



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 22, 2025 – 02:13 pm BST

PDB ID : 9FSU / pdb_00009fsu
Title : Yeast 20S proteasome with human beta1i (1-51) in complex with epoxyketone inhibitor 42
Authors : Maurits, E.; Huber, E.M.; Dekker, P.M.; Wang, X.; Heinemeyer, W.; Florea, B.I.; Groll, M.; Overkleeft, H.S.
Deposited on : 2024-06-21
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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

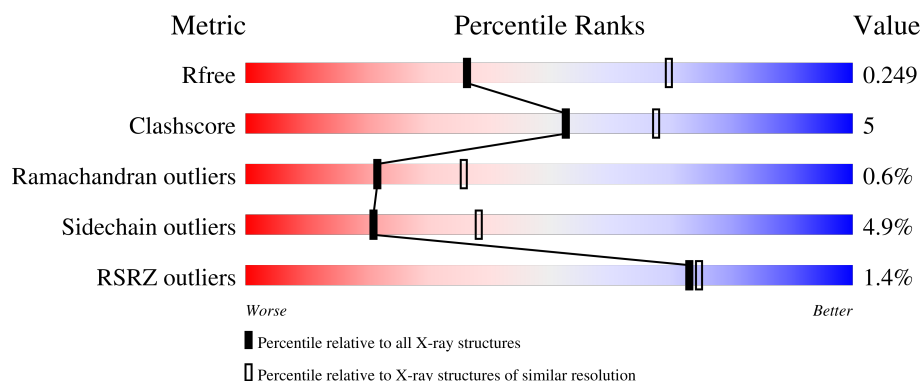
1 Overall quality at a glance

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}	164625	1606 (2.78-2.74)
Clashscore	180529	1689 (2.78-2.74)
Ramachandran outliers	177936	1665 (2.78-2.74)
Sidechain outliers	177891	1665 (2.78-2.74)
RSRZ outliers	164620	1606 (2.78-2.74)

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	
1	O	250	
2	B	258	
2	P	258	

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Mol	Chain	Length	Quality of chain
3	C	254	
3	Q	254	
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	211	
11	Y	211	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	196	

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 49865 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	241	Total	C	N	O	S	0	0	0
			1890	1181	331	374	4			
3	Q	241	Total	C	N	O	S	0	0	0
			1890	1181	331	374	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	242	Total	C	N	O	S	0	0	0
			1861	1162	314	378	7			
4	R	242	Total	C	N	O	S	0	0	0
			1861	1162	314	378	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			
5	S	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	244	Total	C	N	O	S	0	0	0
			1896	1205	330	357	4			
6	T	244	Total	C	N	O	S	0	0	0
			1896	1205	330	357	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			
7	U	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			
8	V	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	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	196	Total	C	N	O	S	0	0	0
			1570	997	266	301	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	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	224	Total	C	N	O	S	0	0	0
			1753	1108	300	338	7			
13	a	224	Total	C	N	O	S	0	0	0
			1753	1108	300	338	7			

- Molecule 14 is a protein called Proteasome subunit beta type-9, Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	195	Total	C	N	O	S	0	0	0
			1495	946	243	299	7			
14	b	195	Total	C	N	O	S	0	0	0
			1495	946	243	299	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		

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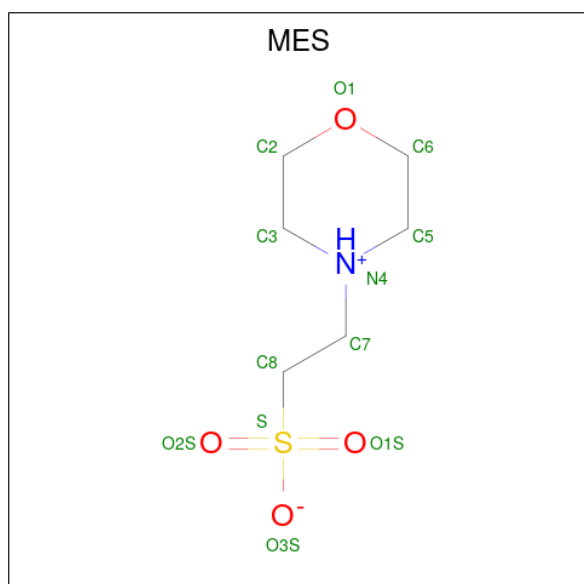
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	I	1	Total	Mg	0	0
			1	1		
15	J	1	Total	Mg	0	0
			1	1		
15	K	1	Total	Mg	0	0
			1	1		
15	N	1	Total	Mg	0	0
			1	1		
15	V	1	Total	Mg	0	0
			1	1		
15	W	1	Total	Mg	0	0
			1	1		
15	Y	1	Total	Mg	0	0
			1	1		
15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

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

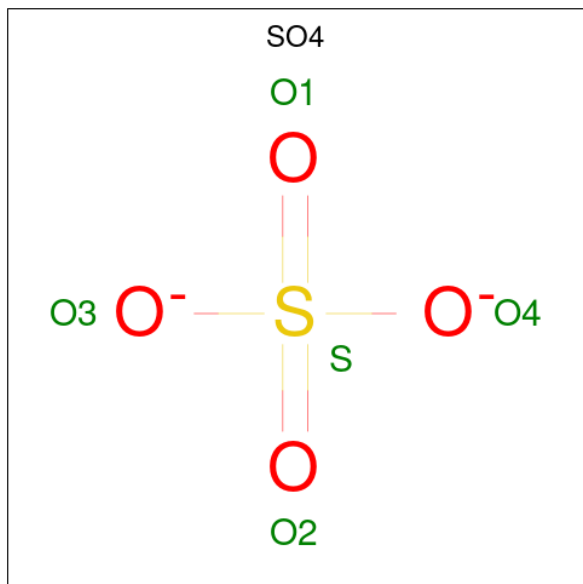
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	G	1	Total	Cl	0	0
			1	1		
16	U	1	Total	Cl	0	0
			1	1		

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



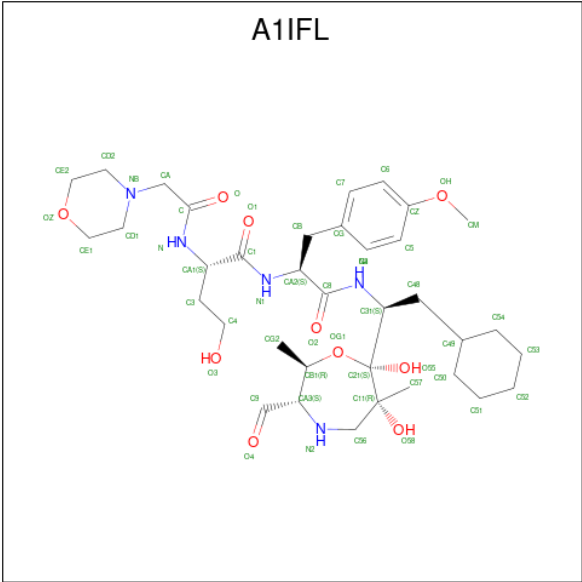
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	J	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
17	V	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
17	X	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 18 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 19 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
19	K	1	Total	C	N	O	0	0
			51	36	5	10		
19	N	1	Total	C	N	O	0	0
			51	36	5	10		
19	Y	1	Total	C	N	O	0	0
			51	36	5	10		
19	b	1	Total	C	N	O	0	0
			51	36	5	10		

- Molecule 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	9	Total	O	0	0
			9	9		
20	B	9	Total	O	0	0
			9	9		
20	C	8	Total	O	0	0
			8	8		
20	D	10	Total	O	0	0
			10	10		
20	E	6	Total	O	0	0
			6	6		
20	F	15	Total	O	0	0
			15	15		
20	G	7	Total	O	0	0
			7	7		
20	H	10	Total	O	0	0
			10	10		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	I	10	Total 10	O 10	0	0
20	J	12	Total 12	O 12	0	0
20	K	15	Total 15	O 15	0	0
20	L	11	Total 11	O 11	0	0
20	M	12	Total 12	O 12	0	0
20	N	9	Total 9	O 9	0	0
20	O	6	Total 6	O 6	0	0
20	P	8	Total 8	O 8	0	0
20	Q	5	Total 5	O 5	0	0
20	R	1	Total 1	O 1	0	0
20	S	6	Total 6	O 6	0	0
20	T	7	Total 7	O 7	0	0
20	U	9	Total 9	O 9	0	0
20	V	9	Total 9	O 9	0	0
20	W	8	Total 8	O 8	0	0
20	X	10	Total 10	O 10	0	0
20	Y	13	Total 13	O 13	0	0
20	Z	11	Total 11	O 11	0	0
20	a	11	Total 11	O 11	0	0
20	b	14	Total 14	O 14	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: 




- Molecule 1: Proteasome subunit alpha type-2

Chain O: 




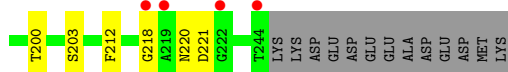
- Molecule 2: Proteasome subunit alpha type-3

Chain B: 




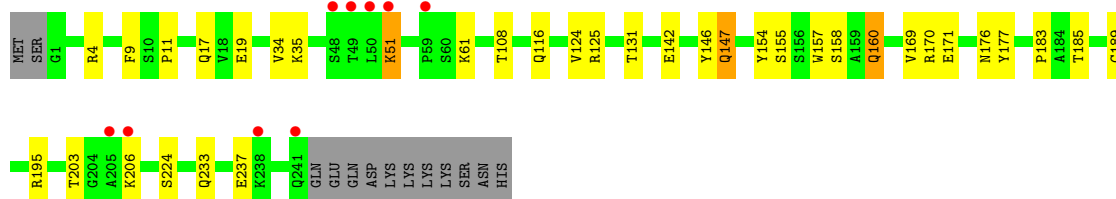
- Molecule 2: Proteasome subunit alpha type-3

Chain P: 




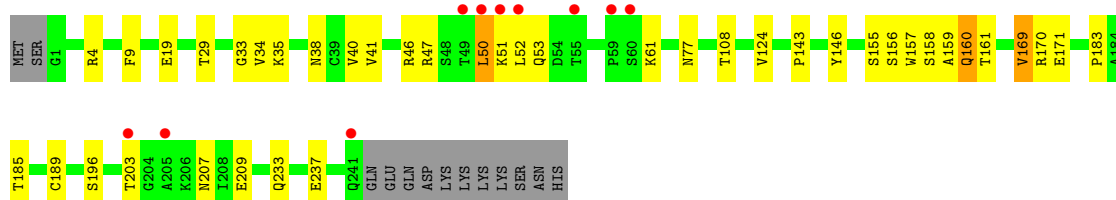
- Molecule 3: Proteasome subunit alpha type-4

Chain C: 




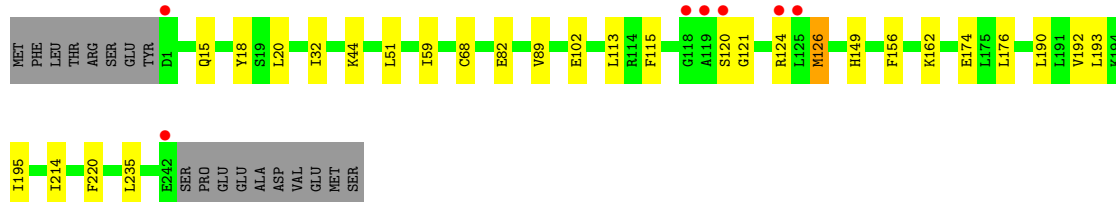
• Molecule 3: Proteasome subunit alpha type-4

Chain Q: 




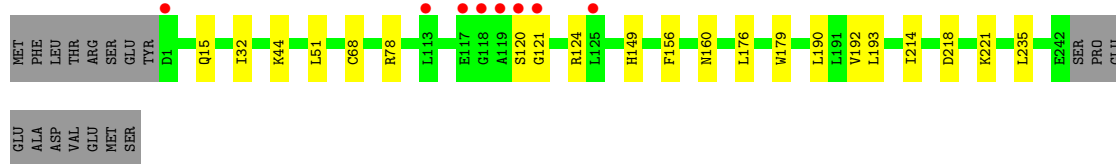
• Molecule 4: Proteasome subunit alpha type-5

Chain D: 




• Molecule 4: Proteasome subunit alpha type-5

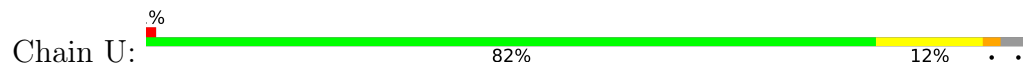
Chain R: 

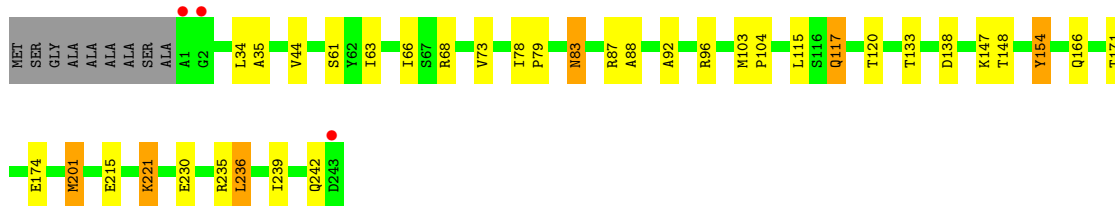


• Molecule 5: Proteasome subunit alpha type-6

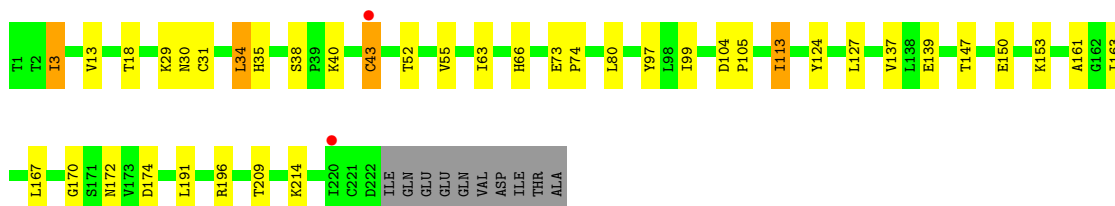
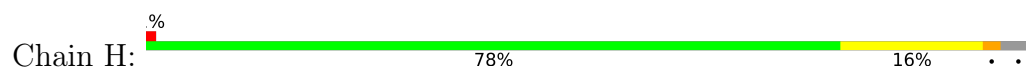
Chain E: 



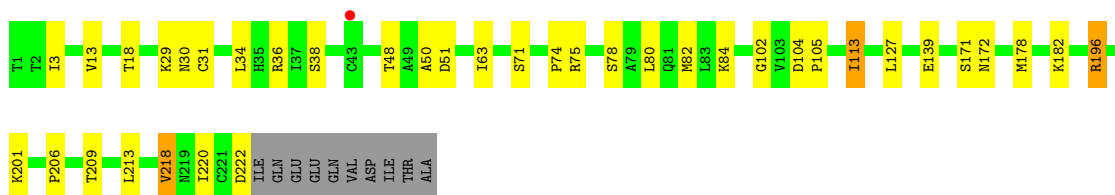
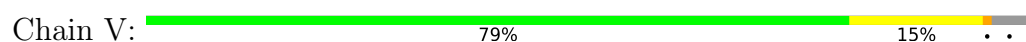




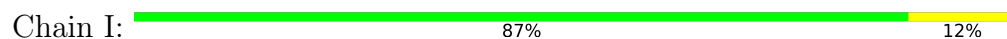
• Molecule 8: Proteasome subunit beta type-2



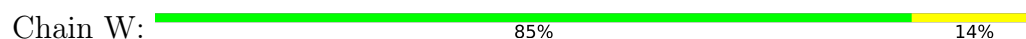
• Molecule 8: Proteasome subunit beta type-2



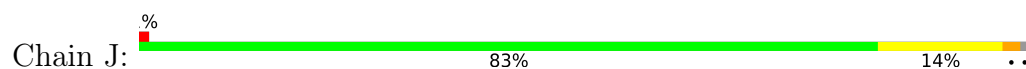
• Molecule 9: Proteasome subunit beta type-3



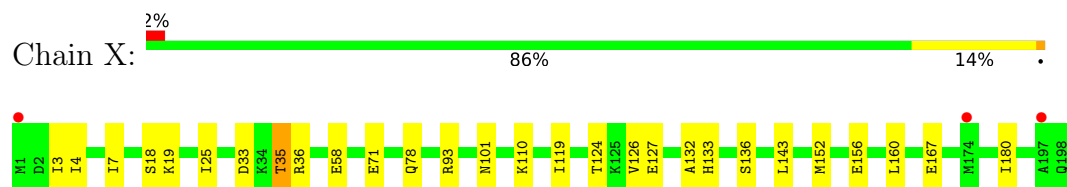
• Molecule 9: Proteasome subunit beta type-3



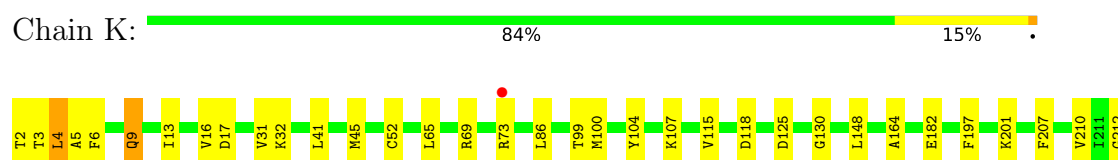
• Molecule 10: Proteasome subunit beta type-4



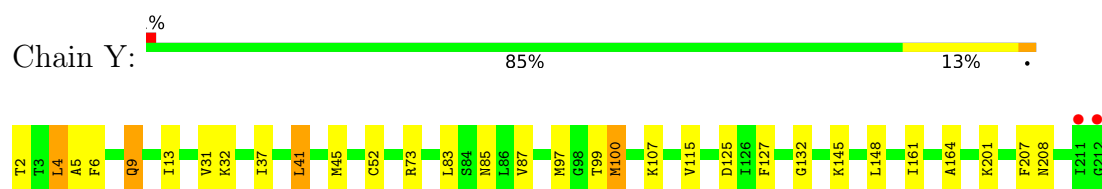
- Molecule 10: Proteasome subunit beta type-4



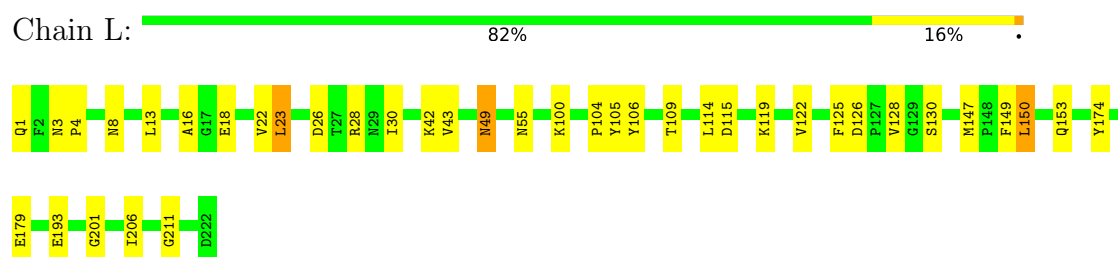
- Molecule 11: Proteasome subunit beta type-5



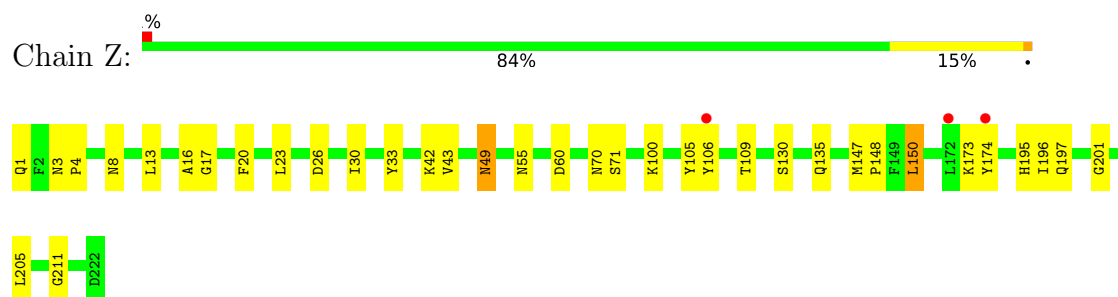
- Molecule 11: Proteasome subunit beta type-5



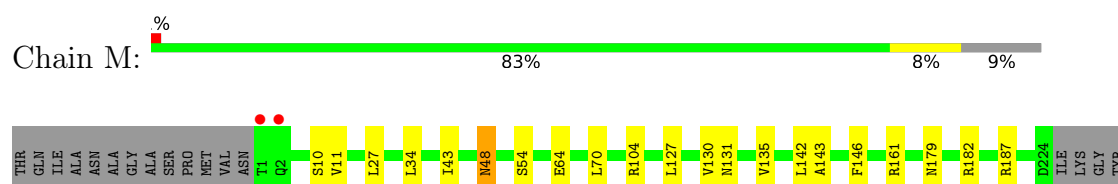
- Molecule 12: Proteasome subunit beta type-6



- Molecule 12: Proteasome subunit beta type-6

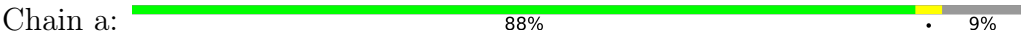


- Molecule 13: Proteasome subunit beta type-7

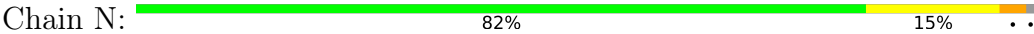


GLY
THR
GLN
LYS
ILE

• Molecule 13: Proteasome subunit beta type-7

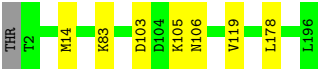


• Molecule 14: Proteasome subunit beta type-9,Proteasome subunit beta type-1



L178
E184
L196

• Molecule 14: Proteasome subunit beta type-9,Proteasome subunit beta type-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.94Å 301.90Å 145.06Å 90.00° 113.05° 90.00°	Depositor
Resolution (Å)	30.00 – 2.75 30.00 – 2.75	Depositor EDS
% Data completeness (in resolution range)	97.1 (30.00-2.75) 97.1 (30.00-2.75)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.76Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.203 , 0.245 0.211 , 0.249	Depositor DCC
R_{free} test set	13480 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	67.3	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 32.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	49865	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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: MES, MG, SO4, A1IFL, 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	0.68	0/1952	0.79	0/2642
1	O	0.68	0/1952	0.79	0/2642
2	B	0.67	0/1934	0.81	1/2618 (0.0%)
2	P	0.67	0/1934	0.81	0/2618
3	C	0.68	0/1919	0.81	0/2598
3	Q	0.68	0/1919	0.79	0/2598
4	D	0.68	0/1886	0.81	0/2541
4	R	0.68	0/1886	0.78	0/2541
5	E	0.67	0/1823	0.79	0/2463
5	S	0.68	0/1823	0.78	0/2463
6	F	0.68	0/1936	0.78	0/2614
6	T	0.69	0/1936	0.79	0/2614
7	G	0.67	0/1959	0.82	0/2652
7	U	0.67	0/1959	0.83	0/2652
8	H	0.67	0/1715	0.82	0/2326
8	V	0.66	0/1715	0.80	0/2326
9	I	0.70	0/1611	0.80	0/2174
9	W	0.68	0/1611	0.79	0/2174
10	J	0.66	0/1598	0.81	0/2154
10	X	0.66	0/1613	0.80	0/2173
11	K	0.68	0/1674	0.82	0/2264
11	Y	0.68	0/1674	0.82	0/2264
12	L	0.65	0/1795	0.80	0/2420
12	Z	0.66	0/1795	0.78	0/2420
13	M	0.67	0/1783	0.82	0/2420
13	a	0.68	0/1783	0.84	0/2420
14	N	0.69	0/1524	0.80	0/2063
14	b	0.69	0/1524	0.80	0/2063
All	All	0.68	0/50233	0.80	1/67917 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	69	ASN	CB-CA-C	-5.98	98.44	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	16	0
1	O	1915	0	1929	16	0
2	B	1904	0	1904	30	0
2	P	1904	0	1904	17	0
3	C	1890	0	1903	22	0
3	Q	1890	0	1903	24	0
4	D	1861	0	1839	14	0
4	R	1861	0	1839	9	0
5	E	1795	0	1800	13	0
5	S	1795	0	1800	19	0
6	F	1896	0	1889	17	0
6	T	1896	0	1889	17	0
7	G	1921	0	1913	30	0
7	U	1921	0	1913	25	0
8	H	1684	0	1688	19	0
8	V	1684	0	1688	24	0
9	I	1581	0	1574	15	0
9	W	1581	0	1574	23	0
10	J	1570	0	1577	20	0
10	X	1585	0	1590	14	0
11	K	1637	0	1585	24	0
11	Y	1637	0	1585	19	0
12	L	1757	0	1711	22	0
12	Z	1757	0	1711	18	0
13	M	1753	0	1754	12	0
13	a	1753	0	1754	0	0
14	N	1495	0	1450	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	b	1495	0	1450	0	0
15	G	1	0	0	0	0
15	I	1	0	0	0	0
15	J	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	1	0
16	U	1	0	0	0	0
17	J	12	0	13	4	0
17	V	12	0	13	1	0
17	X	12	0	13	0	0
18	K	5	0	0	0	0
18	N	5	0	0	0	0
18	Y	5	0	0	0	0
18	b	5	0	0	0	0
19	K	51	0	0	6	0
19	N	51	0	0	3	0
19	Y	51	0	0	3	0
19	b	51	0	0	0	0
20	A	9	0	0	0	0
20	B	9	0	0	0	0
20	C	8	0	0	0	0
20	D	10	0	0	0	0
20	E	6	0	0	0	0
20	F	15	0	0	0	0
20	G	7	0	0	0	0
20	H	10	0	0	0	0
20	I	10	0	0	0	0
20	J	12	0	0	0	0
20	K	15	0	0	0	0
20	L	11	0	0	0	0
20	M	12	0	0	1	0
20	N	9	0	0	0	0
20	O	6	0	0	0	0
20	P	8	0	0	0	0
20	Q	5	0	0	2	0
20	R	1	0	0	0	0
20	S	6	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	T	7	0	0	0	0
20	U	9	0	0	1	0
20	V	9	0	0	0	0
20	W	8	0	0	0	0
20	X	10	0	0	0	0
20	Y	13	0	0	0	0
20	Z	11	0	0	0	0
20	a	11	0	0	0	0
20	b	14	0	0	0	0
All	All	49865	0	49084	451	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 451 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)
7:U:92:ALA:HA	7:U:103:MET:HE2	1.53	0.89
2:P:66:TYR:CD2	2:P:87:ILE:HD13	2.07	0.89
14:N:2:THR:HG21	14:N:162:ALA:CB	2.03	0.88
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.46	0.81
6:T:91:GLU:HG2	6:T:111:ARG:HB3	1.64	0.80

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%)	240 (97%)	6 (2%)	2 (1%)	16	29
1	O	248/250 (99%)	238 (96%)	7 (3%)	3 (1%)	11	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	242/258 (94%)	229 (95%)	11 (4%)	2 (1%)	16	29
2	P	242/258 (94%)	226 (93%)	12 (5%)	4 (2%)	7	13
3	C	239/254 (94%)	225 (94%)	12 (5%)	2 (1%)	16	29
3	Q	239/254 (94%)	220 (92%)	16 (7%)	3 (1%)	10	17
4	D	240/260 (92%)	229 (95%)	8 (3%)	3 (1%)	10	17
4	R	240/260 (92%)	226 (94%)	12 (5%)	2 (1%)	16	29
5	E	231/234 (99%)	219 (95%)	9 (4%)	3 (1%)	10	17
5	S	231/234 (99%)	220 (95%)	8 (4%)	3 (1%)	10	17
6	F	242/288 (84%)	234 (97%)	8 (3%)	0	100	100
6	T	242/288 (84%)	234 (97%)	6 (2%)	2 (1%)	16	29
7	G	241/252 (96%)	231 (96%)	9 (4%)	1 (0%)	30	47
7	U	241/252 (96%)	233 (97%)	7 (3%)	1 (0%)	30	47
8	H	220/232 (95%)	214 (97%)	6 (3%)	0	100	100
8	V	220/232 (95%)	210 (96%)	9 (4%)	1 (0%)	25	41
9	I	202/205 (98%)	192 (95%)	10 (5%)	0	100	100
9	W	202/205 (98%)	193 (96%)	9 (4%)	0	100	100
10	J	194/198 (98%)	184 (95%)	8 (4%)	2 (1%)	13	23
10	X	196/198 (99%)	185 (94%)	11 (6%)	0	100	100
11	K	209/211 (99%)	199 (95%)	10 (5%)	0	100	100
11	Y	209/211 (99%)	201 (96%)	8 (4%)	0	100	100
12	L	220/222 (99%)	206 (94%)	13 (6%)	1 (0%)	25	41
12	Z	220/222 (99%)	208 (94%)	11 (5%)	1 (0%)	25	41
13	M	222/246 (90%)	213 (96%)	9 (4%)	0	100	100
13	a	222/246 (90%)	213 (96%)	9 (4%)	0	100	100
14	N	193/196 (98%)	182 (94%)	10 (5%)	1 (0%)	25	41
14	b	193/196 (98%)	184 (95%)	9 (5%)	0	100	100
All	All	6288/6612 (95%)	5988 (95%)	263 (4%)	37 (1%)	22	36

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	120	SER
1	O	50	LYS

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Mol	Chain	Res	Type
1	A	2	THR
2	B	51	VAL
2	B	221	ASP

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	59
1	O	209/209 (100%)	203 (97%)	6 (3%)	37	59
2	B	203/216 (94%)	188 (93%)	15 (7%)	11	20
2	P	203/216 (94%)	189 (93%)	14 (7%)	13	23
3	C	213/226 (94%)	200 (94%)	13 (6%)	15	28
3	Q	213/226 (94%)	204 (96%)	9 (4%)	25	44
4	D	198/215 (92%)	188 (95%)	10 (5%)	20	36
4	R	198/215 (92%)	190 (96%)	8 (4%)	27	47
5	E	192/193 (100%)	179 (93%)	13 (7%)	13	24
5	S	192/193 (100%)	181 (94%)	11 (6%)	17	32
6	F	201/239 (84%)	189 (94%)	12 (6%)	16	29
6	T	201/239 (84%)	190 (94%)	11 (6%)	18	33
7	G	207/210 (99%)	199 (96%)	8 (4%)	27	48
7	U	207/210 (99%)	195 (94%)	12 (6%)	17	31
8	H	181/190 (95%)	167 (92%)	14 (8%)	10	19
8	V	181/190 (95%)	168 (93%)	13 (7%)	12	22
9	I	172/173 (99%)	168 (98%)	4 (2%)	45	67
9	W	172/173 (99%)	168 (98%)	4 (2%)	45	67
10	J	174/175 (99%)	168 (97%)	6 (3%)	32	54
10	X	175/175 (100%)	167 (95%)	8 (5%)	23	41
11	K	168/168 (100%)	162 (96%)	6 (4%)	30	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	Y	168/168 (100%)	159 (95%)	9 (5%)	18	34
12	L	185/185 (100%)	176 (95%)	9 (5%)	21	38
12	Z	185/185 (100%)	177 (96%)	8 (4%)	25	44
13	M	192/208 (92%)	186 (97%)	6 (3%)	35	56
13	a	192/208 (92%)	184 (96%)	8 (4%)	25	44
14	N	160/161 (99%)	152 (95%)	8 (5%)	20	37
14	b	160/161 (99%)	153 (96%)	7 (4%)	24	43
All	All	5311/5536 (96%)	5053 (95%)	258 (5%)	21	38

5 of 258 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	Y	87	VAL
12	Z	71	SER
10	J	71	GLU
9	I	182	TRP
13	a	7	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 152 such sidechains are listed below:

Mol	Chain	Res	Type
7	U	114	ASN
12	Z	195	HIS
7	U	186	ASN
10	X	37	GLN
13	a	194	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 11 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
18	SO4	N	202	-	4,4,4	0.39	0	6,6,6	0.05	0
18	SO4	K	302	-	4,4,4	0.37	0	6,6,6	0.05	0
18	SO4	b	201	-	4,4,4	0.59	0	6,6,6	0.10	0
17	MES	X	201	-	12,12,12	0.79	0	14,16,16	0.45	0
19	A1IFL	N	203	14	47,54,54	1.18	2 (4%)	52,75,75	0.99	3 (5%)
19	A1IFL	b	202	14	47,54,54	1.42	3 (6%)	52,75,75	1.16	3 (5%)
19	A1IFL	K	303	11	47,54,54	1.52	6 (12%)	52,75,75	1.18	4 (7%)
18	SO4	Y	302	-	4,4,4	0.36	0	6,6,6	0.07	0
19	A1IFL	Y	303	11	47,54,54	1.48	5 (10%)	52,75,75	1.11	1 (1%)
17	MES	V	302	-	12,12,12	0.81	0	14,16,16	0.37	0
17	MES	J	202	-	12,12,12	0.71	0	14,16,16	0.50	0

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
19	A1IFL	N	203	14	-	11/37/85/85	0/3/4/4
19	A1IFL	b	202	14	-	10/37/85/85	0/3/4/4
17	MES	X	201	-	-	4/6/14/14	0/1/1/1
19	A1IFL	K	303	11	-	13/37/85/85	0/3/4/4
19	A1IFL	Y	303	11	-	14/37/85/85	0/3/4/4
17	MES	V	302	-	-	3/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	MES	J	202	-	-	4/6/14/14	0/1/1/1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	K	303	A1IFL	CB-CG	-6.74	1.35	1.51
19	b	202	A1IFL	CB-CG	-6.29	1.36	1.51
19	Y	303	A1IFL	CB-CG	-6.25	1.36	1.51
19	N	203	A1IFL	CB-CG	-5.21	1.38	1.51
19	b	202	A1IFL	O58-C11	-3.49	1.39	1.44

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Y	303	A1IFL	CM-OH-CZ	-4.47	107.82	117.51
19	b	202	A1IFL	C-CA-NB	-3.20	105.92	113.36
19	K	303	A1IFL	CM-OH-CZ	-2.89	111.25	117.51
19	K	303	A1IFL	CA-NB-CD2	-2.85	106.68	111.09
19	K	303	A1IFL	C57-C11-C56	-2.66	102.91	109.02

There are no chirality outliers.

5 of 59 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	J	202	MES	C8-C7-N4-C3
17	J	202	MES	C7-C8-S-O1S
17	V	302	MES	C7-C8-S-O2S
17	V	302	MES	C7-C8-S-O3S
17	X	201	MES	C8-C7-N4-C3

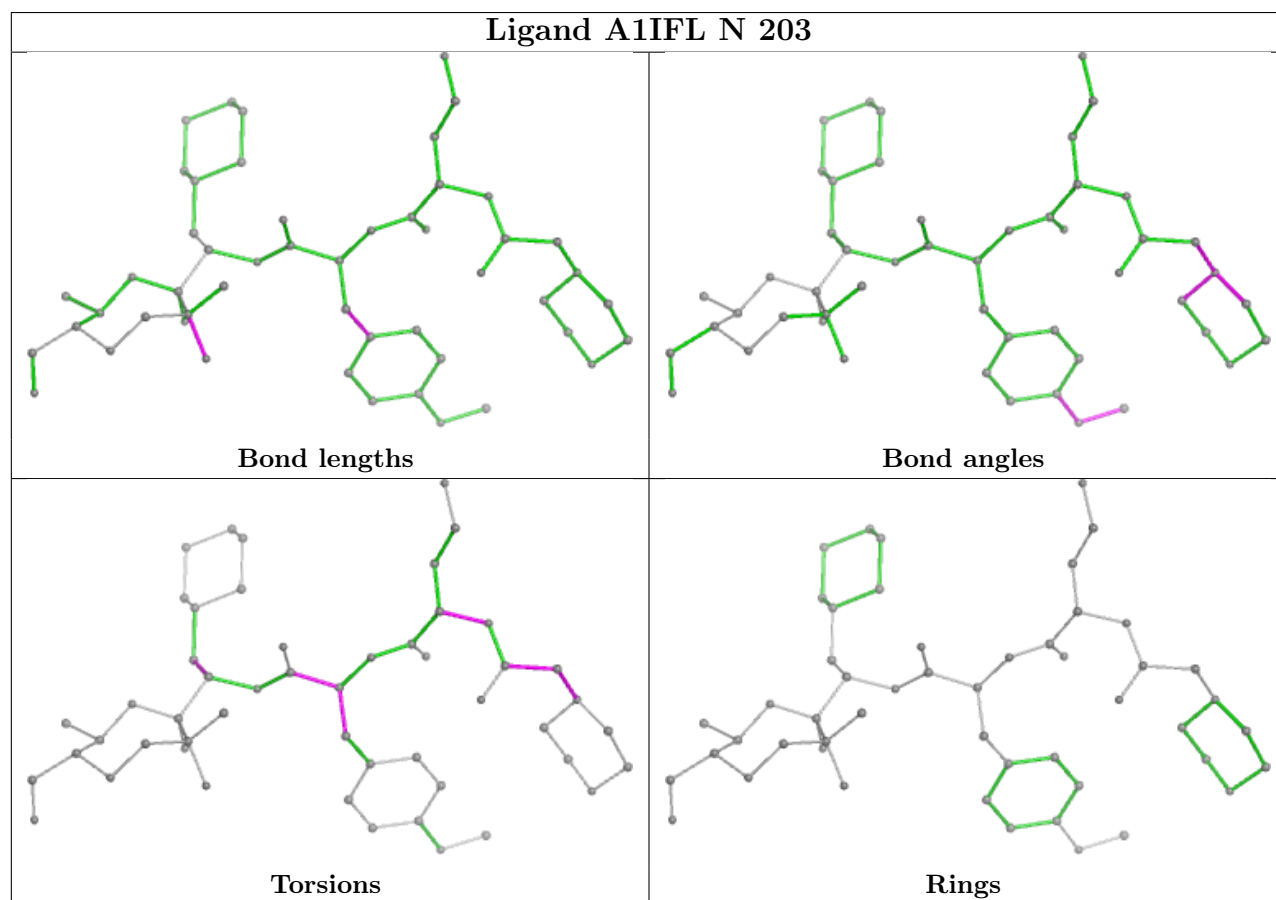
There are no ring outliers.

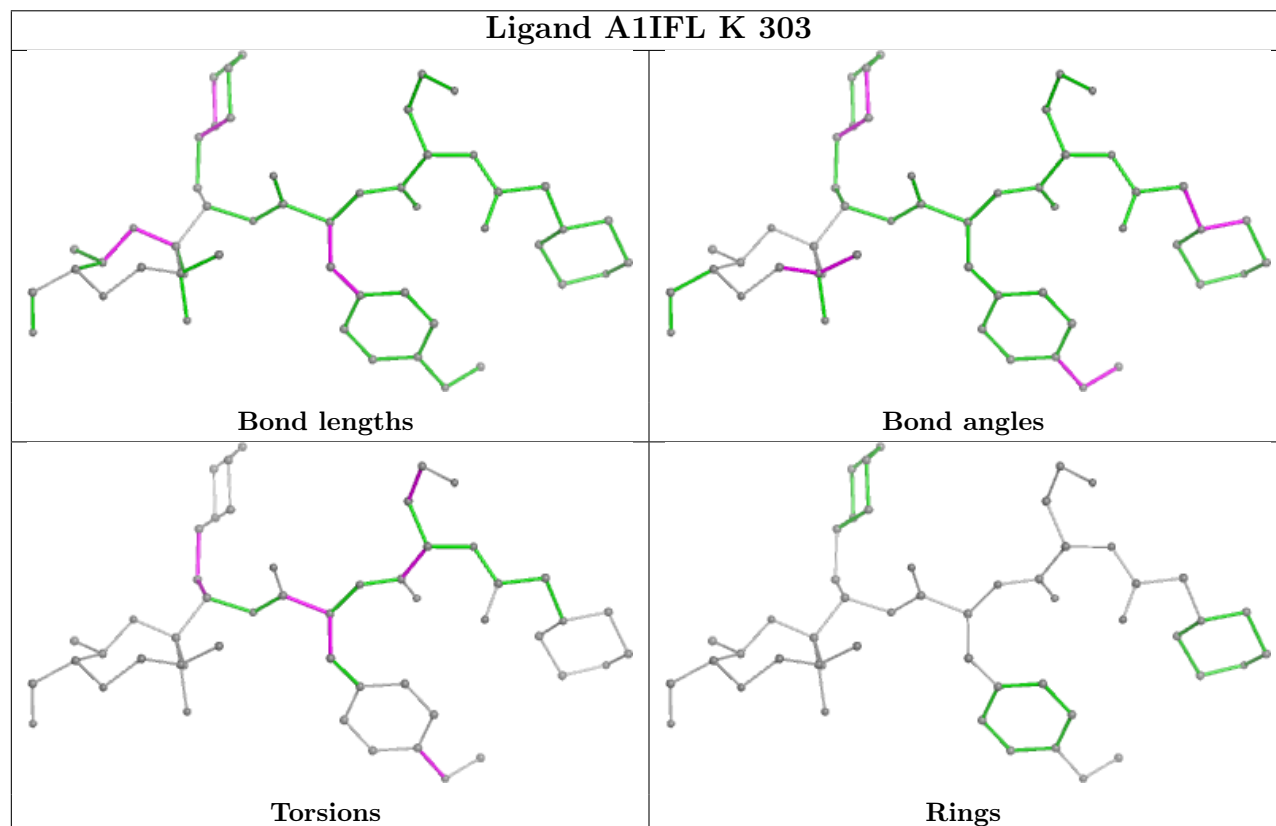
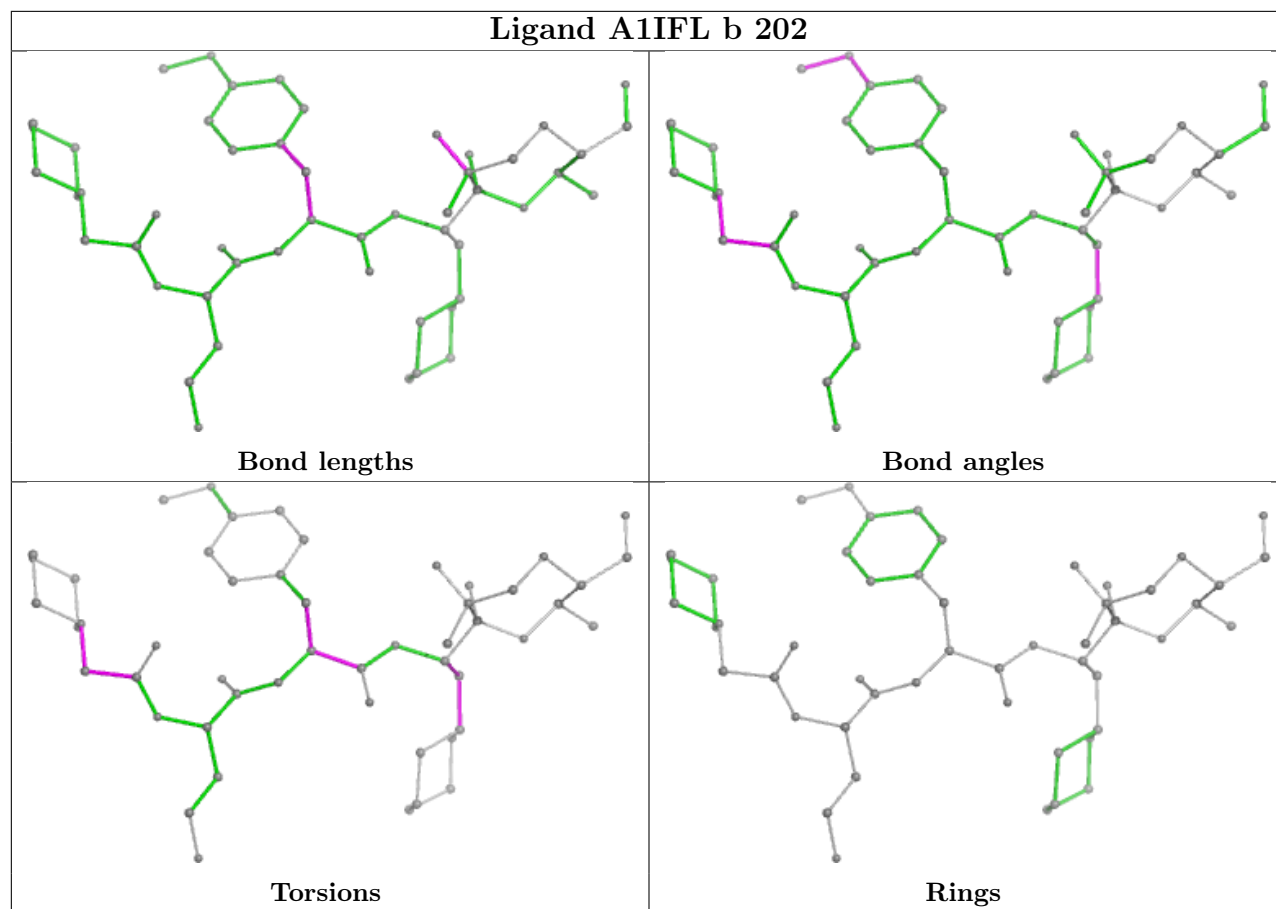
5 monomers are involved in 15 short contacts:

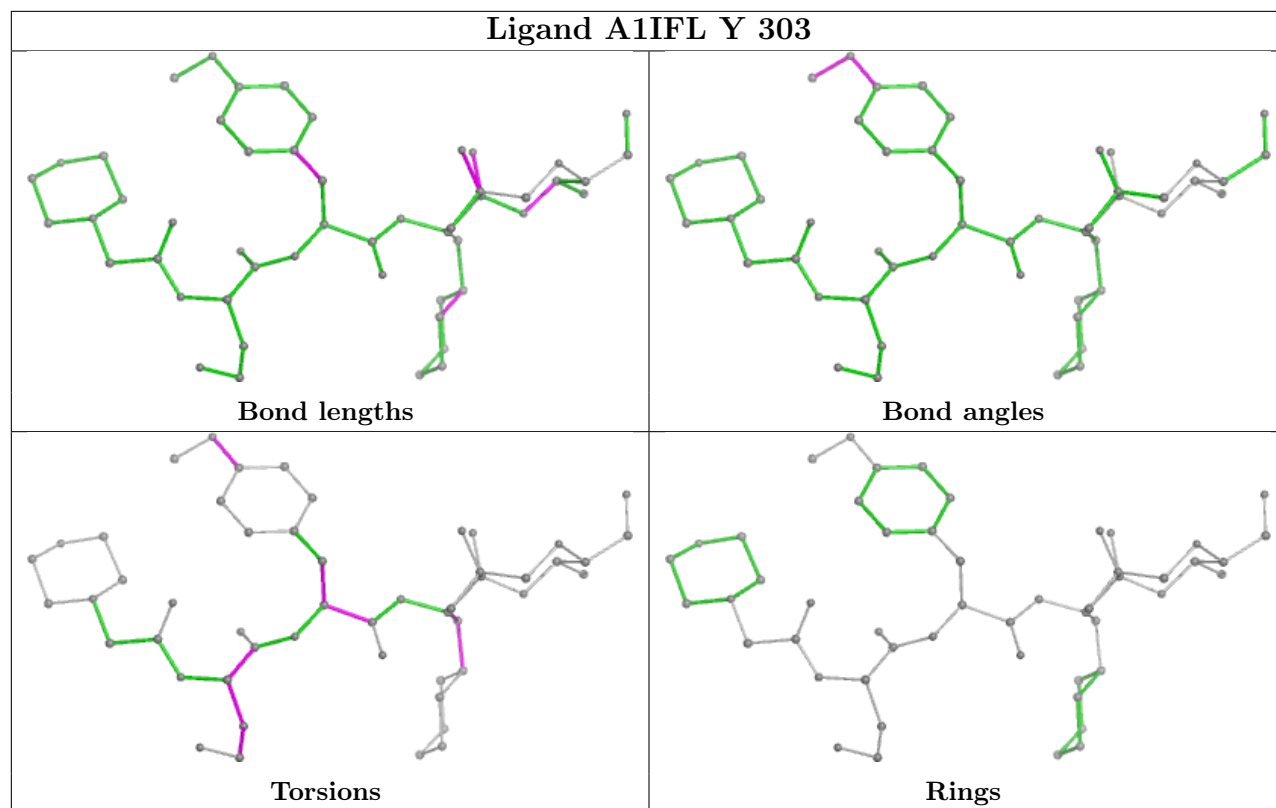
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	N	203	A1IFL	3	0
19	K	303	A1IFL	6	0
19	Y	303	A1IFL	3	0
17	V	302	MES	1	0
17	J	202	MES	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/250 (100%)	-0.18	1 (0%) 89 90	60, 76, 107, 143	0
1	O	250/250 (100%)	-0.12	1 (0%) 89 90	67, 86, 119, 154	0
2	B	244/258 (94%)	0.02	5 (2%) 64 65	64, 80, 124, 161	0
2	P	244/258 (94%)	0.05	8 (3%) 49 51	69, 86, 131, 179	0
3	C	241/254 (94%)	0.01	9 (3%) 45 47	62, 85, 141, 164	0
3	Q	241/254 (94%)	0.07	10 (4%) 42 44	74, 94, 154, 165	0
4	D	242/260 (93%)	0.02	7 (2%) 54 55	65, 86, 123, 173	0
4	R	242/260 (93%)	0.06	8 (3%) 49 51	67, 90, 126, 187	0
5	E	233/234 (99%)	0.05	2 (0%) 81 83	69, 88, 121, 164	0
5	S	233/234 (99%)	0.20	8 (3%) 48 50	71, 96, 133, 159	0
6	F	244/288 (84%)	-0.08	1 (0%) 89 90	58, 80, 117, 147	0
6	T	244/288 (84%)	-0.04	3 (1%) 76 78	65, 86, 127, 152	0
7	G	243/252 (96%)	-0.22	4 (1%) 70 71	58, 73, 107, 168	0
7	U	243/252 (96%)	-0.17	3 (1%) 76 78	64, 79, 109, 146	0
8	H	222/232 (95%)	-0.03	2 (0%) 81 83	59, 73, 98, 126	0
8	V	222/232 (95%)	-0.09	1 (0%) 87 89	62, 78, 98, 133	0
9	I	204/205 (99%)	-0.23	1 (0%) 87 89	56, 72, 94, 114	0
9	W	204/205 (99%)	-0.23	0 100 100	60, 74, 98, 123	0
10	J	196/198 (98%)	-0.22	2 (1%) 79 82	59, 72, 96, 140	0
10	X	198/198 (100%)	-0.19	3 (1%) 71 73	62, 75, 97, 165	0
11	K	211/211 (100%)	-0.23	1 (0%) 87 89	61, 73, 97, 111	0
11	Y	211/211 (100%)	-0.24	2 (0%) 81 83	60, 72, 94, 120	0
12	L	222/222 (100%)	-0.15	0 100 100	60, 76, 101, 121	0
12	Z	222/222 (100%)	-0.12	3 (1%) 73 75	56, 76, 102, 161	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	224/246 (91%)	-0.23	2 (0%) 81 83	58, 73, 96, 147	0
13	a	224/246 (91%)	-0.23	1 (0%) 89 90	60, 72, 92, 136	0
14	N	195/196 (99%)	-0.12	0 100 100	57, 70, 97, 138	0
14	b	195/196 (99%)	-0.17	0 100 100	58, 72, 100, 145	0
All	All	6344/6612 (95%)	-0.10	88 (1%) 73 75	56, 79, 120, 187	0

The worst 5 of 88 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	R	119	ALA	7.0
3	Q	50	LEU	6.6
4	D	118	GLY	6.6
4	R	120	SER	6.0
4	D	119	ALA	5.8

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 monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
17	MES	V	302	12/12	0.76	0.22	121,131,138,145	0
15	MG	I	301	1/1	0.82	0.45	97,97,97,97	0
18	SO4	b	201	5/5	0.82	0.15	135,137,141,144	0
15	MG	Z	301	1/1	0.87	0.18	82,82,82,82	0
18	SO4	N	202	5/5	0.89	0.24	105,113,119,123	0
19	A1IFL	K	303	51/51	0.90	0.12	63,67,78,79	0
17	MES	J	202	12/12	0.91	0.17	86,94,100,102	0

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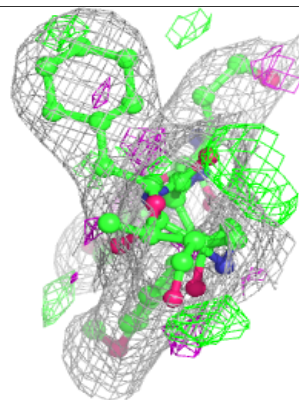
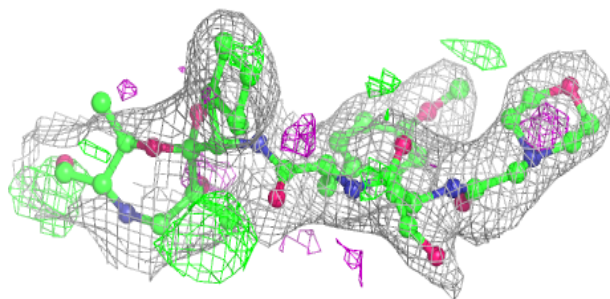
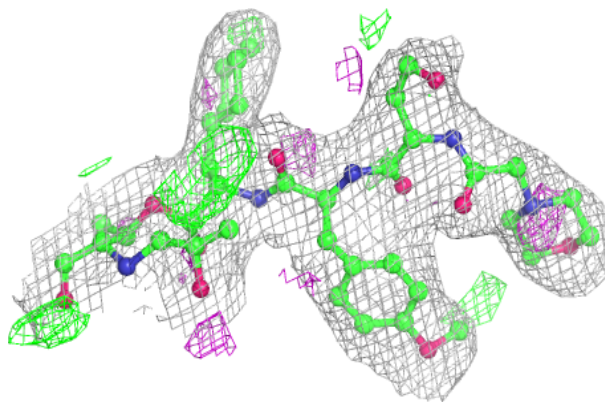
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
19	A1IFL	N	203	51/51	0.91	0.10	58,61,81,85	0
19	A1IFL	Y	303	51/51	0.91	0.11	63,68,75,76	0
19	A1IFL	b	202	51/51	0.91	0.11	65,67,86,89	0
18	SO4	Y	302	5/5	0.92	0.19	109,117,118,118	0
18	SO4	K	302	5/5	0.92	0.21	101,102,111,115	0
17	MES	X	201	12/12	0.92	0.13	81,86,90,92	0
15	MG	K	301	1/1	0.93	0.07	69,69,69,69	0
15	MG	V	301	1/1	0.93	0.07	83,83,83,83	0
15	MG	N	201	1/1	0.94	0.07	51,51,51,51	0
16	CL	U	301	1/1	0.95	0.09	62,62,62,62	0
15	MG	G	301	1/1	0.95	0.09	82,82,82,82	0
15	MG	W	301	1/1	0.95	0.10	68,68,68,68	0
15	MG	J	201	1/1	0.95	0.21	48,48,48,48	0
15	MG	Y	301	1/1	0.96	0.06	74,74,74,74	0
16	CL	G	302	1/1	0.97	0.07	61,61,61,61	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.

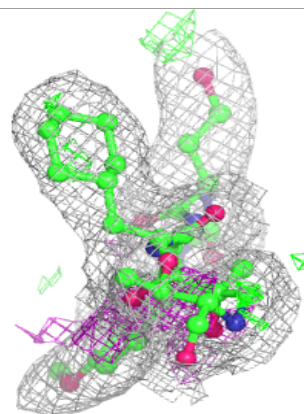
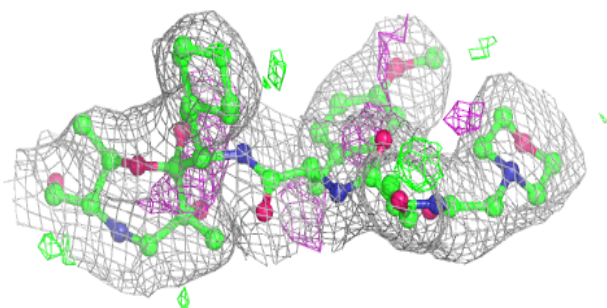
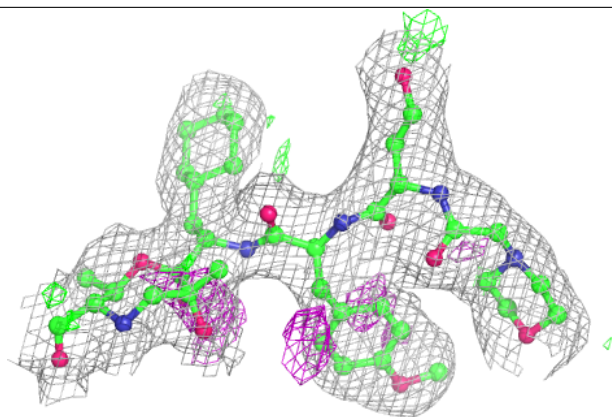
Electron density around A1IFL K 303:

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

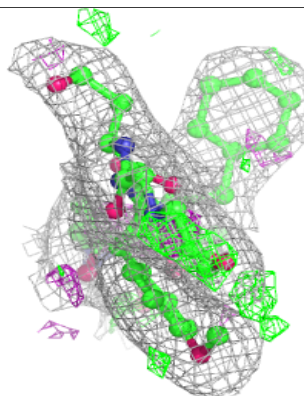
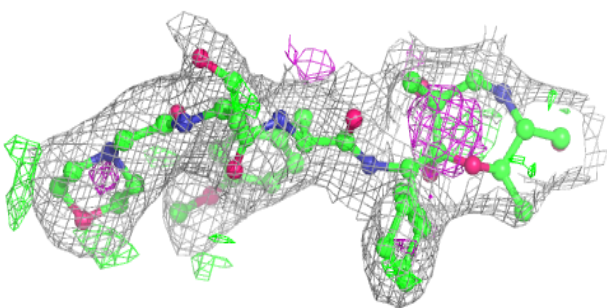
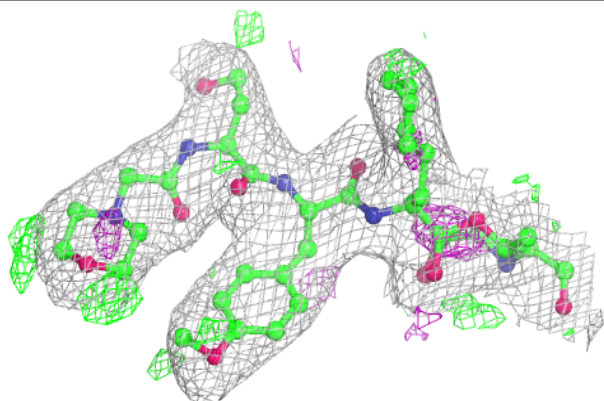


Electron density around A1IFL N 203:

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

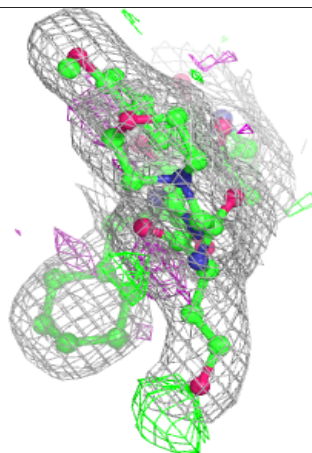
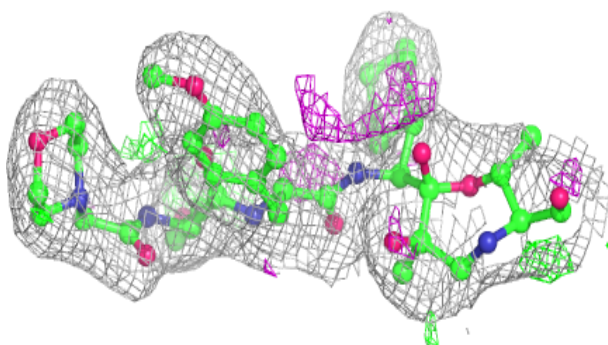
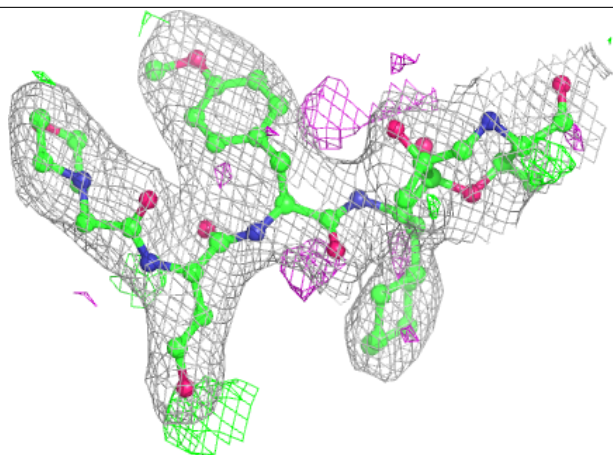
**Electron density around A1IFL Y 303:**

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



Electron density around A1IFL b 202:

$2mF_o-DF_c$ (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.