



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 06:46 PM UTC

PDB ID : 9FST / pdb_00009fst
Title : Yeast 20S proteasome with human beta1i (1-51) in complex with epoxyketone inhibitor LU-001i
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	:	4-5-2 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

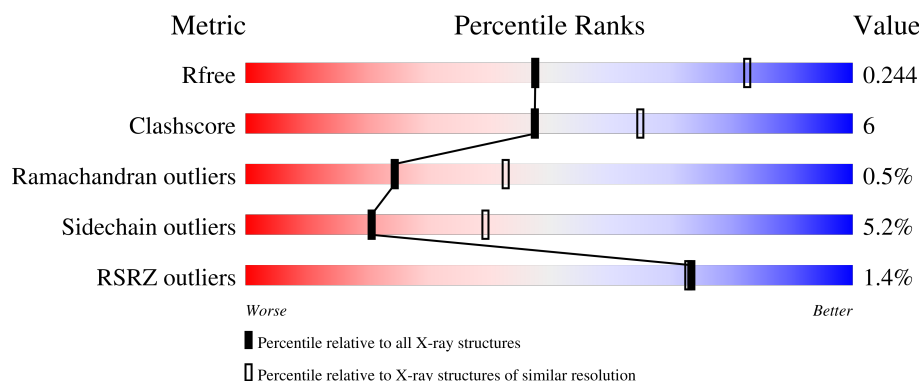
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

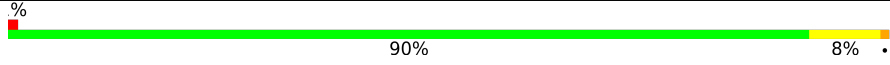
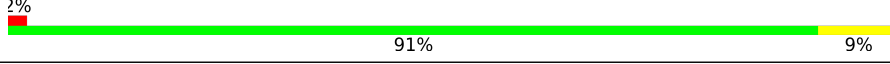
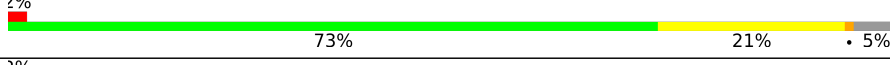
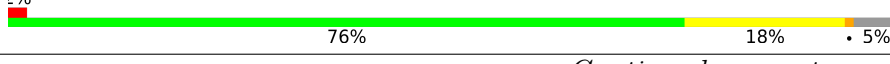
The reported resolution of this entry is 2.75 Å.

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	 2% 90% 8%
1	O	250	 2% 91% 9%
2	B	258	 2% 73% 21% 5%
2	P	258	 2% 76% 18% 5%

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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	195	
14	b	195	

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 49773 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	1	0
			1914	1207	324	380	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	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	1	0
			1767	1121	306	336	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	225	Total	C	N	O	S	0	0	0
			1761	1114	301	339	7			
13	a	228	Total	C	N	O	S	0	0	0
			1786	1131	305	343	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 CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	G	1	Total Cl 1 1	0	0

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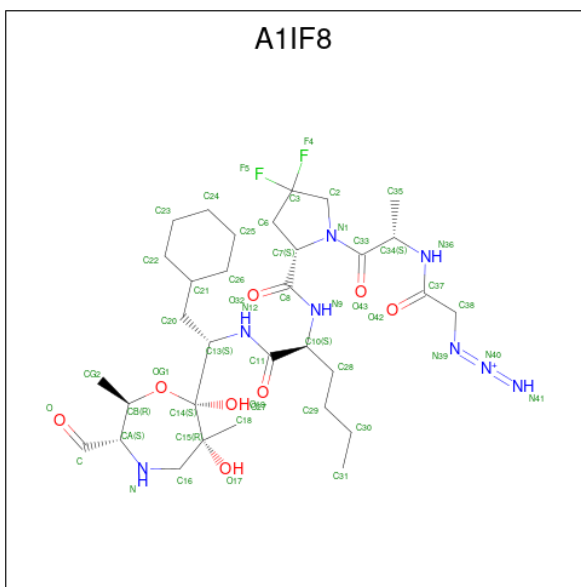
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	H	1	Total 1	Cl 1	0	0
15	U	1	Total 1	Cl 1	0	0
15	V	1	Total 1	Cl 1	0	0

- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

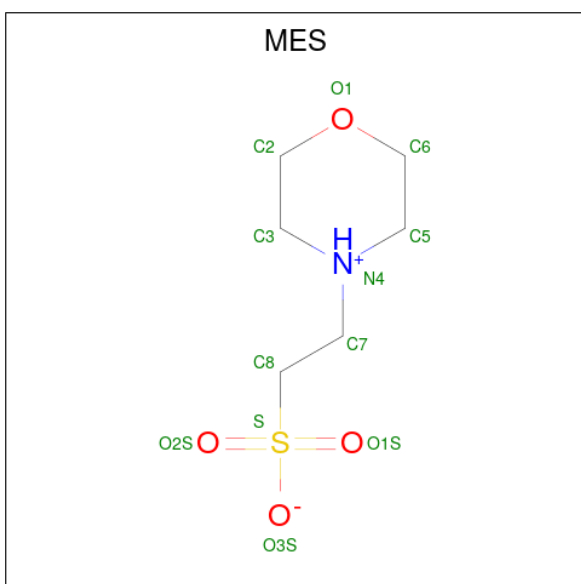
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	G	1	Total 1	Mg 1	0	0
16	I	1	Total 1	Mg 1	0	0
16	K	1	Total 1	Mg 1	0	0
16	N	1	Total 1	Mg 1	0	0
16	W	1	Total 1	Mg 1	0	0
16	X	1	Total 1	Mg 1	0	0
16	Y	1	Total 1	Mg 1	0	0
16	Z	1	Total 1	Mg 1	0	0

- Molecule 17 is azanylidene-[2-[[[(2S)-1-[(2S)-2-[[[(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]-1-oxidanylidene-hexan-2-yl]carbamoyl]-4,4-bis(fluoranyl)pyrrolidin-1-yl]-1-oxidanylidene-propan-2-yl]amino]-2-oxidanylidene-ethyl]imino-azanium (CCD ID: A1IF8) (formula: C₃₂H₅₃F₂N₈O₈) (labeled as "Ligand of Interest" by depositor).



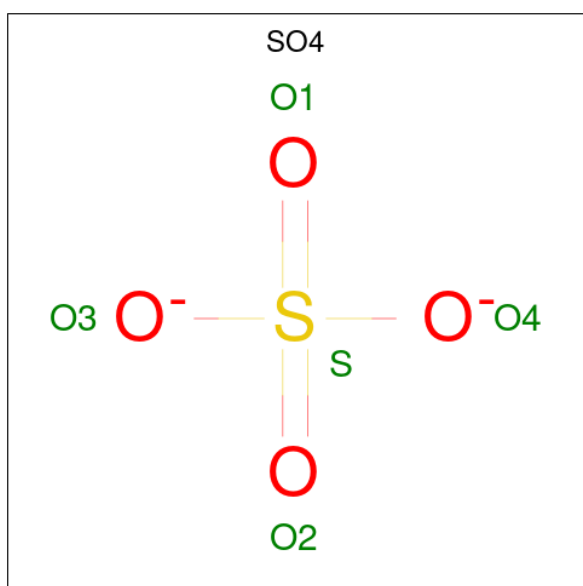
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	K	1	Total 50	C 32	F 2	N 8	O 8	0	0
17	N	1	Total 50	C 32	F 2	N 8	O 8	0	0
17	Y	1	Total 50	C 32	F 2	N 8	O 8	0	0
17	b	1	Total 50	C 32	F 2	N 8	O 8	0	0

- Molecule 18 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	K	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
18	M	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
18	Y	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
18	a	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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



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

- Molecule 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	6	Total	O	0	0
			6	6		
20	B	9	Total	O	0	0
			9	9		
20	C	7	Total	O	0	0
			7	7		
20	D	7	Total	O	0	0
			7	7		
20	E	4	Total	O	0	0
			4	4		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	F	6	Total O 6 6	0	0
20	G	17	Total O 17 17	0	0
20	H	10	Total O 10 10	0	0
20	I	10	Total O 10 10	0	0
20	J	11	Total O 11 11	0	0
20	K	11	Total O 11 11	0	0
20	L	10	Total O 10 10	0	0
20	M	17	Total O 17 17	0	0
20	N	4	Total O 4 4	0	0
20	O	3	Total O 3 3	0	0
20	P	5	Total O 5 5	0	0
20	Q	9	Total O 9 9	0	0
20	R	5	Total O 5 5	0	0
20	S	4	Total O 4 4	0	0
20	T	11	Total O 11 11	0	0
20	U	11	Total O 11 11	0	0
20	V	13	Total O 13 13	0	0
20	W	11	Total O 11 11	0	0
20	X	13	Total O 13 13	0	0
20	Y	14	Total O 14 14	0	0
20	Z	13	Total O 13 13	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	a	12	Total	O	0	0
			12	12		
20	b	18	Total	O	0	0
			18	18		

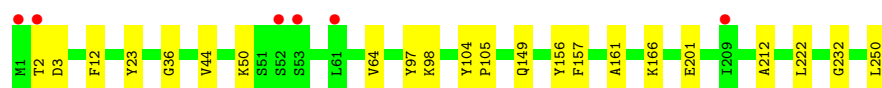
3 Residue-property plots [i](#)

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.

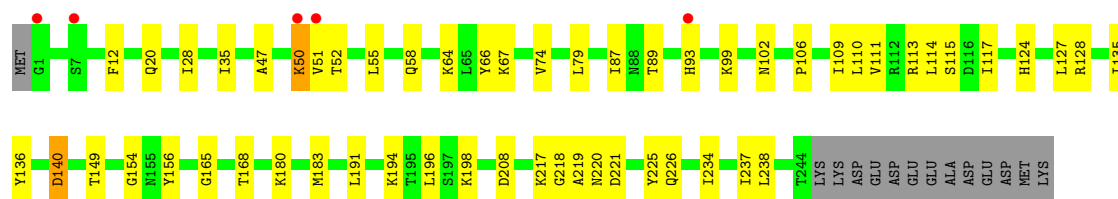
- Molecule 1: Proteasome subunit alpha type-2



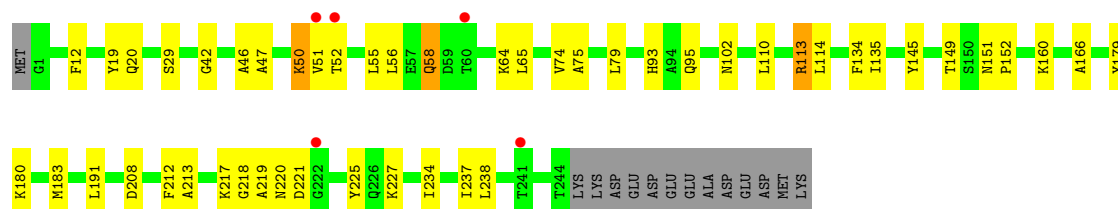
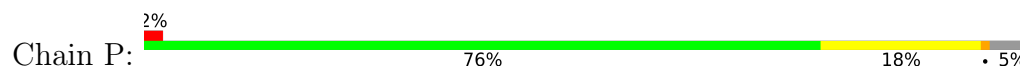
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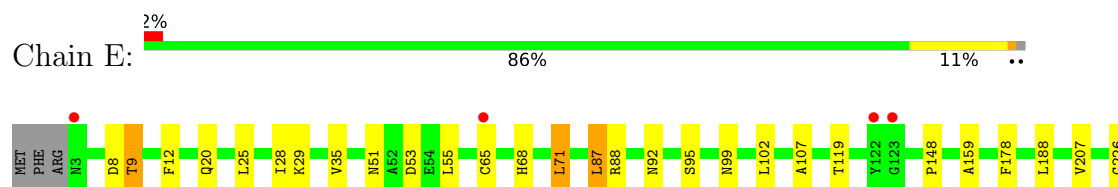
- Molecule 2: Proteasome subunit alpha type-3



- Molecule 2: Proteasome subunit alpha type-3

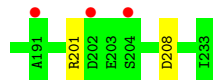
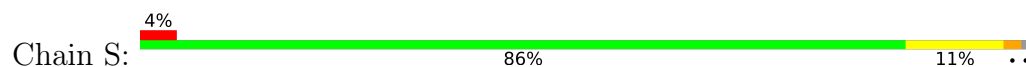


- Molecule 3: Proteasome subunit alpha type-4

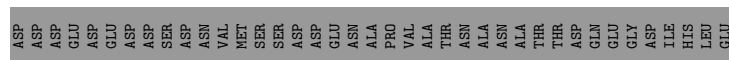
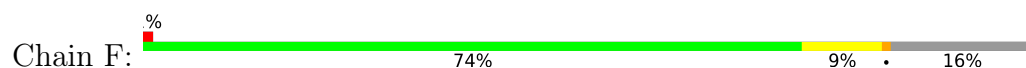




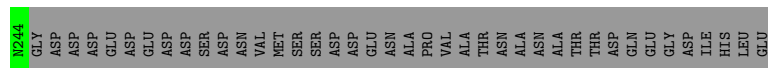
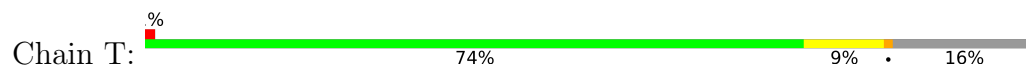
• Molecule 5: Proteasome subunit alpha type-6



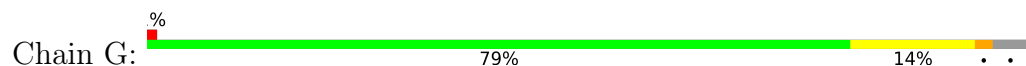
• Molecule 6: Probable proteasome subunit alpha type-7



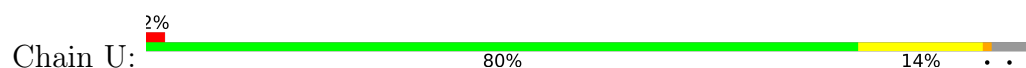
• Molecule 6: Probable proteasome subunit alpha type-7

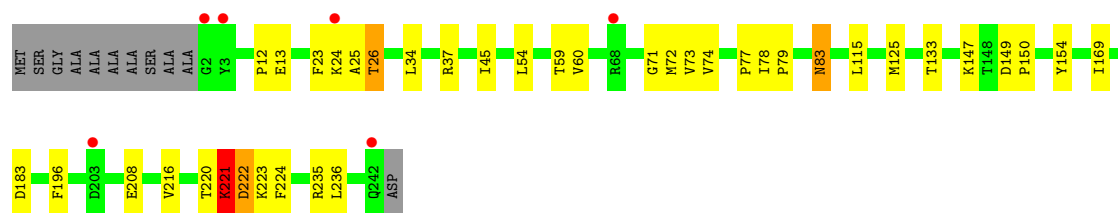


• Molecule 7: Proteasome subunit alpha type-1

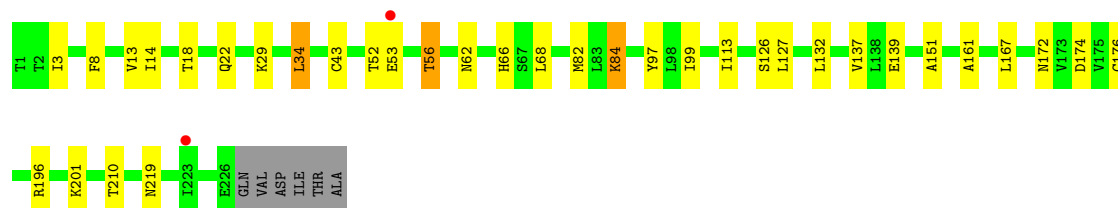
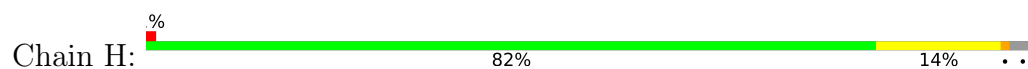


• Molecule 7: Proteasome subunit alpha type-1

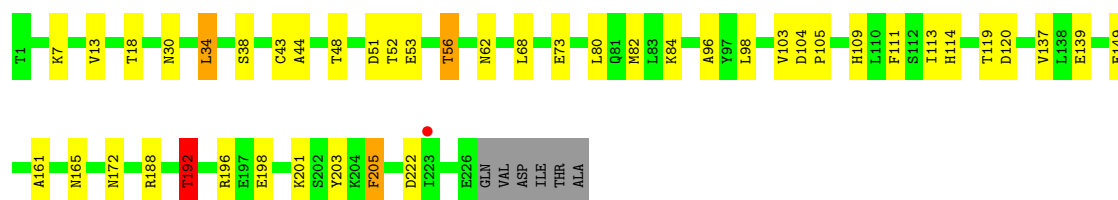
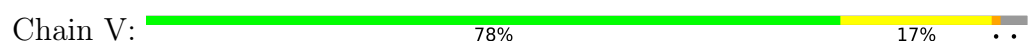




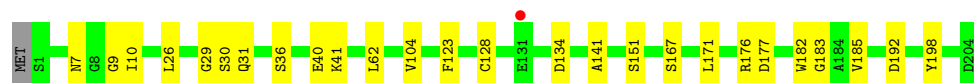
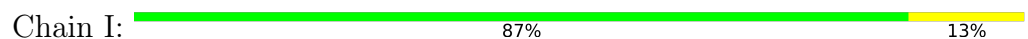
• Molecule 8: Proteasome subunit beta type-2



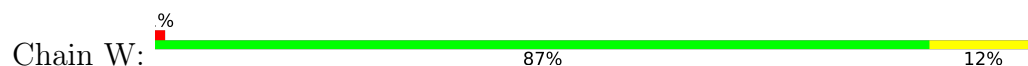
• Molecule 8: Proteasome subunit beta type-2



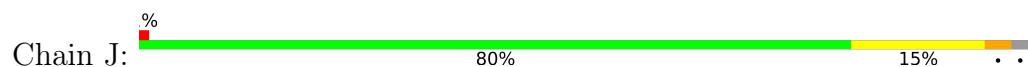
• Molecule 9: Proteasome subunit beta type-3

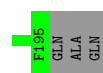


• Molecule 9: Proteasome subunit beta type-3

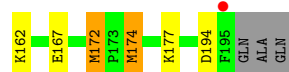
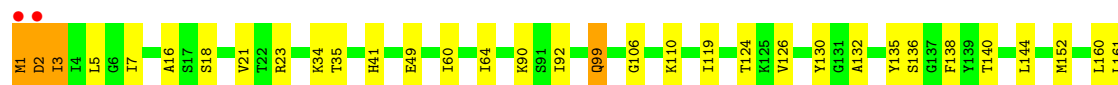
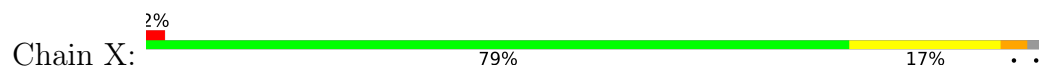


• Molecule 10: Proteasome subunit beta type-4

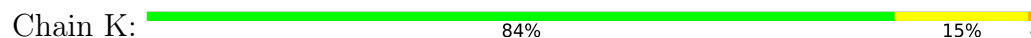




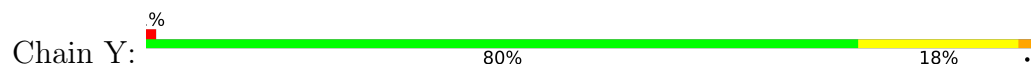
• Molecule 10: Proteasome subunit beta type-4



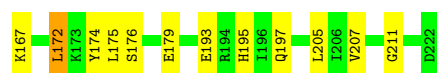
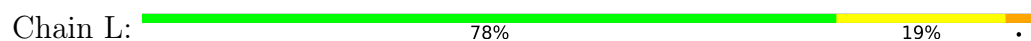
• Molecule 11: Proteasome subunit beta type-5



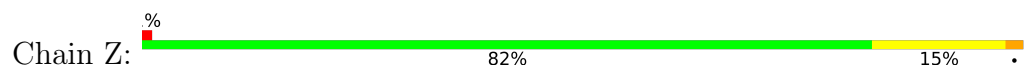
• Molecule 11: Proteasome subunit beta type-5

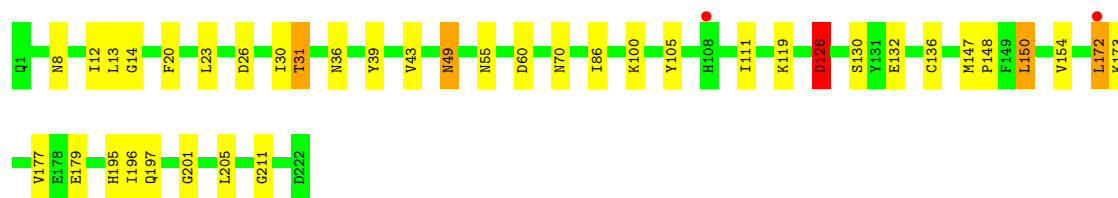


• Molecule 12: Proteasome subunit beta type-6

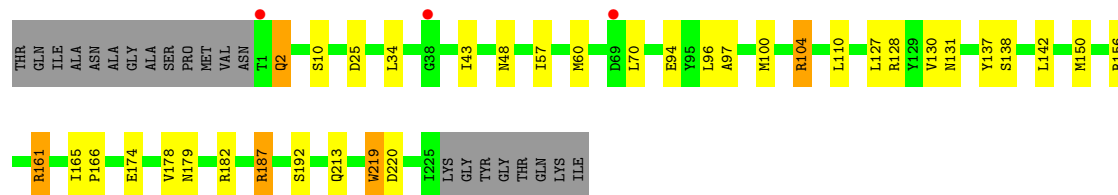
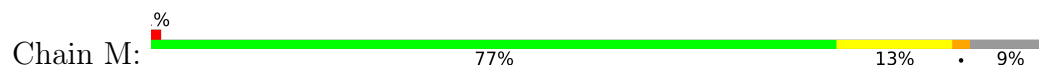


• Molecule 12: Proteasome subunit beta type-6

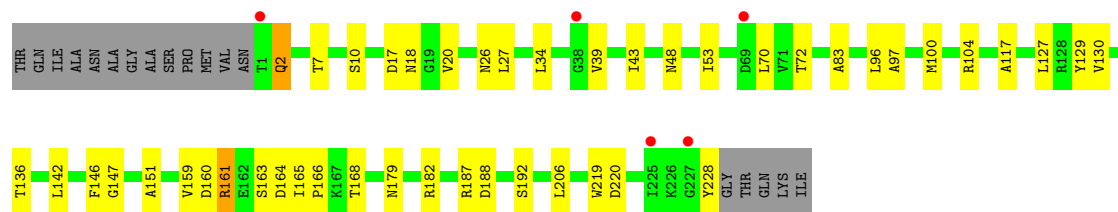
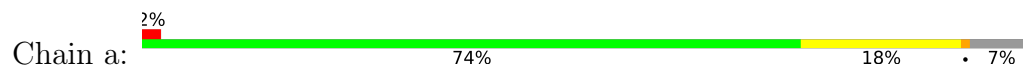




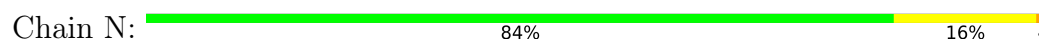
- Molecule 13: Proteasome subunit beta type-7



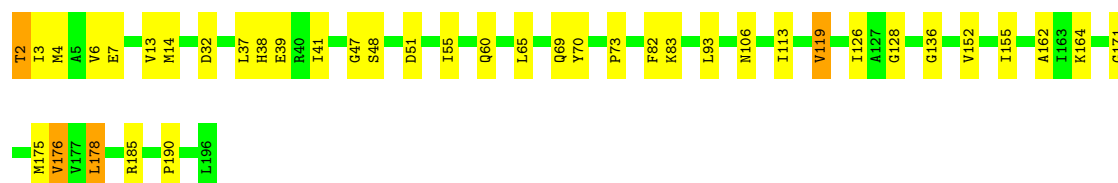
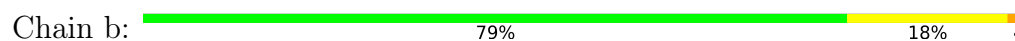
- Molecule 13: Proteasome subunit beta type-7



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



- 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	135.37Å 300.16Å 143.97Å 90.00° 112.78° 90.00°	Depositor
Resolution (Å)	30.00 – 2.75 30.00 – 2.75	Depositor EDS
% Data completeness (in resolution range)	96.8 (30.00-2.75) 96.8 (30.00-2.75)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.76Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.205 , 0.245 0.209 , 0.244	Depositor DCC
R_{free} test set	13235 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	63.6	Xtriage
Anisotropy	0.507	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 33.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	49773	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% 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, SO4, A1IF8, CL, 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	1.02	0/1952	1.41	0/2642
1	O	1.02	0/1952	1.44	0/2642
2	B	1.02	0/1945	1.44	0/2633
2	P	1.04	0/1934	1.44	0/2618
3	C	1.03	0/1910	1.46	0/2586
3	Q	1.06	1/1910 (0.1%)	1.45	0/2586
4	D	1.05	0/1837	1.49	0/2475
4	R	1.05	0/1837	1.46	0/2475
5	E	1.03	0/1800	1.43	0/2433
5	S	1.02	0/1800	1.44	0/2433
6	F	1.01	0/1932	1.47	4/2609 (0.2%)
6	T	1.07	2/1932 (0.1%)	1.46	1/2609 (0.0%)
7	G	1.02	0/1945	1.45	4/2634 (0.2%)
7	U	1.05	0/1945	1.48	6/2634 (0.2%)
8	H	1.03	0/1750	1.43	0/2373
8	V	1.03	0/1750	1.46	1/2373 (0.0%)
9	I	1.03	0/1611	1.43	2/2174 (0.1%)
9	W	1.02	0/1611	1.41	0/2174
10	J	0.99	0/1589	1.39	0/2142
10	X	0.97	0/1589	1.44	2/2142 (0.1%)
11	K	1.01	0/1674	1.44	4/2264 (0.2%)
11	Y	1.02	0/1674	1.42	1/2264 (0.0%)
12	L	0.99	0/1795	1.40	1/2420 (0.0%)
12	Z	1.00	0/1806	1.43	3/2435 (0.1%)
13	M	1.00	0/1791	1.43	4/2431 (0.2%)
13	a	1.01	0/1817	1.41	3/2465 (0.1%)
14	N	1.02	0/1524	1.43	0/2063
14	b	1.03	1/1524 (0.1%)	1.44	2/2063 (0.1%)
All	All	1.02	4/50136 (0.0%)	1.44	38/67792 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	T	164	GLY	C-O	5.65	1.31	1.23
3	Q	75	GLY	C-O	5.58	1.28	1.24
14	b	47	GLY	C-O	5.48	1.27	1.24
6	T	26	ALA	C-O	5.15	1.30	1.24

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	V	192	THR	CB-CA-C	7.56	121.84	111.41
7	U	222	ASP	CA-C-N	7.02	134.94	121.54
7	U	222	ASP	C-N-CA	7.02	134.94	121.54
6	F	77	LEU	CA-C-N	6.96	124.63	120.24
6	F	77	LEU	C-N-CA	6.96	124.63	120.24

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	14	0
1	O	1915	0	1929	8	0
2	B	1914	0	1910	32	0
2	P	1904	0	1904	24	0
3	C	1881	0	1895	15	0
3	Q	1881	0	1895	13	0
4	D	1813	0	1797	20	0
4	R	1813	0	1797	21	0
5	E	1773	0	1775	18	0
5	S	1773	0	1775	22	0
6	F	1892	0	1883	14	0
6	T	1892	0	1883	14	0
7	G	1907	0	1901	22	0
7	U	1907	0	1901	21	0
8	H	1719	0	1719	19	0
8	V	1719	0	1719	30	0
9	I	1581	0	1574	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	W	1581	0	1574	16	0
10	J	1561	0	1569	24	0
10	X	1561	0	1569	27	0
11	K	1637	0	1585	27	0
11	Y	1637	0	1585	28	0
12	L	1757	0	1711	37	0
12	Z	1767	0	1717	32	0
13	M	1761	0	1765	22	0
13	a	1786	0	1790	29	0
14	N	1495	0	1450	23	0
14	b	1495	0	1450	29	0
15	G	1	0	0	0	0
15	H	1	0	0	0	0
15	U	1	0	0	0	0
15	V	1	0	0	1	0
16	G	1	0	0	0	0
16	I	1	0	0	0	0
16	K	1	0	0	0	0
16	N	1	0	0	0	0
16	W	1	0	0	0	0
16	X	1	0	0	0	0
16	Y	1	0	0	0	0
16	Z	1	0	0	0	0
17	K	50	0	0	2	0
17	N	50	0	0	1	0
17	Y	50	0	0	2	0
17	b	50	0	0	3	0
18	K	12	0	13	0	0
18	M	12	0	13	0	0
18	Y	12	0	13	1	0
18	a	12	0	13	3	0
19	N	5	0	0	1	0
20	A	6	0	0	0	0
20	B	9	0	0	0	0
20	C	7	0	0	0	0
20	D	7	0	0	0	0
20	E	4	0	0	0	0
20	F	6	0	0	0	0
20	G	17	0	0	1	0
20	H	10	0	0	0	0
20	I	10	0	0	0	0
20	J	11	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	K	11	0	0	0	0
20	L	10	0	0	0	0
20	M	17	0	0	1	0
20	N	4	0	0	0	0
20	O	3	0	0	0	0
20	P	5	0	0	0	0
20	Q	9	0	0	0	0
20	R	5	0	0	0	0
20	S	4	0	0	0	0
20	T	11	0	0	0	0
20	U	11	0	0	0	0
20	V	13	0	0	0	0
20	W	11	0	0	0	0
20	X	13	0	0	1	0
20	Y	14	0	0	0	0
20	Z	13	0	0	1	0
20	a	12	0	0	2	0
20	b	18	0	0	0	0
All	All	49773	0	49003	555	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 6.

The worst 5 of 555 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)
12:L:164:THR:O	12:L:167:LYS:HD2	1.61	1.00
10:J:25:ILE:HD11	10:X:135:TYR:CD1	2.03	0.93
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.52	0.91
11:K:5:ALA:HB3	11:K:100:MET:HE2	1.53	0.90
14:N:2:THR:HG21	14:N:162:ALA:CB	2.06	0.86

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%)	239 (96%)	7 (3%)	2 (1%)	16	30
1	O	248/250 (99%)	238 (96%)	6 (2%)	4 (2%)	7	14
2	B	243/258 (94%)	231 (95%)	7 (3%)	5 (2%)	5	11
2	P	242/258 (94%)	231 (96%)	6 (2%)	5 (2%)	5	11
3	C	238/254 (94%)	228 (96%)	6 (2%)	4 (2%)	7	14
3	Q	238/254 (94%)	226 (95%)	9 (4%)	3 (1%)	9	18
4	D	231/260 (89%)	225 (97%)	5 (2%)	1 (0%)	30	50
4	R	231/260 (89%)	224 (97%)	6 (3%)	1 (0%)	30	50
5	E	229/234 (98%)	218 (95%)	11 (5%)	0	100	100
5	S	229/234 (98%)	218 (95%)	11 (5%)	0	100	100
6	F	241/288 (84%)	235 (98%)	6 (2%)	0	100	100
6	T	241/288 (84%)	234 (97%)	7 (3%)	0	100	100
7	G	239/252 (95%)	230 (96%)	8 (3%)	1 (0%)	30	50
7	U	239/252 (95%)	228 (95%)	9 (4%)	2 (1%)	16	30
8	H	224/232 (97%)	214 (96%)	10 (4%)	0	100	100
8	V	224/232 (97%)	217 (97%)	7 (3%)	0	100	100
9	I	202/205 (98%)	192 (95%)	10 (5%)	0	100	100
9	W	202/205 (98%)	192 (95%)	10 (5%)	0	100	100
10	J	193/198 (98%)	187 (97%)	5 (3%)	1 (0%)	24	43
10	X	193/198 (98%)	184 (95%)	9 (5%)	0	100	100
11	K	209/211 (99%)	198 (95%)	11 (5%)	0	100	100
11	Y	209/211 (99%)	199 (95%)	9 (4%)	1 (0%)	24	43
12	L	220/222 (99%)	211 (96%)	9 (4%)	0	100	100
12	Z	221/222 (100%)	213 (96%)	8 (4%)	0	100	100
13	M	223/246 (91%)	215 (96%)	8 (4%)	0	100	100
13	a	226/246 (92%)	216 (96%)	9 (4%)	1 (0%)	30	50
14	N	193/195 (99%)	185 (96%)	8 (4%)	0	100	100
14	b	193/195 (99%)	183 (95%)	10 (5%)	0	100	100
All	All	6269/6610 (95%)	6011 (96%)	227 (4%)	31 (0%)	24	43

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR
2	B	51	VAL
2	B	220	ASN
2	B	221	ASP
3	C	202	GLN

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%)	202 (97%)	7 (3%)	33	57
1	O	209/209 (100%)	205 (98%)	4 (2%)	50	70
2	B	204/216 (94%)	196 (96%)	8 (4%)	28	51
2	P	203/216 (94%)	194 (96%)	9 (4%)	25	47
3	C	212/226 (94%)	196 (92%)	16 (8%)	12	24
3	Q	212/226 (94%)	203 (96%)	9 (4%)	26	49
4	D	194/215 (90%)	179 (92%)	15 (8%)	12	22
4	R	194/215 (90%)	184 (95%)	10 (5%)	21	39
5	E	190/193 (98%)	180 (95%)	10 (5%)	20	39
5	S	190/193 (98%)	181 (95%)	9 (5%)	23	45
6	F	201/239 (84%)	189 (94%)	12 (6%)	17	32
6	T	201/239 (84%)	190 (94%)	11 (6%)	19	37
7	G	206/210 (98%)	192 (93%)	14 (7%)	14	27
7	U	206/210 (98%)	194 (94%)	12 (6%)	18	34
8	H	185/190 (97%)	174 (94%)	11 (6%)	18	33
8	V	185/190 (97%)	170 (92%)	15 (8%)	11	20
9	I	172/173 (99%)	166 (96%)	6 (4%)	32	56
9	W	172/173 (99%)	168 (98%)	4 (2%)	44	66
10	J	173/175 (99%)	161 (93%)	12 (7%)	14	26
10	X	173/175 (99%)	162 (94%)	11 (6%)	16	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	168/168 (100%)	161 (96%)	7 (4%)	26	49
11	Y	168/168 (100%)	159 (95%)	9 (5%)	20	38
12	L	185/185 (100%)	174 (94%)	11 (6%)	18	33
12	Z	186/185 (100%)	178 (96%)	8 (4%)	26	47
13	M	193/208 (93%)	183 (95%)	10 (5%)	21	39
13	a	195/208 (94%)	184 (94%)	11 (6%)	19	36
14	N	160/160 (100%)	153 (96%)	7 (4%)	25	47
14	b	160/160 (100%)	150 (94%)	10 (6%)	16	30
All	All	5306/5534 (96%)	5028 (95%)	278 (5%)	21	39

5 of 278 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	X	3	ILE
10	X	172	MET
13	a	70	LEU
9	I	182	TRP
9	I	31	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 166 such sidechains are listed below:

Mol	Chain	Res	Type
6	T	86	ASN
11	Y	133	GLN
6	T	191	GLN
8	V	66	HIS
12	Z	70	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 21 ligands modelled in this entry, 12 are monoatomic - leaving 9 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	N	202	-	4,4,4	0.37	0	6,6,6	0.06	0
17	A1IF8	b	201	14	45,52,52	3.18	10 (22%)	52,75,75	1.32	5 (9%)
18	MES	K	302	-	12,12,12	0.74	0	15,16,16	0.28	0
17	A1IF8	K	301	11	45,52,52	2.76	10 (22%)	52,75,75	1.27	6 (11%)
18	MES	M	301	-	12,12,12	0.69	0	15,16,16	0.30	0
18	MES	a	301	-	12,12,12	0.67	0	15,16,16	0.41	0
17	A1IF8	N	201	14	45,52,52	3.46	13 (28%)	52,75,75	1.23	6 (11%)
18	MES	Y	302	-	12,12,12	0.72	0	15,16,16	0.36	0
17	A1IF8	Y	301	11	45,52,52	2.72	8 (17%)	52,75,75	1.48	8 (15%)

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	A1IF8	b	201	14	-	14/40/94/94	0/2/3/3
18	MES	K	302	-	-	2/6/14/14	0/1/1/1
17	A1IF8	K	301	11	-	5/40/94/94	0/2/3/3
18	MES	M	301	-	-	0/6/14/14	0/1/1/1
18	MES	a	301	-	-	0/6/14/14	0/1/1/1
17	A1IF8	N	201	14	-	5/40/94/94	0/2/3/3
18	MES	Y	302	-	-	3/6/14/14	0/1/1/1
17	A1IF8	Y	301	11	-	9/40/94/94	0/2/3/3

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	N	201	A1IF8	F4-C3	-13.80	0.84	1.37
17	N	201	A1IF8	F5-C3	-13.16	0.87	1.37
17	b	201	A1IF8	F5-C3	-12.19	0.91	1.37
17	b	201	A1IF8	F4-C3	-10.80	0.96	1.37
17	Y	301	A1IF8	F5-C3	-8.87	1.03	1.37

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	201	A1IF8	C34-N36-C37	3.67	126.70	121.13
17	Y	301	A1IF8	C2-N1-C7	-3.43	105.84	112.74
17	b	201	A1IF8	C28-C10-C11	-3.40	101.80	110.11
17	b	201	A1IF8	C13-N12-C11	-3.09	118.49	123.37
17	Y	301	A1IF8	C13-N12-C11	-3.06	118.54	123.37

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	K	301	A1IF8	O42-C37-C38-N39
17	K	301	A1IF8	N36-C37-C38-N39
17	Y	301	A1IF8	N1-C33-C34-C35
17	Y	301	A1IF8	O43-C33-C34-C35
17	b	201	A1IF8	C20-C13-N12-C11

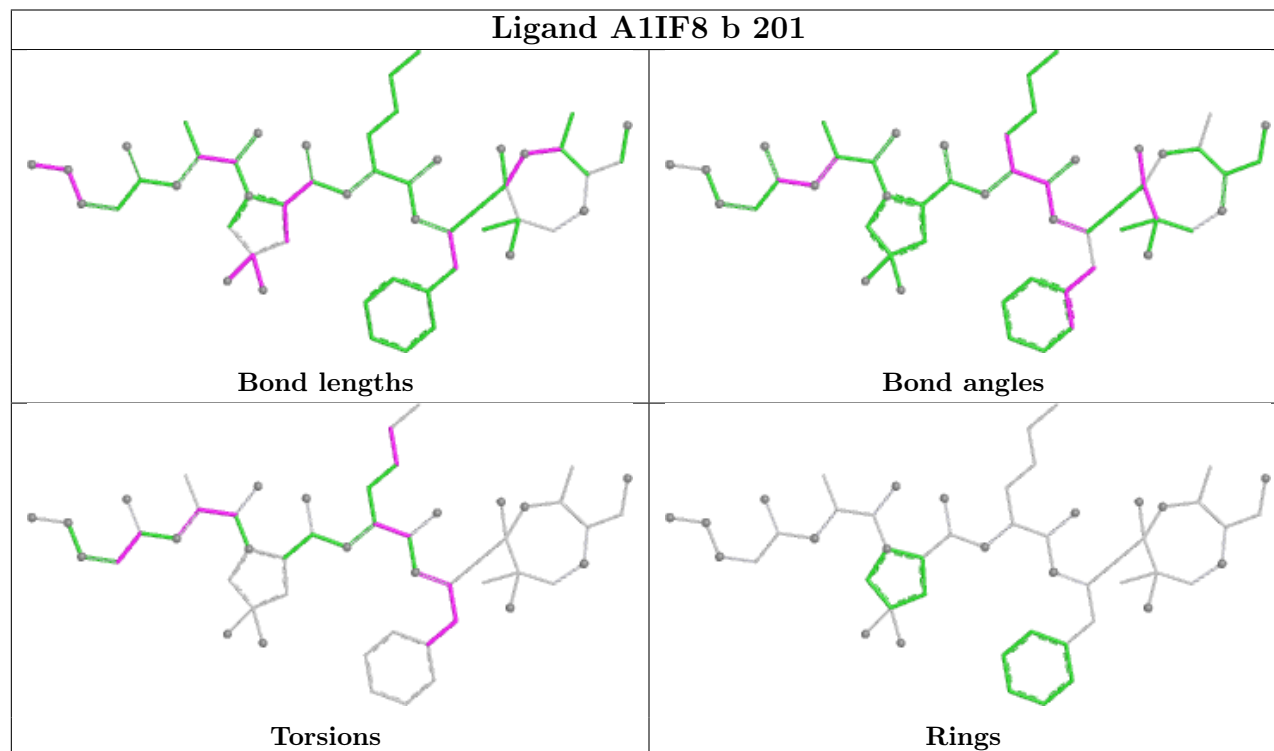
There are no ring outliers.

7 monomers are involved in 13 short contacts:

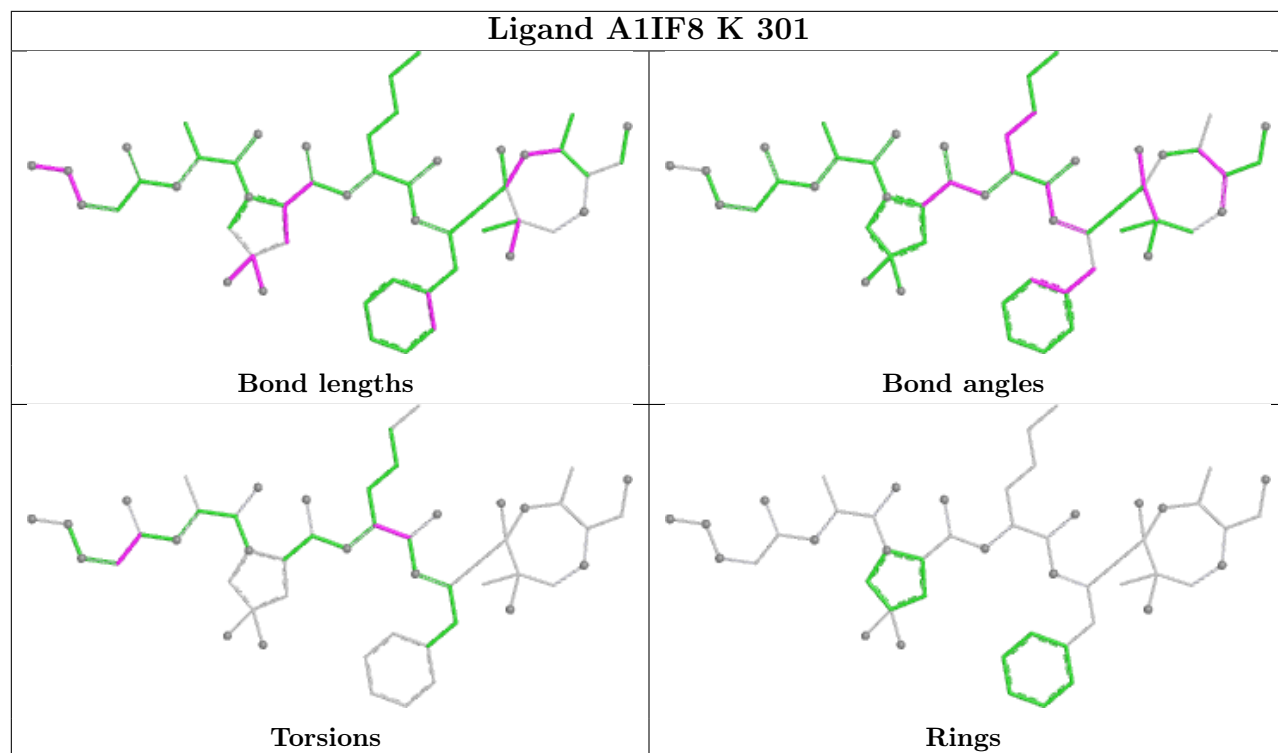
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	N	202	SO4	1	0
17	b	201	A1IF8	3	0
17	K	301	A1IF8	2	0
18	a	301	MES	3	0
17	N	201	A1IF8	1	0
18	Y	302	MES	1	0
17	Y	301	A1IF8	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

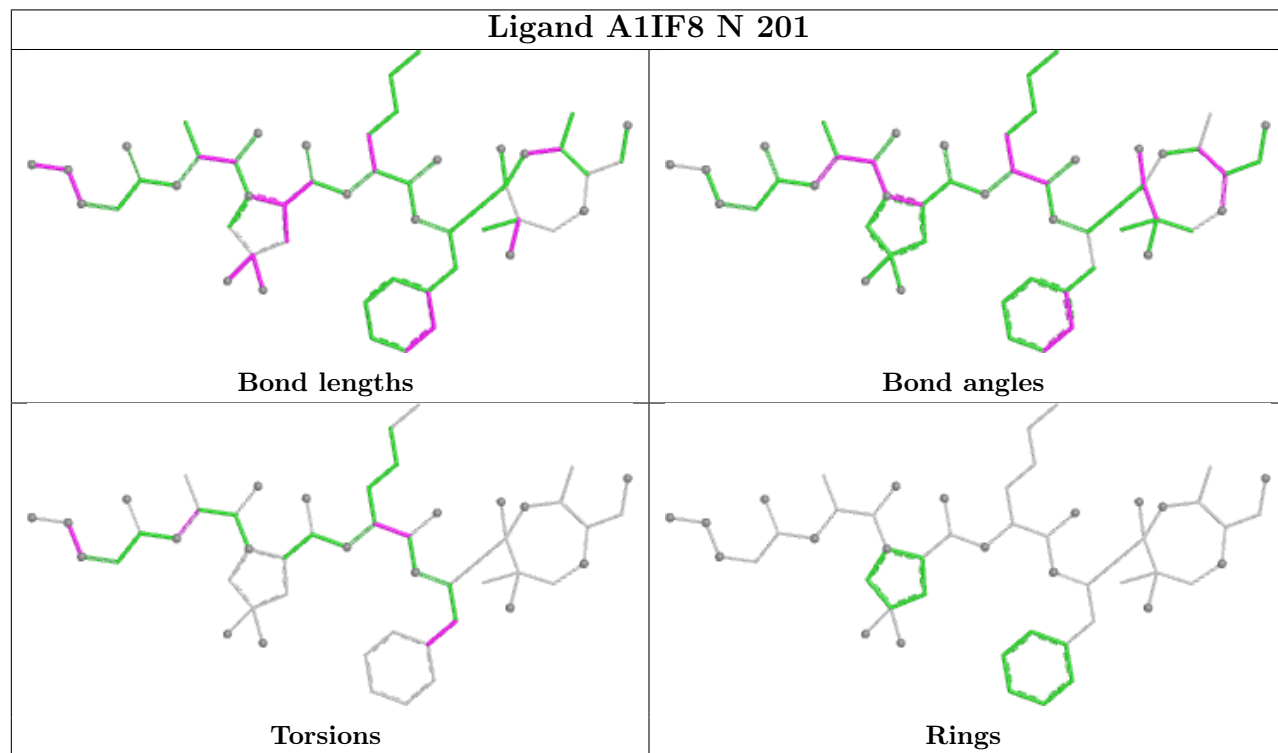
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

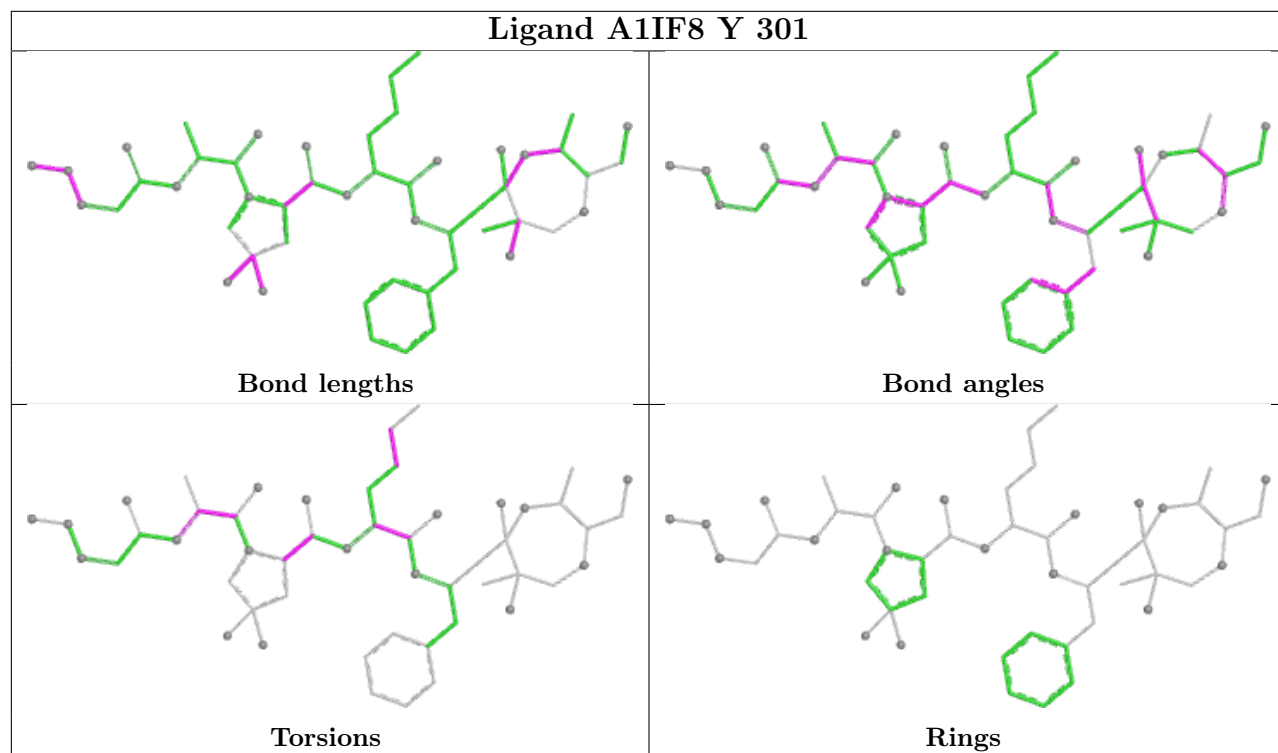


Ligand A1IF8 K 301



Ligand A1IF8 N 201





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	250/250 (100%)	-0.01	2 (0%) 82 82	58, 71, 102, 135	0
1	O	250/250 (100%)	-0.01	6 (2%) 59 57	63, 79, 111, 138	0
2	B	244/258 (94%)	0.16	5 (2%) 65 63	32, 75, 112, 172	1 (0%)
2	P	244/258 (94%)	0.21	5 (2%) 65 63	63, 78, 123, 155	0
3	C	240/254 (94%)	0.17	4 (1%) 69 67	57, 79, 134, 147	0
3	Q	240/254 (94%)	0.37	11 (4%) 37 36	64, 91, 155, 176	0
4	D	235/260 (90%)	0.10	3 (1%) 75 75	61, 79, 100, 135	0
4	R	235/260 (90%)	0.16	4 (1%) 69 67	65, 84, 114, 139	0
5	E	231/234 (98%)	0.13	4 (1%) 69 67	62, 81, 108, 127	0
5	S	231/234 (98%)	0.36	9 (3%) 43 40	69, 89, 124, 139	0
6	F	243/288 (84%)	0.10	3 (1%) 76 76	58, 74, 108, 137	0
6	T	243/288 (84%)	0.12	2 (0%) 82 82	64, 80, 117, 138	0
7	G	241/252 (95%)	-0.07	3 (1%) 76 76	56, 69, 99, 141	0
7	U	241/252 (95%)	0.01	6 (2%) 58 56	61, 74, 100, 131	0
8	H	226/232 (97%)	0.10	2 (0%) 81 81	56, 69, 92, 148	0
8	V	226/232 (97%)	0.10	1 (0%) 88 89	59, 73, 95, 150	0
9	I	204/205 (99%)	-0.07	1 (0%) 87 87	54, 68, 89, 104	0
9	W	204/205 (99%)	-0.05	2 (0%) 79 79	53, 66, 89, 105	0
10	J	195/198 (98%)	-0.05	2 (1%) 79 79	56, 68, 91, 121	0
10	X	195/198 (98%)	-0.08	3 (1%) 72 71	59, 69, 88, 125	0
11	K	211/211 (100%)	-0.10	0 100 100	53, 65, 85, 99	0
11	Y	211/211 (100%)	-0.04	2 (0%) 81 81	58, 70, 91, 111	0
12	L	222/222 (100%)	0.02	1 (0%) 87 87	56, 69, 90, 112	0
12	Z	222/222 (100%)	0.12	2 (0%) 81 81	31, 71, 95, 118	1 (0%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	225/246 (91%)	-0.07	3 (1%) 75 75	54, 68, 86, 115	0
13	a	228/246 (92%)	-0.06	5 (2%) 62 60	54, 66, 87, 120	0
14	N	195/195 (100%)	-0.02	0 100 100	54, 66, 89, 119	0
14	b	195/195 (100%)	-0.03	0 100 100	56, 67, 89, 118	0
All	All	6327/6610 (95%)	0.06	91 (1%) 73 73	31, 73, 111, 176	2 (0%)

The worst 5 of 91 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	50	LEU	8.3
2	P	51	VAL	5.2
3	Q	49	THR	5.0
1	A	1	MET	4.7
2	B	1	GLY	4.3

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.

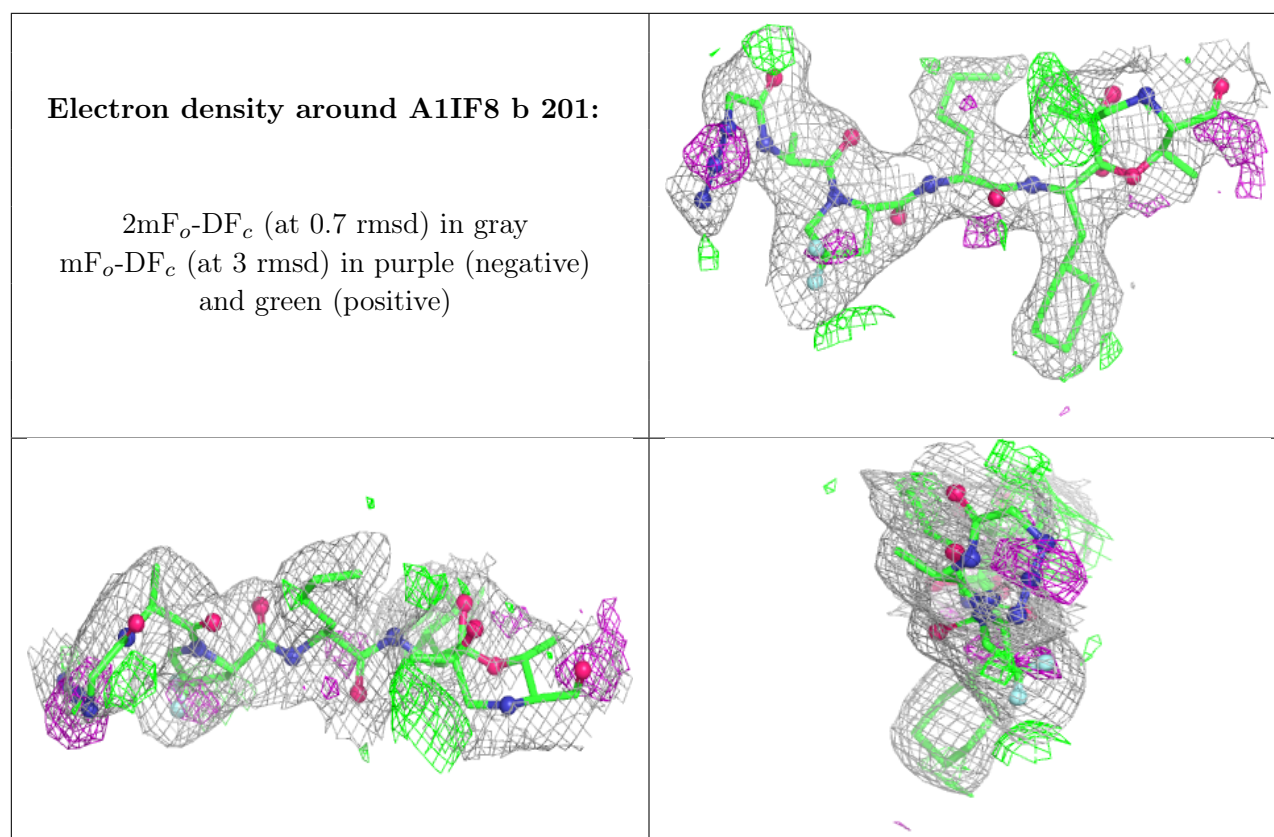
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
18	MES	M	301	12/12	0.77	0.22	140,142,154,158	0
16	MG	I	301	1/1	0.78	0.39	95,95,95,95	0
18	MES	a	301	12/12	0.79	0.18	125,130,140,141	0
16	MG	Z	301	1/1	0.80	0.31	79,79,79,79	0
19	SO4	N	202	5/5	0.85	0.30	120,121,125,132	0
17	A1IF8	b	201	50/50	0.87	0.12	61,65,93,99	0
17	A1IF8	Y	301	50/50	0.87	0.15	65,74,97,100	0

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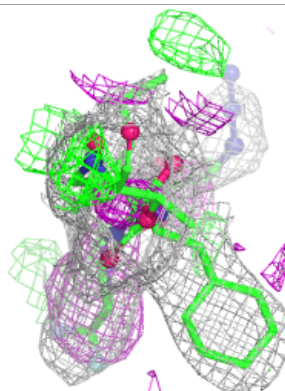
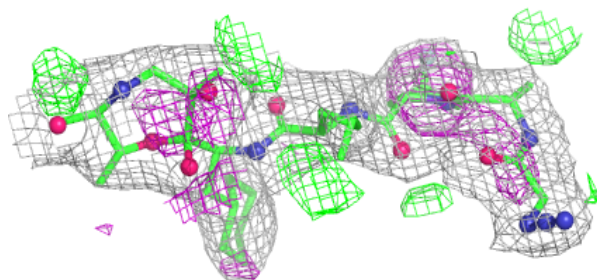
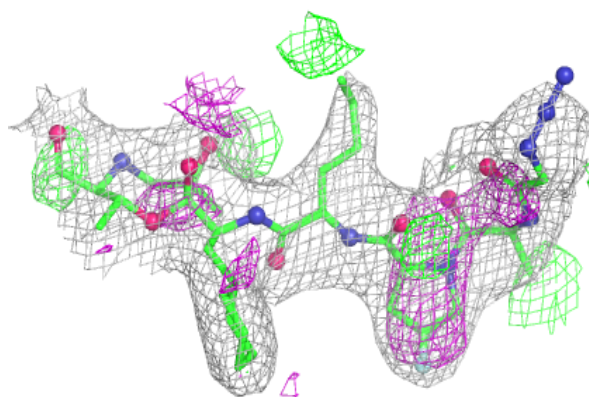
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	CL	V	301	1/1	0.88	0.15	96,96,96,96	0
18	MES	Y	302	12/12	0.89	0.16	89,90,97,101	0
16	MG	N	203	1/1	0.90	0.11	55,55,55,55	0
17	A1IF8	K	301	50/50	0.90	0.12	59,68,99,100	0
17	A1IF8	N	201	50/50	0.91	0.10	55,59,82,91	0
18	MES	K	302	12/12	0.91	0.15	81,86,94,104	0
16	MG	W	301	1/1	0.92	0.11	72,72,72,72	0
15	CL	H	301	1/1	0.96	0.17	77,77,77,77	0
16	MG	X	201	1/1	0.96	0.17	38,38,38,38	0
15	CL	G	301	1/1	0.96	0.07	59,59,59,59	0
15	CL	U	301	1/1	0.97	0.09	64,64,64,64	0
16	MG	Y	303	1/1	0.97	0.05	80,80,80,80	0
16	MG	K	303	1/1	0.97	0.04	73,73,73,73	0
16	MG	G	302	1/1	0.98	0.05	67,67,67,67	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.

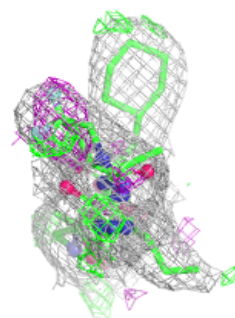
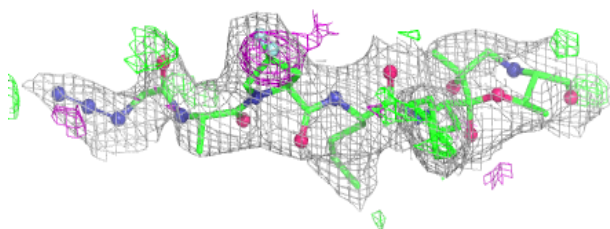
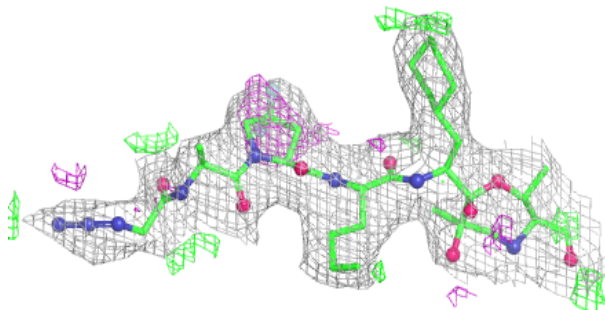


Electron density around A1IF8 Y 301:

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

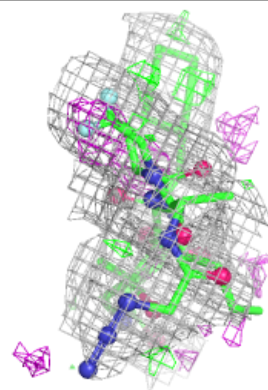
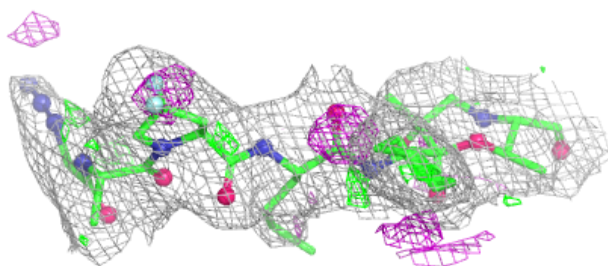
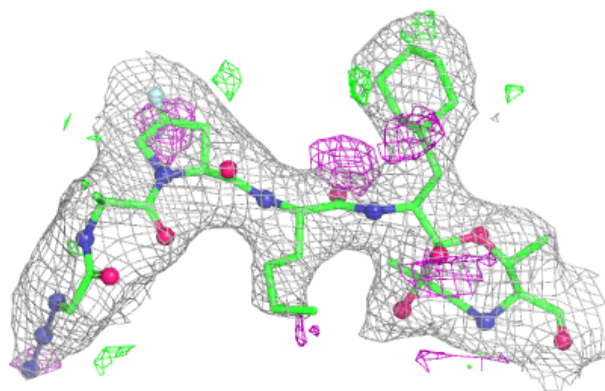
**Electron density around A1IF8 K 301:**

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



Electron density around A1IF8 N 201:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.