 (96%)	9 (4%)	24	46
7	G	206/210 (98%)	195 (95%)	11 (5%)	20	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	U	206/210 (98%)	197 (96%)	9 (4%)	25	47
8	H	183/183 (100%)	172 (94%)	11 (6%)	17	32
8	V	180/183 (98%)	169 (94%)	11 (6%)	17	31
9	I	172/173 (99%)	169 (98%)	3 (2%)	53	71
9	W	172/173 (99%)	163 (95%)	9 (5%)	21	39
10	J	173/175 (99%)	160 (92%)	13 (8%)	12	24
10	X	173/175 (99%)	162 (94%)	11 (6%)	16	29
11	K	168/168 (100%)	164 (98%)	4 (2%)	43	65
11	Y	168/168 (100%)	159 (95%)	9 (5%)	20	38
12	L	185/185 (100%)	175 (95%)	10 (5%)	20	38
12	Z	185/185 (100%)	175 (95%)	10 (5%)	20	38
13	M	200/208 (96%)	191 (96%)	9 (4%)	24	46
13	a	200/208 (96%)	188 (94%)	12 (6%)	17	32
14	N	162/162 (100%)	156 (96%)	6 (4%)	30	54
14	b	162/162 (100%)	155 (96%)	7 (4%)	26	47
All	All	5313/5524 (96%)	5051 (95%)	262 (5%)	22	43

5 of 262 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	Y	195	GLU
12	Z	136	CYS
14	b	119	VAL
11	K	4	LEU
10	J	163	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 171 such sidechains are listed below:

Mol	Chain	Res	Type
5	S	116	GLN
10	X	55	GLN
6	T	19	GLN
7	U	172	ASN
11	Y	209	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 23 ligands modelled in this entry, 11 are monoatomic - leaving 12 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	$\# Z > 2$
19	SO4	K	303	-	4,4,4	0.33	0	6,6,6	0.08	0
19	SO4	N	202	-	4,4,4	0.33	0	6,6,6	0.07	0
17	MES	K	302	-	12,12,12	0.67	0	15,16,16	0.40	0
17	MES	V	302	-	12,12,12	0.70	0	15,16,16	0.51	0
18	A1IFL	Y	304	11	49,54,54	1.74	7 (14%)	58,75,75	1.23	6 (10%)
18	A1IFL	H	302	8	49,54,54	1.33	2 (4%)	58,75,75	1.27	7 (12%)
19	SO4	b	201	-	4,4,4	0.33	0	6,6,6	0.11	0
17	MES	H	301	-	12,12,12	0.72	0	15,16,16	0.42	0
18	A1IFL	K	304	11	49,54,54	1.62	6 (12%)	58,75,75	1.34	4 (6%)
19	SO4	Y	303	-	4,4,4	0.33	0	6,6,6	0.07	0
17	MES	Y	302	-	12,12,12	0.66	0	15,16,16	0.39	0
18	A1IFL	V	303	8	49,54,54	1.73	7 (14%)	58,75,75	1.33	8 (13%)

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	MES	K	302	-	-	2/6/14/14	0/1/1/1
17	MES	V	302	-	-	2/6/14/14	0/1/1/1
18	A1IFL	Y	304	11	-	7/37/85/85	0/3/4/4
18	A1IFL	H	302	8	-	9/37/85/85	0/3/4/4
17	MES	H	301	-	-	1/6/14/14	0/1/1/1
18	A1IFL	K	304	11	-	8/37/85/85	0/3/4/4
17	MES	Y	302	-	-	3/6/14/14	0/1/1/1
18	A1IFL	V	303	8	-	8/37/85/85	0/3/4/4

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	V	303	A1IFL	OG1-CB1	-6.65	1.34	1.43
18	K	304	A1IFL	CB-CG	-6.52	1.35	1.51
18	Y	304	A1IFL	CB-CG	-6.15	1.36	1.51
18	Y	304	A1IFL	O58-C11	-5.95	1.36	1.44
18	H	302	A1IFL	CB-CG	-5.94	1.37	1.51

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	K	304	A1IFL	C4-C3-CA1	-6.46	103.78	113.53
18	H	302	A1IFL	C4-C3-CA1	-4.60	106.59	113.53
18	V	303	A1IFL	CB1-CA3-N2	-4.08	102.57	111.75
18	Y	304	A1IFL	C4-C3-CA1	-3.96	107.56	113.53
18	V	303	A1IFL	O58-C11-C57	-3.71	102.99	108.87

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

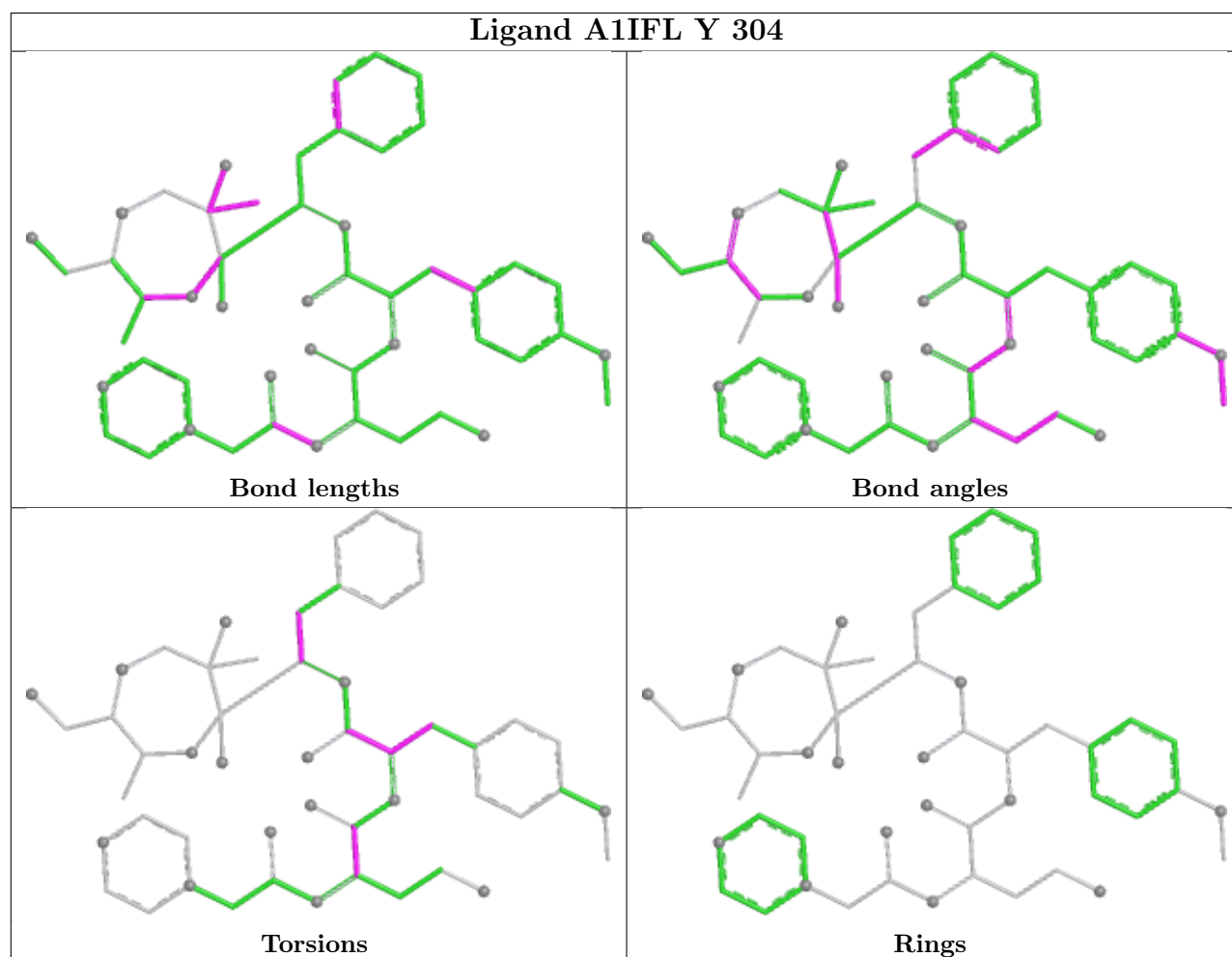
Mol	Chain	Res	Type	Atoms
17	H	301	MES	N4-C7-C8-S
17	Y	302	MES	C7-C8-S-O2S
18	H	302	A1IFL	CA1-C3-C4-O3
18	H	302	A1IFL	C31-C48-C49-C54
18	K	304	A1IFL	C21-C31-C48-C49

There are no ring outliers.

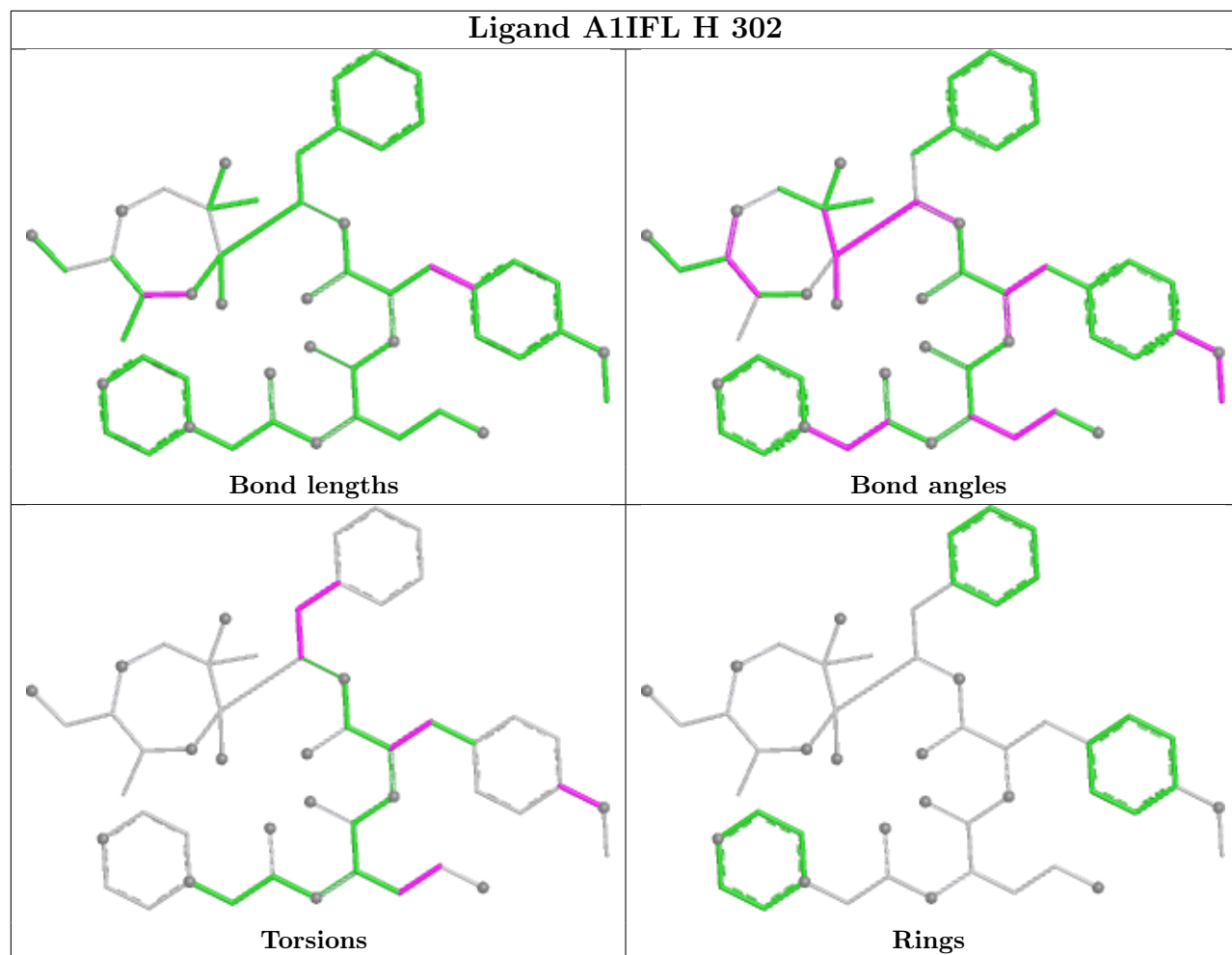
5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	K	302	MES	1	0
18	Y	304	A1IFL	2	0
18	H	302	A1IFL	1	0
18	K	304	A1IFL	2	0
18	V	303	A1IFL	3	0

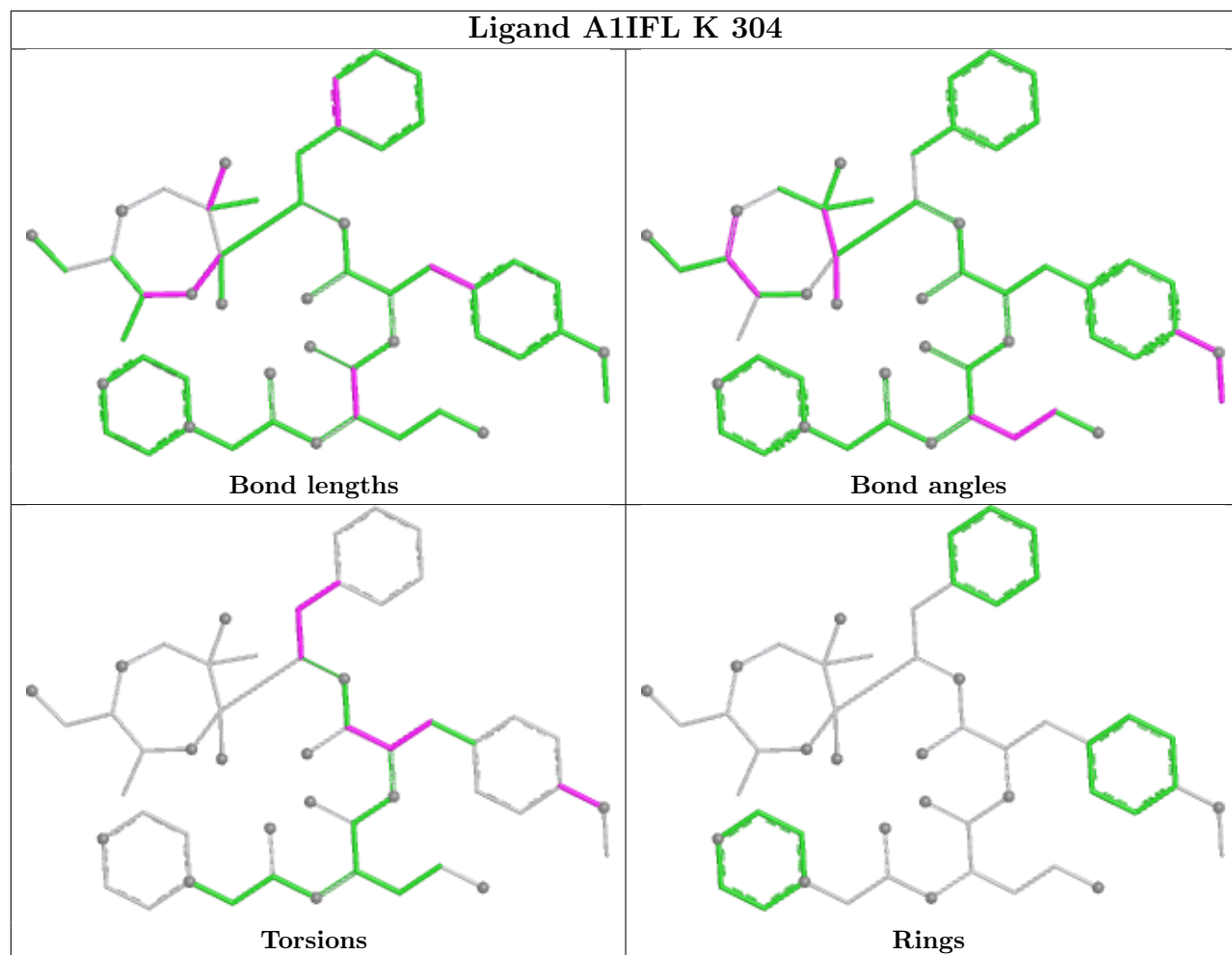
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

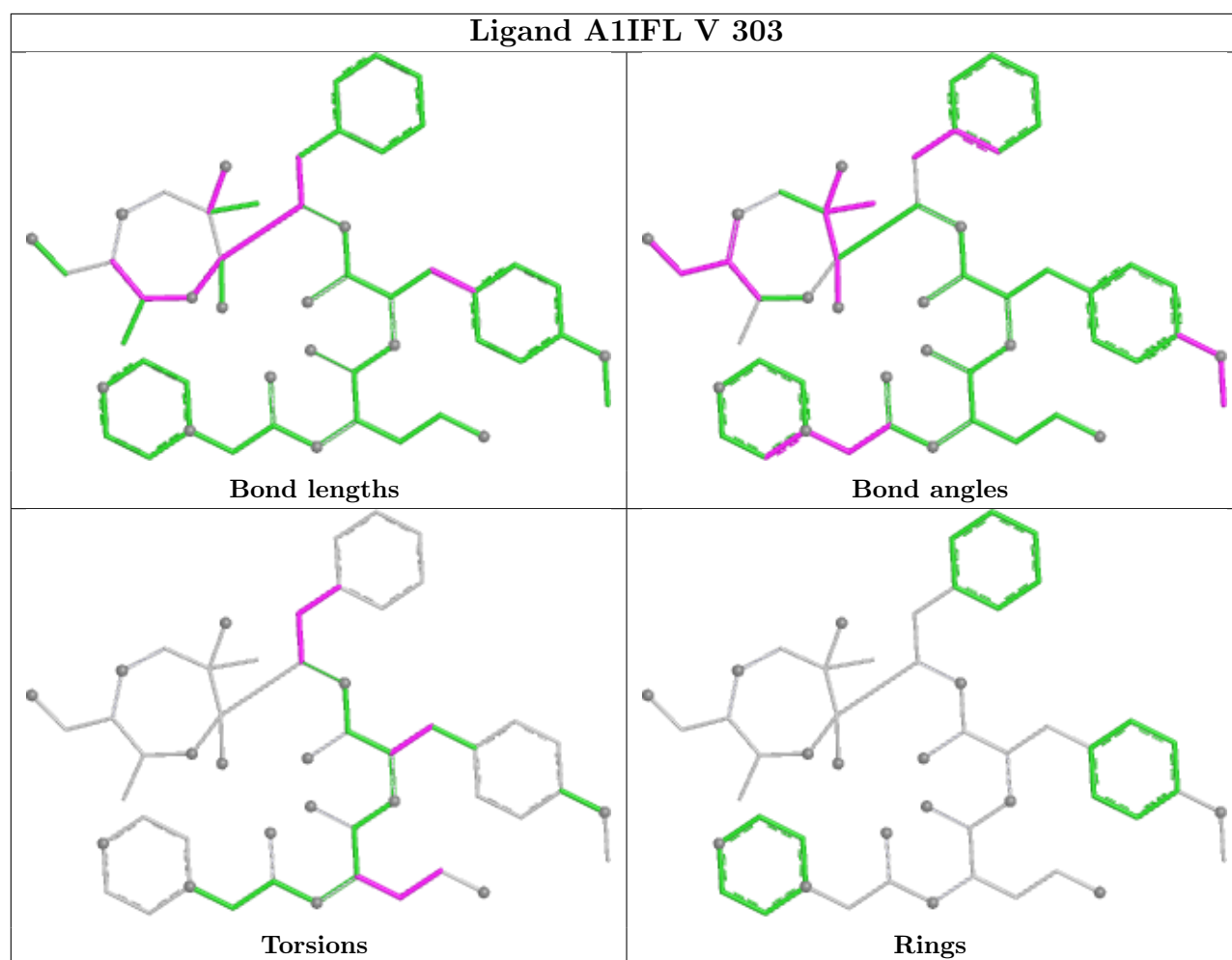


Ligand A1IFL H 302



Ligand A1IFL K 304





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	9 (3%) 46 44	49, 64, 99, 127	0
1	O	250/250 (100%)	0.35	11 (4%) 39 38	54, 74, 108, 127	0
2	B	244/258 (94%)	0.47	11 (4%) 38 37	53, 69, 107, 149	0
2	P	244/258 (94%)	0.45	11 (4%) 38 37	57, 72, 118, 144	0
3	C	240/254 (94%)	0.49	13 (5%) 31 31	53, 73, 131, 143	0
3	Q	240/254 (94%)	0.70	24 (10%) 12 12	58, 83, 150, 160	0
4	D	235/260 (90%)	0.26	7 (2%) 52 50	54, 71, 93, 123	0
4	R	235/260 (90%)	0.55	10 (4%) 40 38	59, 77, 106, 131	0
5	E	231/234 (98%)	0.36	3 (1%) 75 75	56, 73, 100, 121	0
5	S	231/234 (98%)	0.62	9 (3%) 43 40	59, 80, 115, 131	0
6	F	243/288 (84%)	0.37	4 (1%) 70 69	49, 68, 107, 130	0
6	T	243/288 (84%)	0.32	8 (3%) 49 47	54, 72, 108, 139	0
7	G	241/252 (95%)	0.26	4 (1%) 69 67	49, 64, 90, 126	0
7	U	241/252 (95%)	0.21	4 (1%) 69 67	53, 68, 91, 126	0
8	H	225/225 (100%)	0.22	7 (3%) 51 49	49, 60, 86, 162	0
8	V	222/225 (98%)	0.25	3 (1%) 73 73	51, 62, 84, 141	0
9	I	204/205 (99%)	0.26	1 (0%) 87 87	45, 60, 78, 96	0
9	W	204/205 (99%)	0.06	1 (0%) 87 87	49, 60, 77, 97	0
10	J	195/198 (98%)	0.29	4 (2%) 63 61	50, 61, 82, 104	0
10	X	195/198 (98%)	0.23	5 (2%) 57 55	53, 64, 82, 120	0
11	K	211/211 (100%)	0.08	0 100 100	49, 59, 78, 87	0
11	Y	211/211 (100%)	0.21	1 (0%) 87 87	52, 62, 83, 98	0
12	L	222/222 (100%)	0.22	1 (0%) 87 87	47, 61, 85, 100	0
12	Z	222/222 (100%)	0.16	1 (0%) 87 87	50, 62, 87, 101	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	0.22	4 (1%) 69 67	30, 60, 79, 90	1 (0%)
13	a	233/246 (94%)	0.29	2 (0%) 81 81	29, 61, 76, 84	1 (0%)
14	N	196/196 (100%)	0.11	2 (1%) 79 79	48, 57, 78, 101	0
14	b	196/196 (100%)	0.18	2 (1%) 79 79	48, 59, 83, 106	0
All	All	6337/6598 (96%)	0.31	162 (2%) 57 55	29, 66, 104, 162	2 (0%)

The worst 5 of 162 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	51	VAL	7.4
3	Q	50	LEU	6.1
3	Q	49	THR	5.8
8	V	223	ILE	5.5
1	O	229	THR	5.3

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
15	MG	Z	301	1/1	0.77	0.18	73,73,73,73	0
17	MES	V	302	12/12	0.87	0.18	55,58,59,59	12
15	MG	I	301	1/1	0.88	0.25	87,87,87,87	0
17	MES	Y	302	12/12	0.88	0.21	47,51,53,56	12
18	A1IFL	H	302	51/51	0.88	0.13	56,61,72,73	0
18	A1IFL	V	303	51/51	0.88	0.13	60,64,69,69	0
18	A1IFL	K	304	51/51	0.90	0.12	49,51,59,60	0

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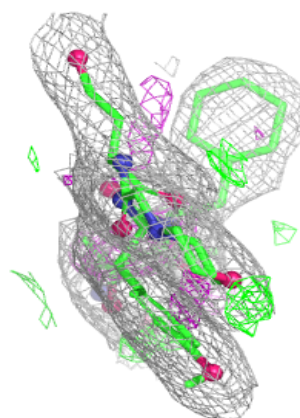
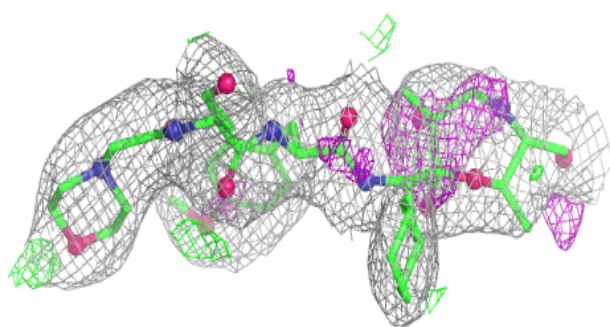
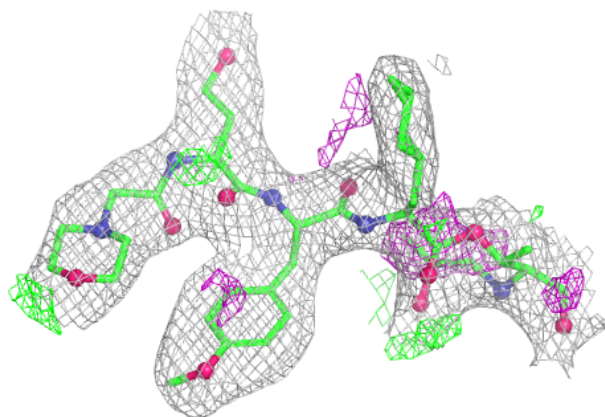
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
19	SO4	N	202	5/5	0.90	0.18	81,83,84,85	5
19	SO4	b	201	5/5	0.91	0.18	64,64,67,71	5
17	MES	H	301	12/12	0.92	0.17	50,51,51,52	12
16	CL	U	301	1/1	0.93	0.10	55,55,55,55	0
15	MG	N	201	1/1	0.93	0.11	64,64,64,64	0
17	MES	K	302	12/12	0.93	0.16	45,47,50,50	12
18	A1IFL	Y	304	51/51	0.93	0.10	53,54,65,66	0
15	MG	Y	301	1/1	0.93	0.09	70,70,70,70	0
19	SO4	Y	303	5/5	0.93	0.17	92,93,97,102	0
15	MG	G	301	1/1	0.93	0.08	61,61,61,61	0
15	MG	K	301	1/1	0.94	0.07	65,65,65,65	0
16	CL	G	302	1/1	0.94	0.11	49,49,49,49	0
16	CL	N	203	1/1	0.94	0.17	79,79,79,79	0
15	MG	W	301	1/1	0.96	0.09	66,66,66,66	0
15	MG	V	301	1/1	0.96	0.07	75,75,75,75	0
19	SO4	K	303	5/5	0.96	0.20	92,95,95,96	0

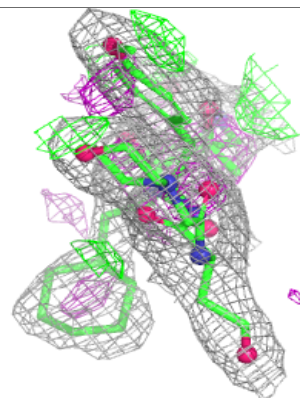
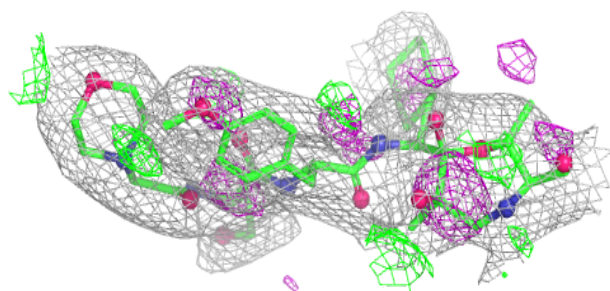
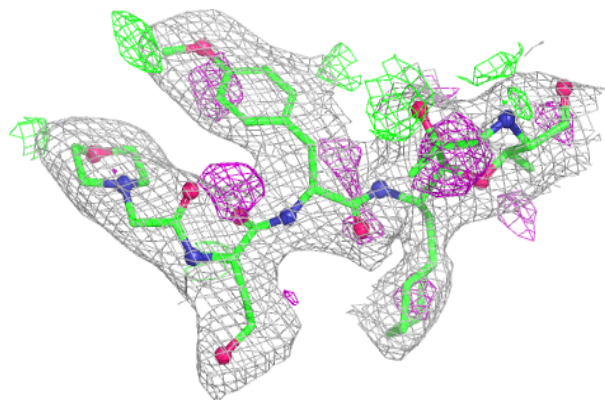
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1IFL H 302:

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

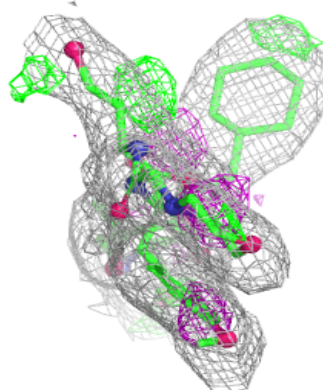
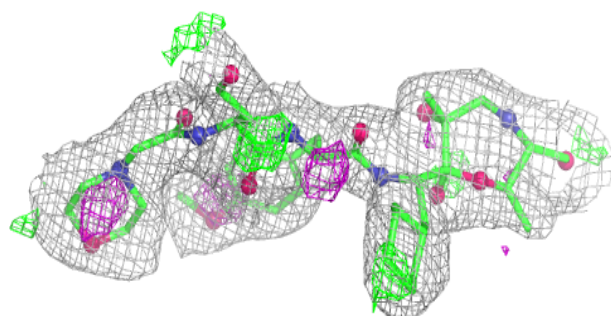
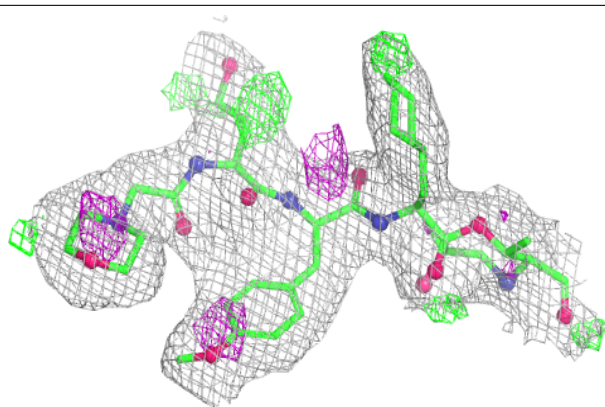
**Electron density around A1IFL V 303:**

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

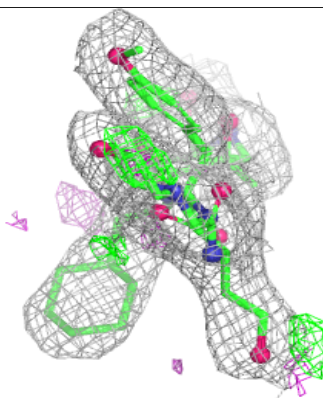
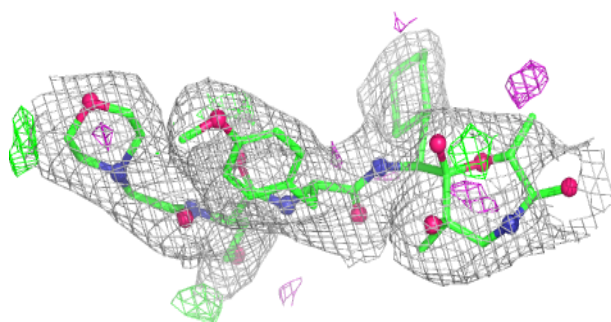
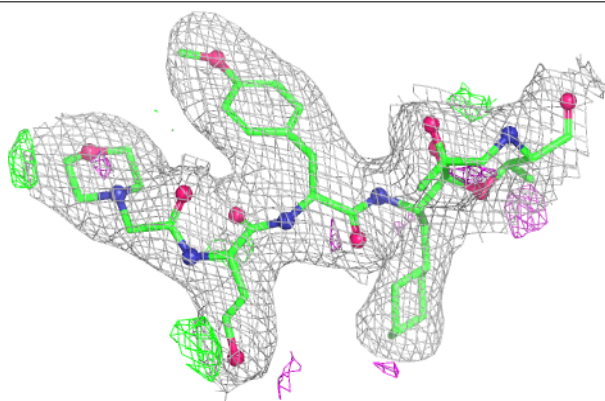


Electron density around A1IFL K 304:

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

**Electron density around A1IFL Y 304:**

$2mF_o-DF_c$ (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.