



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 03:27 AM UTC

PDB ID : 4EU2 / pdb_00004eu2
Title : Crystal structure of 20s proteasome with novel inhibitor K-7174
Authors : Kikuchi, J.; Shibayama, N.; Yamada, S.; Wada, T.; Nobuyoshi, M.; Izumi, T.; Akutsu, M.; Kano, Y.; Ohki, M.; Sugiyama, K.; Park, S.-Y.; Furukawa, Y.
Deposited on : 2012-04-25
Resolution : 2.51 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

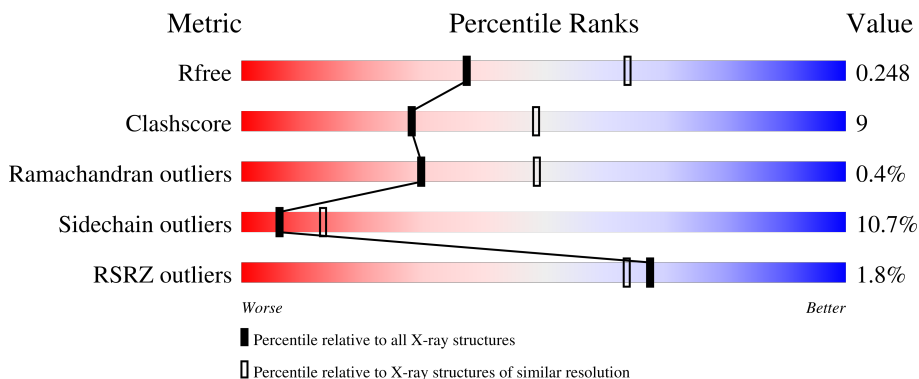
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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.



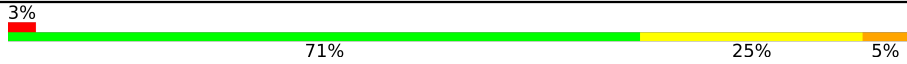

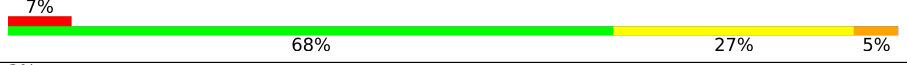



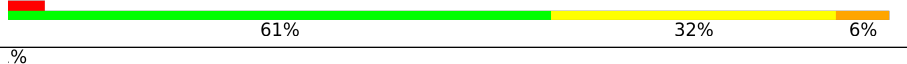

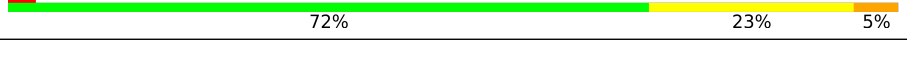


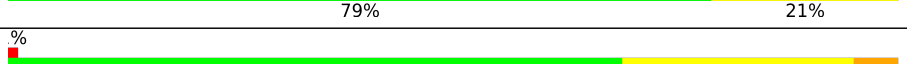

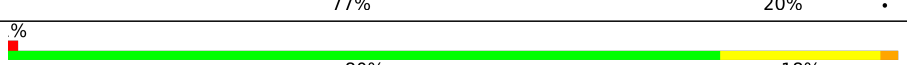

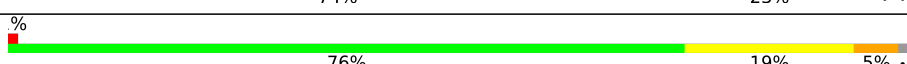
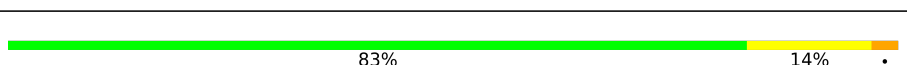
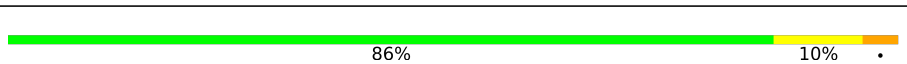
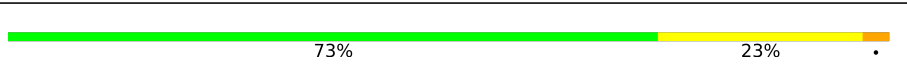



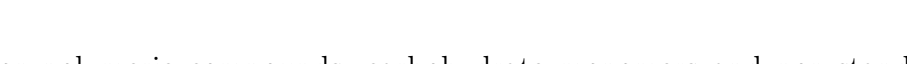
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	241	 72% 24% 2% 2%
1	O	241	 67% 30% 2% 2%
2	B	250	 83% 12% 2% 2%
2	P	250	 65% 30% 2% 2%
3	C	244	 71% 26% 2% 3%

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Mol	Chain	Length	Quality of chain
3	Q	244	 3% 71% 25% 5%
4	D	241	 4% 73% 24% .
4	R	241	 7% 68% 27% 5%
5	E	242	 3% 70% 25% 5%
5	S	242	 5% 69% 25% 6%
6	F	233	 % 69% 27% .
6	T	233	 4% 61% 32% 6%
7	G	244	 % 73% 24% .
7	U	244	 3% 72% 23% 5%
8	H	196	 72% 24% .
8	V	196	 77% 21% .
9	I	222	 % 79% 21%
9	W	222	 % 69% 26% 5%
10	J	204	 77% 20% .
10	X	204	 % 80% 18% .
11	K	198	 % 74% 23% ..
11	Y	198	 % 76% 19% 5% .
12	L	212	 83% 14% .
12	Z	212	 86% 10% .
13	1	222	 73% 23% .
13	M	222	 76% 23% .
14	2	233	 73% 24% .
14	N	233	 77% 20% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	WPI	I	301	-	X	-	-
15	WPI	Z	301	-	X	-	-

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 50701 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 component C7-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	241	Total 1903	C 1212	N 319	O 364	S 8	0	0	0
1	O	241	Total 1903	C 1212	N 319	O 364	S 8	0	0	0

- Molecule 2 is a protein called Proteasome component Y7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	249	Total 1906	C 1213	N 314	O 375	S 4	0	0	0
2	P	249	Total 1906	C 1213	N 314	O 375	S 4	0	0	0

- Molecule 3 is a protein called Proteasome component Y13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	244	Total 1905	C 1201	N 321	O 380	S 3	0	0	0
3	Q	244	Total 1905	C 1201	N 321	O 380	S 3	0	0	0

- Molecule 4 is a protein called Proteasome component PRE6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	241	Total 1891	C 1181	N 331	O 375	S 4	0	0	0
4	R	241	Total 1891	C 1181	N 331	O 375	S 4	0	0	0

- Molecule 5 is a protein called Proteasome component PUP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	242	Total	C	N	O	S	0	0	0
			1862	1162	314	379	7			
5	S	242	Total	C	N	O	S	0	0	0
			1862	1162	314	379	7			

- Molecule 6 is a protein called Proteasome component PRE5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	232	Total	C	N	O	S	0	0	0
			1784	1120	311	349	4			
6	T	232	Total	C	N	O	S	0	0	0
			1784	1120	311	349	4			

- Molecule 7 is a protein called Proteasome component C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	244	Total	C	N	O	S	0	0	0
			1897	1205	330	358	4			
7	U	244	Total	C	N	O	S	0	0	0
			1897	1205	330	358	4			

- Molecule 8 is a protein called Proteasome component PRE3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
8	V	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

- Molecule 9 is a protein called Proteasome component PUP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			
9	W	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			

- Molecule 10 is a protein called Proteasome component PUP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

- Molecule 11 is a protein called Proteasome component C11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	196	Total	C	N	O	S	0	0	0
			1570	997	266	301	6			
11	Y	196	Total	C	N	O	S	0	0	0
			1570	997	266	301	6			

- Molecule 12 is a protein called Proteasome component PRE2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	212	Total	C	N	O	S	0	0	0
			1646	1045	282	312	7			
12	Z	212	Total	C	N	O	S	0	0	0
			1646	1045	282	312	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	33	ARG	LYS	conflict	UNP P30656
Z	33	ARG	LYS	conflict	UNP P30656

- Molecule 13 is a protein called Proteasome component C5.

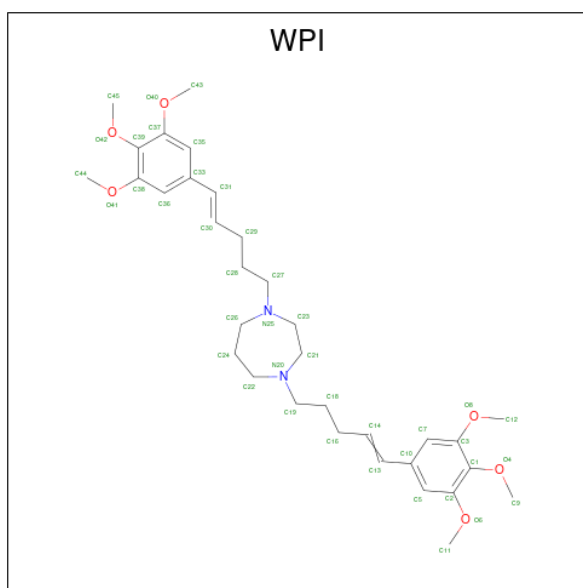
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
13	1	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

- Molecule 14 is a protein called Proteasome component PRE4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
14	2	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

- Molecule 15 is 1,4-bis[(4E)-5-(3,4,5-trimethoxyphenyl)pent-4-en-1-yl]-1,4-diazepane (CCD

ID: WPI (formula: C₃₃H₄₈N₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
15	H	1	Total	C	N	O		
			41	33	2	6	0	0
15	I	1	Total	C	N	O		
			41	33	2	6	0	0
15	L	1	Total	C	N	O		
			41	33	2	6	0	0
15	V	1	Total	C	N	O		
			41	33	2	6	0	0
15	W	1	Total	C	N	O		
			41	33	2	6	0	0
15	Z	1	Total	C	N	O		
			41	33	2	6	0	0

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	47	Total	O		
			47	47	0	0
16	B	27	Total	O		
			27	27	0	0
16	C	34	Total	O		
			34	34	0	0
16	D	35	Total	O		
			35	35	0	0
16	E	30	Total	O		
			30	30	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	F	18	Total 18	O 18	0	0
16	G	36	Total 36	O 36	0	0
16	H	34	Total 34	O 34	0	0
16	I	29	Total 29	O 29	0	0
16	J	47	Total 47	O 47	0	0
16	K	34	Total 34	O 34	0	0
16	L	46	Total 46	O 46	0	0
16	M	51	Total 51	O 51	0	0
16	N	44	Total 44	O 44	0	0
16	O	33	Total 33	O 33	0	0
16	P	32	Total 32	O 32	0	0
16	Q	33	Total 33	O 33	0	0
16	R	18	Total 18	O 18	0	0
16	S	23	Total 23	O 23	0	0
16	T	19	Total 19	O 19	0	0
16	U	38	Total 38	O 38	0	0
16	V	47	Total 47	O 47	0	0
16	W	36	Total 36	O 36	0	0
16	X	36	Total 36	O 36	0	0
16	Y	49	Total 49	O 49	0	0
16	Z	41	Total 41	O 41	0	0

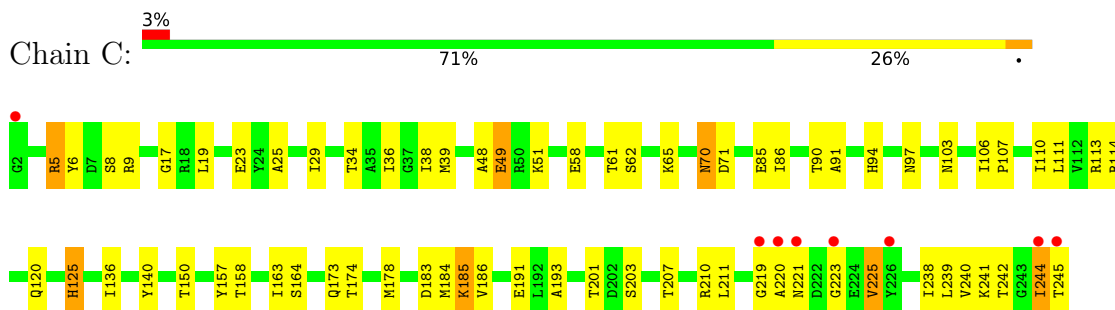
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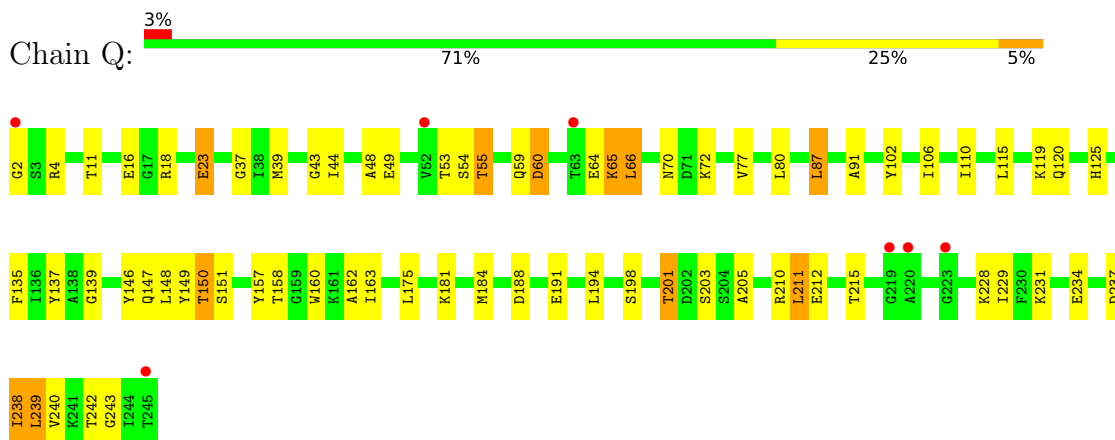
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	1	41	Total O 41 41	0	0
16	2	51	Total O 51 51	0	0



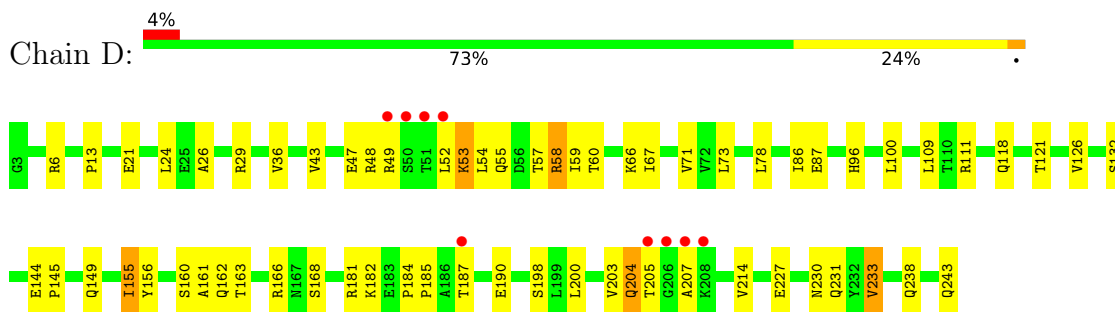
- Molecule 3: Proteasome component Y13



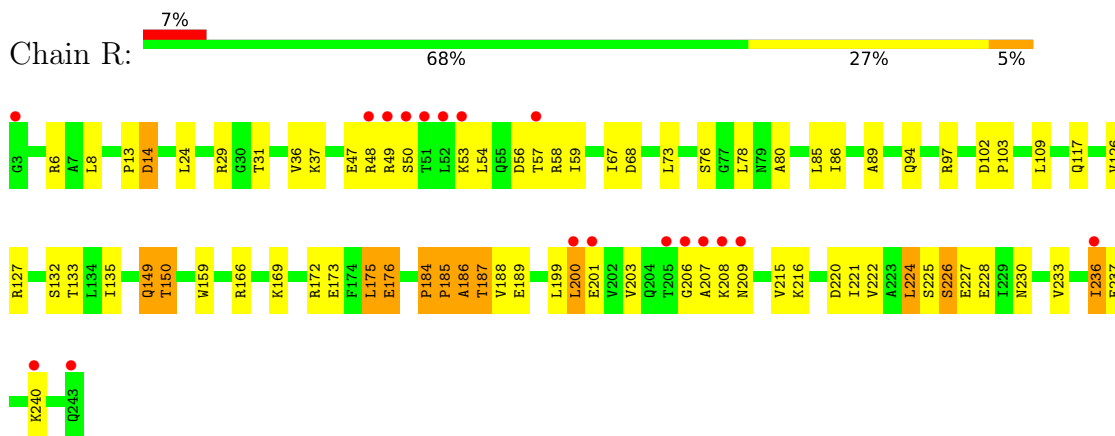
- Molecule 3: Proteasome component Y13



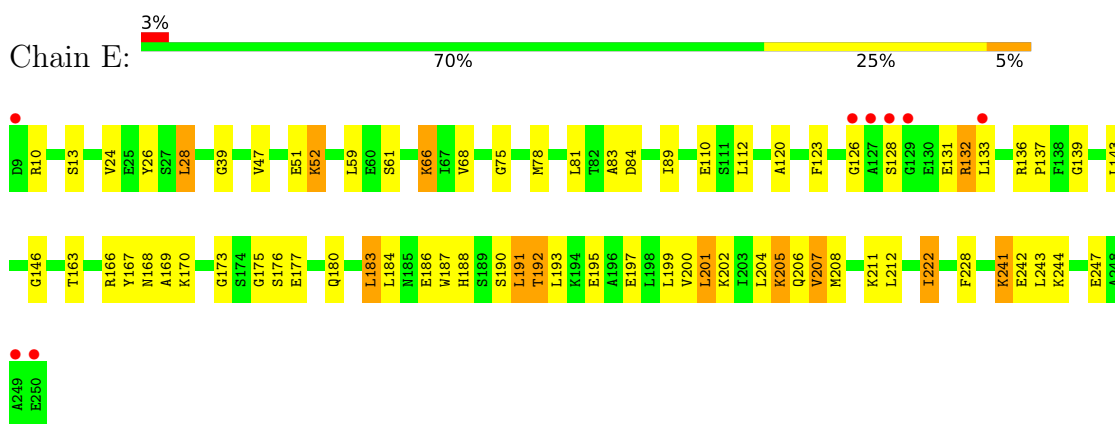
- Molecule 4: Proteasome component PRE6



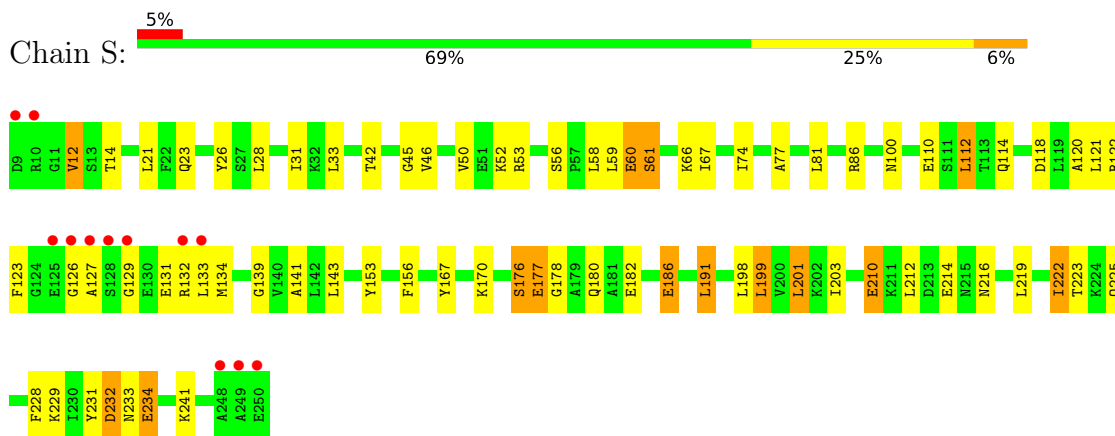
- Molecule 4: Proteasome component PRE6



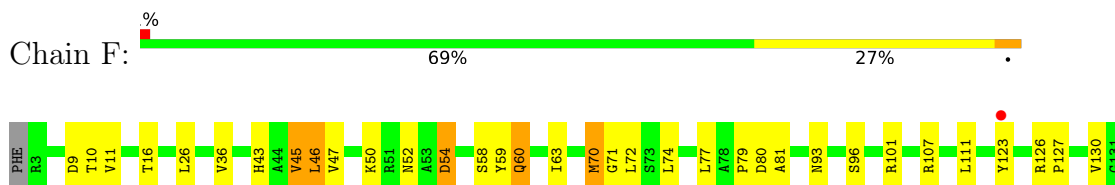
• Molecule 5: Proteasome component PUP2

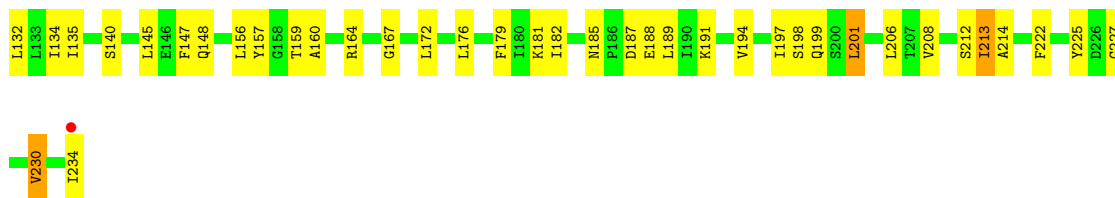


• Molecule 5: Proteasome component PUP2

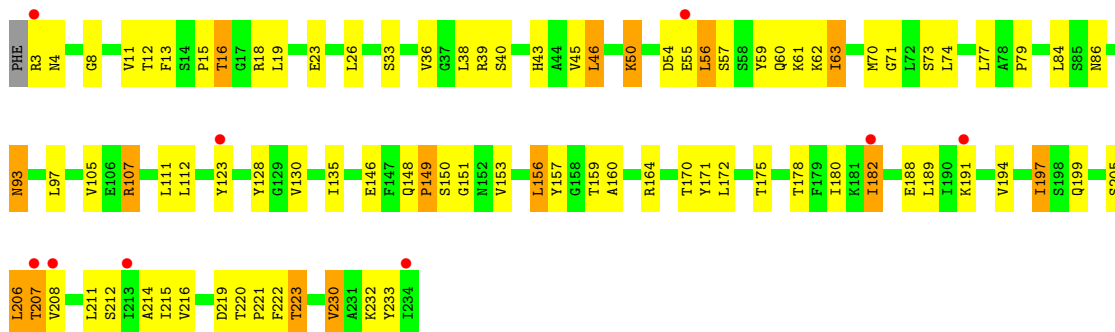


• Molecule 6: Proteasome component PRE5

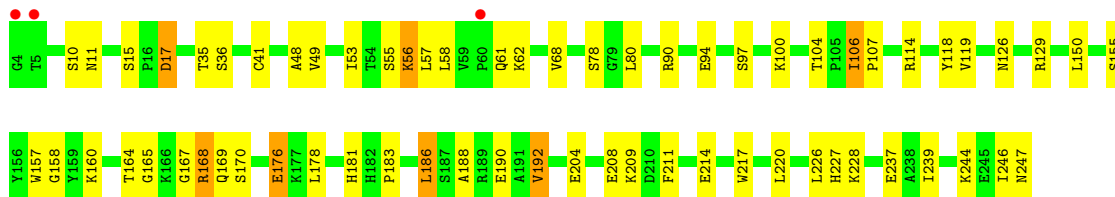
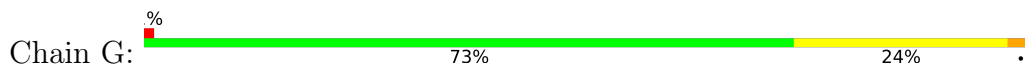




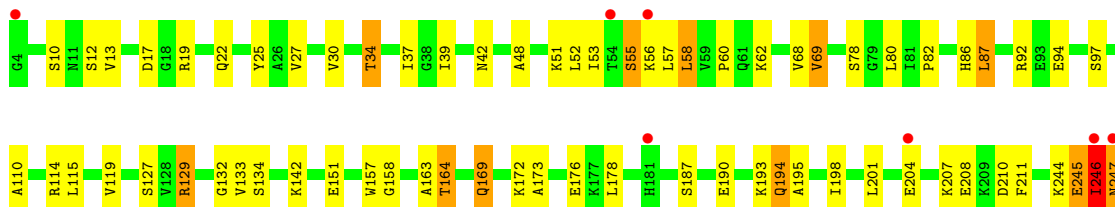
- Molecule 6: Proteasome component PRE5



- Molecule 7: Proteasome component C1



- Molecule 7: Proteasome component C1

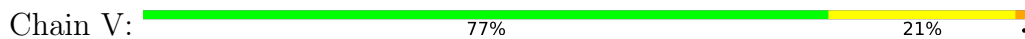


- Molecule 8: Proteasome component PRE3

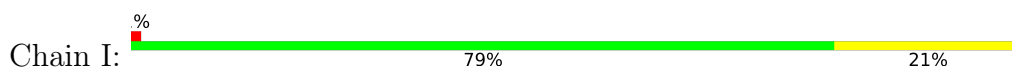




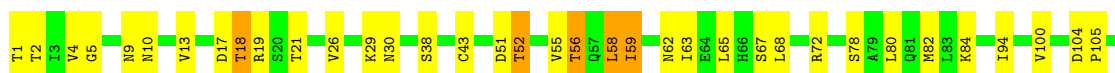
- Molecule 8: Proteasome component PRE3



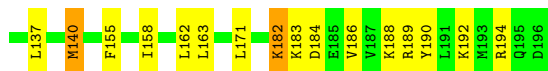
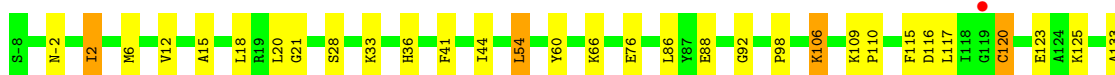
- Molecule 9: Proteasome component PUP1



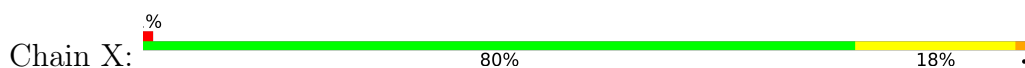
- Molecule 9: Proteasome component PUP1

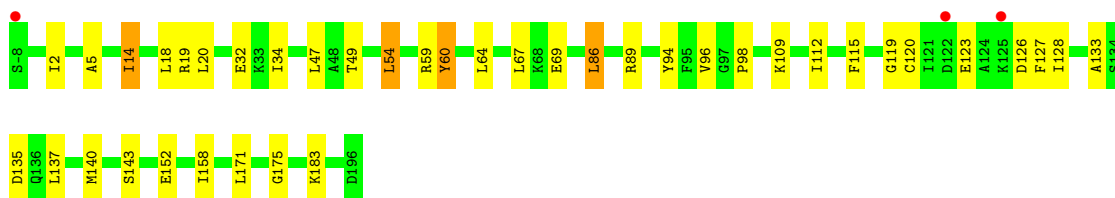


- Molecule 10: Proteasome component PUP3

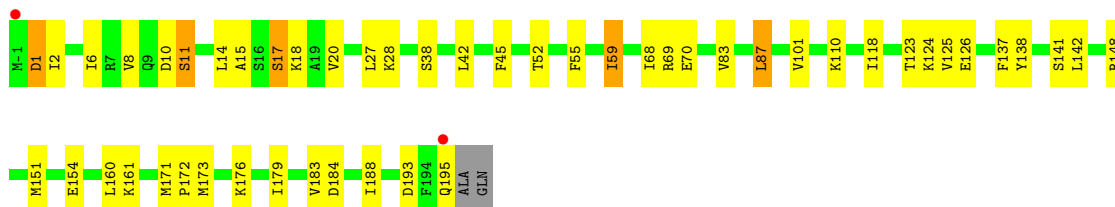


- Molecule 10: Proteasome component PUP3

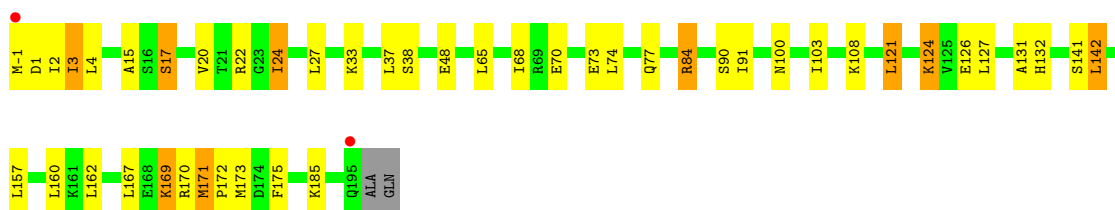
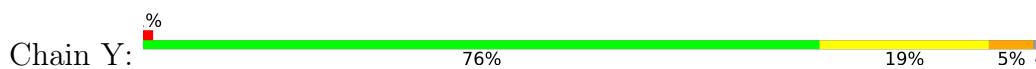




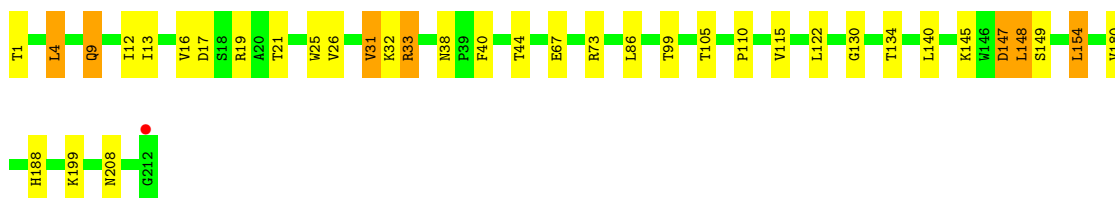
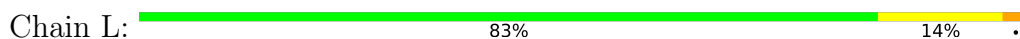
- Molecule 11: Proteasome component C11



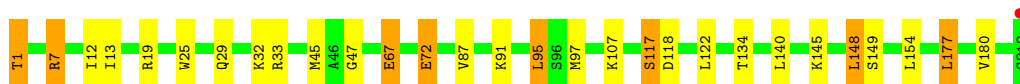
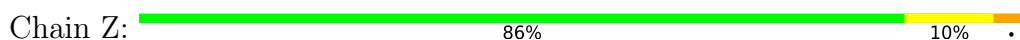
- Molecule 11: Proteasome component C11



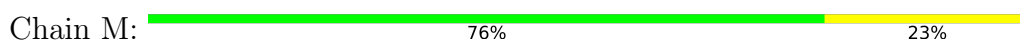
- Molecule 12: Proteasome component PRE2

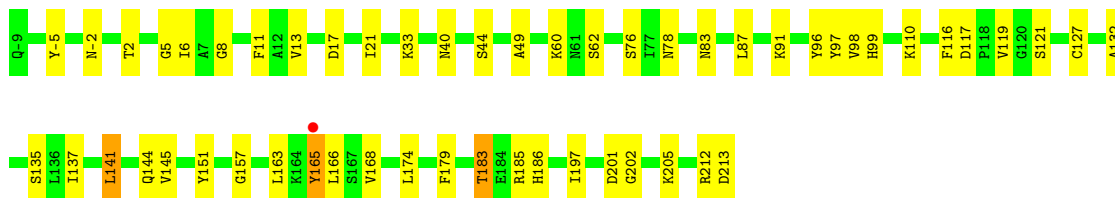


- Molecule 12: Proteasome component PRE2

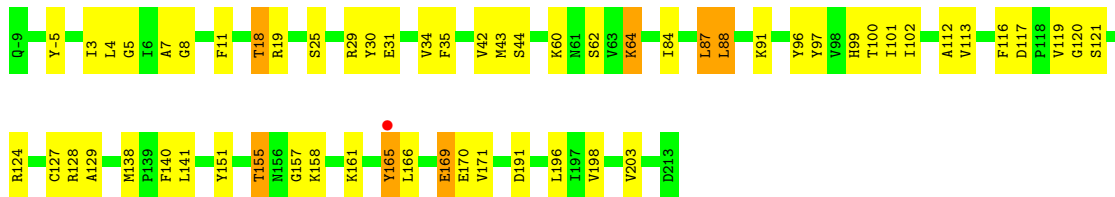


- Molecule 13: Proteasome component C5

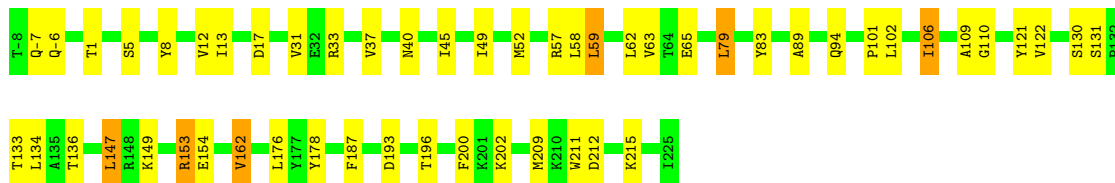
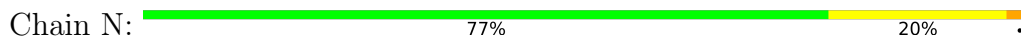




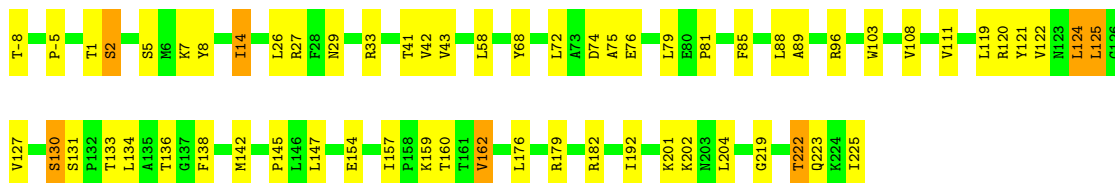
• Molecule 13: Proteasome component C5



• Molecule 14: Proteasome component PRE4



• Molecule 14: Proteasome component PRE4



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	134.26Å 301.36Å 143.96Å 90.00° 112.86° 90.00°	Depositor
Resolution (Å)	45.70 – 2.51 45.70 – 2.51	Depositor EDS
% Data completeness (in resolution range)	87.6 (45.70-2.51) 87.6 (45.70-2.51)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.51Å)	Xtrriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, R_{free}	0.202 , 0.255 0.197 , 0.248	Depositor DCC
R_{free} test set	15842 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtrriage
Anisotropy	0.909	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 29.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	50701	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% 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: WPI

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	0.55	0/1941	0.98	7/2629 (0.3%)
1	O	0.57	0/1941	0.89	2/2629 (0.1%)
2	B	0.54	0/1943	0.89	2/2631 (0.1%)
2	P	0.53	0/1943	0.91	1/2631 (0.0%)
3	C	0.53	0/1935	0.87	3/2618 (0.1%)
3	Q	0.53	0/1935	0.89	1/2618 (0.0%)
4	D	0.52	0/1920	0.88	1/2598 (0.0%)
4	R	0.54	0/1920	0.88	2/2598 (0.1%)
5	E	0.54	0/1887	0.86	2/2541 (0.1%)
5	S	0.49	0/1887	0.85	0/2541
6	F	0.49	0/1811	0.85	3/2447 (0.1%)
6	T	0.50	0/1811	0.92	4/2447 (0.2%)
7	G	0.49	0/1937	0.87	2/2614 (0.1%)
7	U	0.50	0/1937	0.91	3/2614 (0.1%)
8	H	0.55	0/1541	0.93	2/2087 (0.1%)
8	V	0.55	0/1541	0.91	0/2087
9	I	0.58	0/1716	0.92	0/2326
9	W	0.54	0/1716	0.90	2/2326 (0.1%)
10	J	0.52	0/1611	0.84	0/2174
10	X	0.55	0/1611	0.89	2/2174 (0.1%)
11	K	0.53	0/1598	0.87	2/2154 (0.1%)
11	Y	0.56	0/1598	0.91	2/2154 (0.1%)
12	L	0.56	0/1683	0.91	2/2277 (0.1%)
12	Z	0.51	0/1683	0.84	0/2277
13	1	0.50	0/1795	0.91	3/2420 (0.1%)
13	M	0.54	0/1795	0.90	2/2420 (0.1%)
14	2	0.57	0/1855	0.88	1/2514 (0.0%)
14	N	0.54	0/1855	0.89	0/2514
All	All	0.53	0/50346	0.89	51/68060 (0.1%)

There are no bond length outliers.

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	ILE	CB-CA-C	-8.36	105.48	114.35
1	A	87	ILE	N-CA-CB	8.20	115.67	110.50
1	A	158	ASP	CA-C-N	-7.81	111.78	120.45
1	A	158	ASP	C-N-CA	-7.81	111.78	120.45
12	L	38	ASN	CA-C-N	-7.72	111.55	120.12

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	1903	0	1898	49	0
1	O	1903	0	1898	53	0
2	B	1906	0	1918	25	0
2	P	1906	0	1918	44	0
3	C	1905	0	1901	35	0
3	Q	1905	0	1901	44	0
4	D	1891	0	1900	38	0
4	R	1891	0	1900	45	0
5	E	1862	0	1836	41	0
5	S	1862	0	1836	42	0
6	F	1784	0	1788	40	0
6	T	1784	0	1788	45	0
7	G	1897	0	1886	30	0
7	U	1897	0	1886	46	0
8	H	1512	0	1481	40	0
8	V	1512	0	1481	30	0
9	I	1685	0	1688	24	0
9	W	1685	0	1688	38	0
10	J	1581	0	1574	21	0
10	X	1581	0	1574	18	0
11	K	1570	0	1577	25	0
11	Y	1570	0	1577	27	0
12	L	1646	0	1595	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	Z	1646	0	1595	19	0
13	1	1757	0	1711	39	0
13	M	1757	0	1711	27	0
14	2	1824	0	1832	36	0
14	N	1824	0	1832	30	0
15	H	41	0	48	5	0
15	I	41	0	48	7	0
15	L	41	0	48	5	0
15	V	41	0	48	11	0
15	W	41	0	48	3	0
15	Z	41	0	48	7	0
16	1	41	0	0	1	0
16	2	51	0	0	2	0
16	A	47	0	0	0	0
16	B	27	0	0	0	0
16	C	34	0	0	0	0
16	D	35	0	0	0	0
16	E	30	0	0	0	0
16	F	18	0	0	0	0
16	G	36	0	0	0	0
16	H	34	0	0	1	0
16	I	29	0	0	0	0
16	J	47	0	0	0	0
16	K	34	0	0	1	0
16	L	46	0	0	0	0
16	M	51	0	0	0	0
16	N	44	0	0	1	0
16	O	33	0	0	1	0
16	P	32	0	0	0	0
16	Q	33	0	0	0	0
16	R	18	0	0	0	0
16	S	23	0	0	1	0
16	T	19	0	0	0	0
16	U	38	0	0	0	0
16	V	47	0	0	0	0
16	W	36	0	0	0	0
16	X	36	0	0	0	0
16	Y	49	0	0	1	0
16	Z	41	0	0	1	0
All	All	50701	0	49458	884	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 9.

The worst 5 of 884 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)
1:O:165:GLY:H	2:P:60:THR:HG21	1.14	1.09
7:U:245:GLU:O	7:U:246:ILE:HG22	1.56	1.04
7:U:246:ILE:HG13	7:U:246:ILE:O	1.60	0.99
8:V:45:ARG:HD2	8:V:52:THR:HG23	1.48	0.94
3:Q:70:ASN:HB3	3:Q:72:LYS:H	1.40	0.87

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	239/241 (99%)	229 (96%)	9 (4%)	1 (0%)	30	49
1	O	239/241 (99%)	230 (96%)	7 (3%)	2 (1%)	16	31
2	B	247/250 (99%)	230 (93%)	17 (7%)	0	100	100
2	P	247/250 (99%)	236 (96%)	9 (4%)	2 (1%)	16	31
3	C	242/244 (99%)	232 (96%)	8 (3%)	2 (1%)	16	31
3	Q	242/244 (99%)	231 (96%)	9 (4%)	2 (1%)	16	31
4	D	239/241 (99%)	224 (94%)	13 (5%)	2 (1%)	16	31
4	R	239/241 (99%)	225 (94%)	11 (5%)	3 (1%)	9	18
5	E	240/242 (99%)	228 (95%)	10 (4%)	2 (1%)	16	31
5	S	240/242 (99%)	222 (92%)	16 (7%)	2 (1%)	16	31
6	F	230/233 (99%)	217 (94%)	13 (6%)	0	100	100
6	T	230/233 (99%)	219 (95%)	10 (4%)	1 (0%)	30	49
7	G	242/244 (99%)	234 (97%)	8 (3%)	0	100	100
7	U	242/244 (99%)	229 (95%)	11 (4%)	2 (1%)	16	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	194/196 (99%)	186 (96%)	8 (4%)	0	100	100
8	V	194/196 (99%)	185 (95%)	9 (5%)	0	100	100
9	I	220/222 (99%)	212 (96%)	8 (4%)	0	100	100
9	W	220/222 (99%)	215 (98%)	4 (2%)	1 (0%)	24	43
10	J	202/204 (99%)	193 (96%)	8 (4%)	1 (0%)	24	43
10	X	202/204 (99%)	195 (96%)	7 (4%)	0	100	100
11	K	194/198 (98%)	185 (95%)	8 (4%)	1 (0%)	24	43
11	Y	194/198 (98%)	185 (95%)	9 (5%)	0	100	100
12	L	210/212 (99%)	203 (97%)	7 (3%)	0	100	100
12	Z	210/212 (99%)	200 (95%)	10 (5%)	0	100	100
13	1	220/222 (99%)	210 (96%)	10 (4%)	0	100	100
13	M	220/222 (99%)	208 (94%)	12 (6%)	0	100	100
14	2	231/233 (99%)	218 (94%)	12 (5%)	1 (0%)	30	49
14	N	231/233 (99%)	221 (96%)	10 (4%)	0	100	100
All	All	6300/6364 (99%)	6002 (95%)	273 (4%)	25 (0%)	30	49

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	131	GLU
5	E	132	ARG
7	U	246	ILE
4	R	185	PRO
4	R	186	ALA

5.3.2 Protein sidechains [i](#)

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	205/205 (100%)	189 (92%)	16 (8%)	11	24
1	O	205/205 (100%)	183 (89%)	22 (11%)	6	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	208/209 (100%)	189 (91%)	19 (9%)	9	19
2	P	208/209 (100%)	177 (85%)	31 (15%)	3	6
3	C	203/203 (100%)	181 (89%)	22 (11%)	6	13
3	Q	203/203 (100%)	180 (89%)	23 (11%)	5	12
4	D	213/213 (100%)	197 (92%)	16 (8%)	12	26
4	R	213/213 (100%)	184 (86%)	29 (14%)	3	8
5	E	198/198 (100%)	176 (89%)	22 (11%)	6	12
5	S	198/198 (100%)	173 (87%)	25 (13%)	4	9
6	F	191/192 (100%)	167 (87%)	24 (13%)	4	9
6	T	191/192 (100%)	153 (80%)	38 (20%)	1	2
7	G	201/201 (100%)	176 (88%)	25 (12%)	4	9
7	U	201/201 (100%)	171 (85%)	30 (15%)	3	6
8	H	162/162 (100%)	151 (93%)	11 (7%)	14	31
8	V	162/162 (100%)	146 (90%)	16 (10%)	7	16
9	I	181/181 (100%)	168 (93%)	13 (7%)	13	28
9	W	181/181 (100%)	155 (86%)	26 (14%)	3	6
10	J	172/172 (100%)	151 (88%)	21 (12%)	5	10
10	X	172/172 (100%)	155 (90%)	17 (10%)	7	16
11	K	174/175 (99%)	157 (90%)	17 (10%)	7	16
11	Y	174/175 (99%)	155 (89%)	19 (11%)	6	13
12	L	169/169 (100%)	155 (92%)	14 (8%)	10	22
12	Z	169/169 (100%)	156 (92%)	13 (8%)	12	25
13	1	185/185 (100%)	174 (94%)	11 (6%)	18	37
13	M	185/185 (100%)	170 (92%)	15 (8%)	11	23
14	2	199/199 (100%)	179 (90%)	20 (10%)	7	15
14	N	199/199 (100%)	184 (92%)	15 (8%)	12	26
All	All	5322/5328 (100%)	4752 (89%)	570 (11%)	6	13

5 of 570 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	V	196	LEU
9	W	68	LEU

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Mol	Chain	Res	Type
8	V	179	THR
11	Y	141	SER
11	K	27	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
12	Z	66	HIS
13	1	46	ASN
14	2	186	ASN
11	K	117	GLN
10	J	164	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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	$\# Z > 2$
15	WPI	Z	301	-	43,43,43	2.16	12 (27%)	51,55,55	3.06	26 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	WPI	W	301	-	43,43,43	2.08	9 (20%)	51,55,55	2.61	19 (37%)
15	WPI	H	300	-	43,43,43	2.13	11 (25%)	51,55,55	3.12	25 (49%)
15	WPI	V	201	-	43,43,43	2.10	9 (20%)	51,55,55	3.04	22 (43%)
15	WPI	L	301	-	43,43,43	2.20	13 (30%)	51,55,55	2.75	23 (45%)
15	WPI	I	301	-	43,43,43	2.08	12 (27%)	51,55,55	2.96	27 (52%)

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
15	WPI	Z	301	-	-	18/28/39/39	0/3/3/3
15	WPI	W	301	-	-	20/28/39/39	0/3/3/3
15	WPI	H	300	-	-	18/28/39/39	0/3/3/3
15	WPI	V	201	-	-	12/28/39/39	0/3/3/3
15	WPI	L	301	-	-	17/28/39/39	0/3/3/3
15	WPI	I	301	-	-	18/28/39/39	0/3/3/3

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	I	301	WPI	C31-C30	7.10	1.53	1.31
15	V	201	WPI	C31-C30	7.09	1.53	1.31
15	W	301	WPI	C31-C30	7.08	1.53	1.31
15	Z	301	WPI	C13-C14	7.00	1.53	1.31
15	Z	301	WPI	C31-C30	6.98	1.53	1.31

The worst 5 of 142 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	H	300	WPI	C29-C30-C31	-7.67	108.47	125.48
15	V	201	WPI	C10-C13-C14	-7.59	108.40	126.99
15	I	301	WPI	C16-C14-C13	-7.39	109.09	125.48
15	H	300	WPI	C22-N20-C21	7.31	132.84	113.22
15	Z	301	WPI	C33-C31-C30	-7.19	109.39	126.99

There are no chirality outliers.

5 of 103 torsion outliers are listed below:

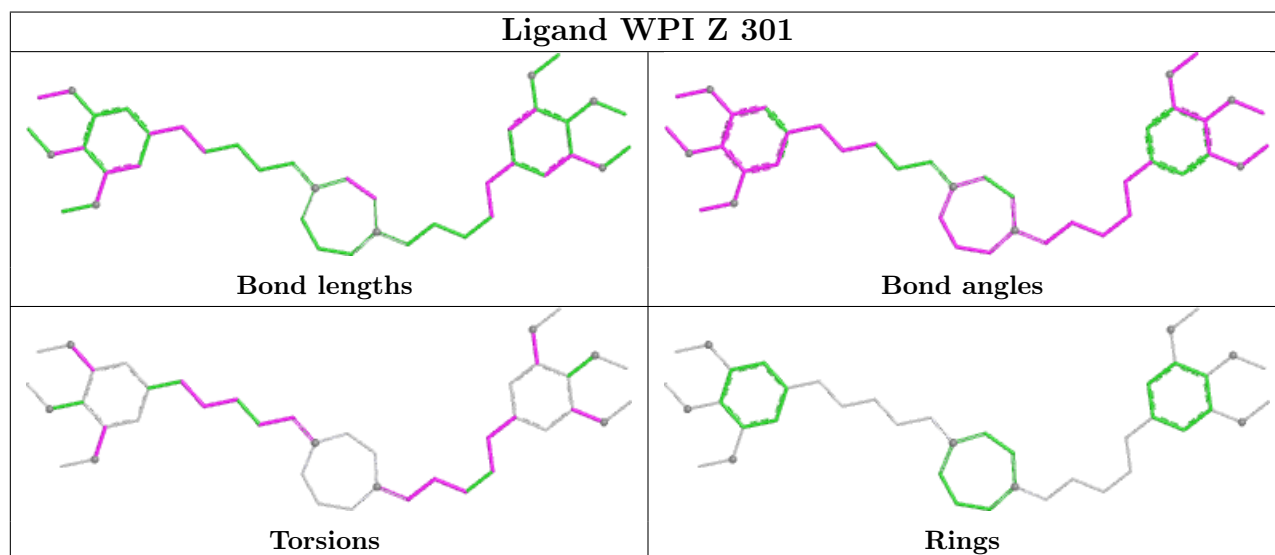
Mol	Chain	Res	Type	Atoms
15	H	300	WPI	C10-C13-C14-C16
15	H	300	WPI	C14-C16-C18-C19
15	H	300	WPI	C18-C19-N20-C22
15	H	300	WPI	C28-C27-N25-C26
15	I	301	WPI	C14-C16-C18-C19

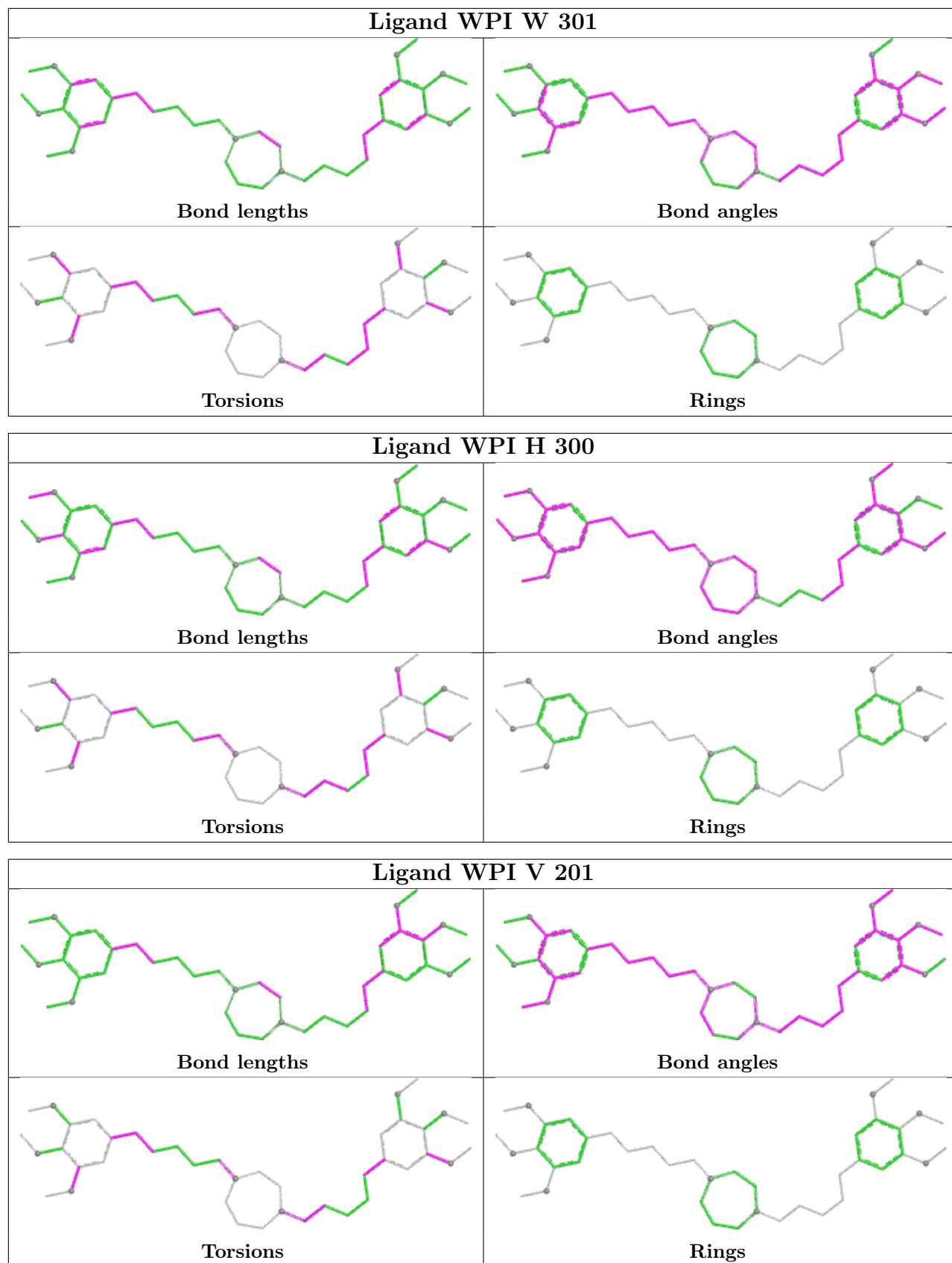
There are no ring outliers.

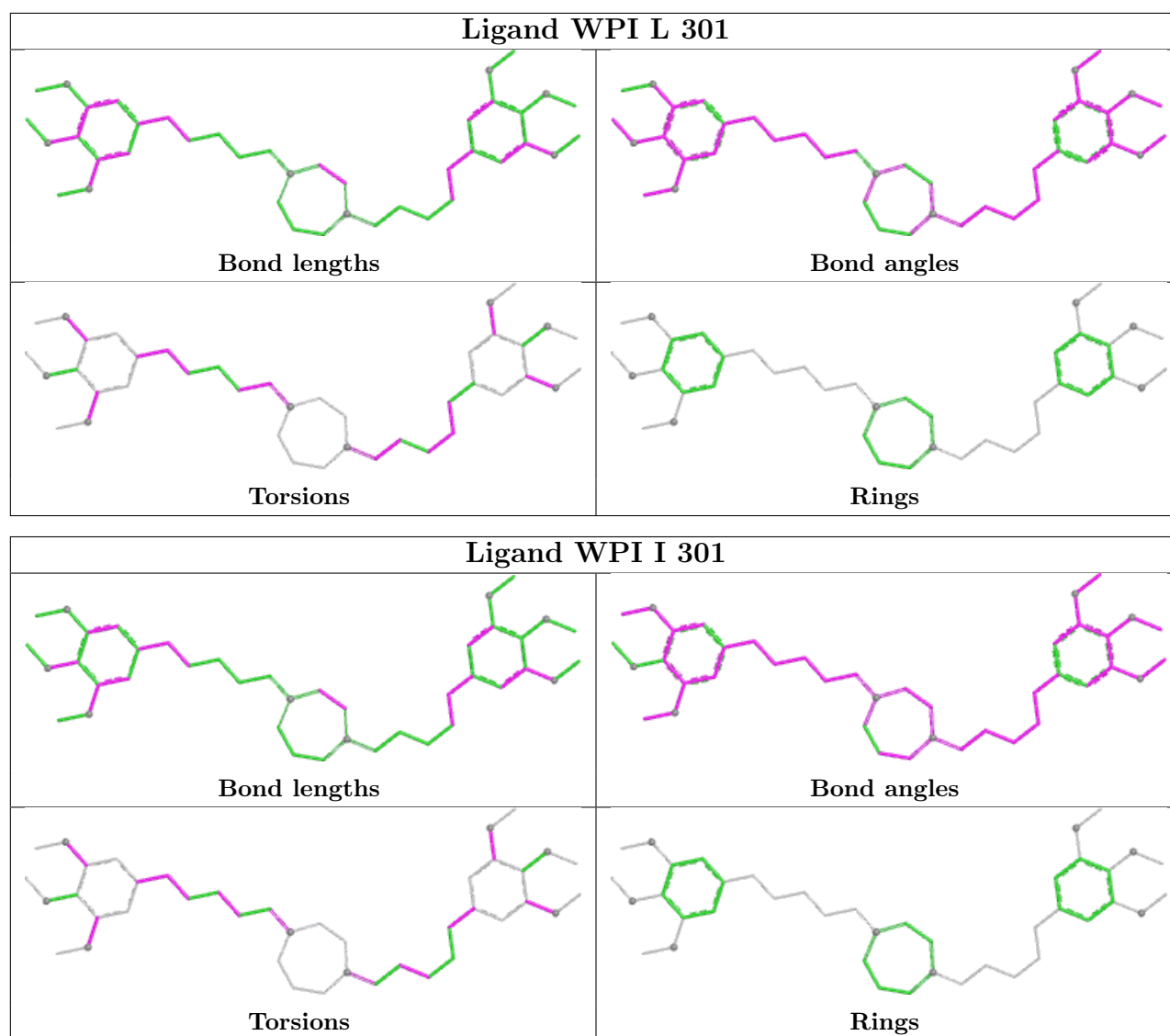
6 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	Z	301	WPI	7	0
15	W	301	WPI	3	0
15	H	300	WPI	5	0
15	V	201	WPI	11	0
15	L	301	WPI	5	0
15	I	301	WPI	7	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	241/241 (100%)	-0.23	3 (1%) 76 73	18, 32, 60, 80	0
1	O	241/241 (100%)	-0.14	3 (1%) 76 73	20, 36, 61, 88	0
2	B	249/250 (99%)	-0.22	4 (1%) 70 67	21, 34, 63, 85	0
2	P	249/250 (99%)	-0.05	6 (2%) 59 55	21, 39, 69, 84	0
3	C	244/244 (100%)	-0.05	8 (3%) 49 45	19, 37, 72, 128	0
3	Q	244/244 (100%)	-0.00	7 (2%) 53 49	18, 37, 71, 110	0
4	D	241/241 (100%)	0.04	9 (3%) 45 40	19, 39, 86, 96	0
4	R	241/241 (100%)	0.36	18 (7%) 20 18	22, 45, 93, 116	0
5	E	242/242 (100%)	0.04	8 (3%) 49 45	20, 40, 69, 122	0
5	S	242/242 (100%)	0.20	12 (4%) 34 30	24, 44, 78, 139	0
6	F	232/233 (99%)	0.14	2 (0%) 81 78	25, 45, 70, 99	0
6	T	232/233 (99%)	0.40	9 (3%) 43 38	25, 47, 75, 96	0
7	G	244/244 (100%)	-0.01	3 (1%) 76 73	22, 40, 71, 85	0
7	U	244/244 (100%)	0.11	7 (2%) 53 49	22, 40, 72, 83	0
8	H	196/196 (100%)	-0.43	0 100 100	19, 27, 46, 64	0
8	V	196/196 (100%)	-0.48	0 100 100	19, 28, 48, 63	0
9	I	222/222 (100%)	-0.31	3 (1%) 73 70	18, 31, 52, 105	0
9	W	222/222 (100%)	-0.31	2 (0%) 81 78	21, 33, 51, 100	0
10	J	204/204 (100%)	-0.43	1 (0%) 87 85	16, 31, 51, 71	0
10	X	204/204 (100%)	-0.42	3 (1%) 72 68	17, 30, 52, 73	0
11	K	196/198 (98%)	-0.45	2 (1%) 79 76	18, 31, 48, 83	0
11	Y	196/198 (98%)	-0.42	2 (1%) 79 76	17, 31, 48, 85	0
12	L	212/212 (100%)	-0.47	1 (0%) 87 85	18, 28, 44, 64	0
12	Z	212/212 (100%)	-0.40	1 (0%) 87 85	20, 31, 50, 69	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1	222/222 (100%)	-0.31	1 (0%) 87 85	18, 32, 58, 74	0
13	M	222/222 (100%)	-0.39	1 (0%) 87 85	18, 31, 52, 71	0
14	2	233/233 (100%)	-0.43	0 100 100	18, 29, 44, 59	0
14	N	233/233 (100%)	-0.44	0 100 100	17, 30, 48, 58	0
All	All	6356/6364 (99%)	-0.17	116 (1%) 67 64	16, 34, 68, 139	0

The worst 5 of 116 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	R	51	THR	7.1
4	R	52	LEU	6.2
5	E	127	ALA	6.1
5	E	133	LEU	5.0
7	U	247	ASN	4.9

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.

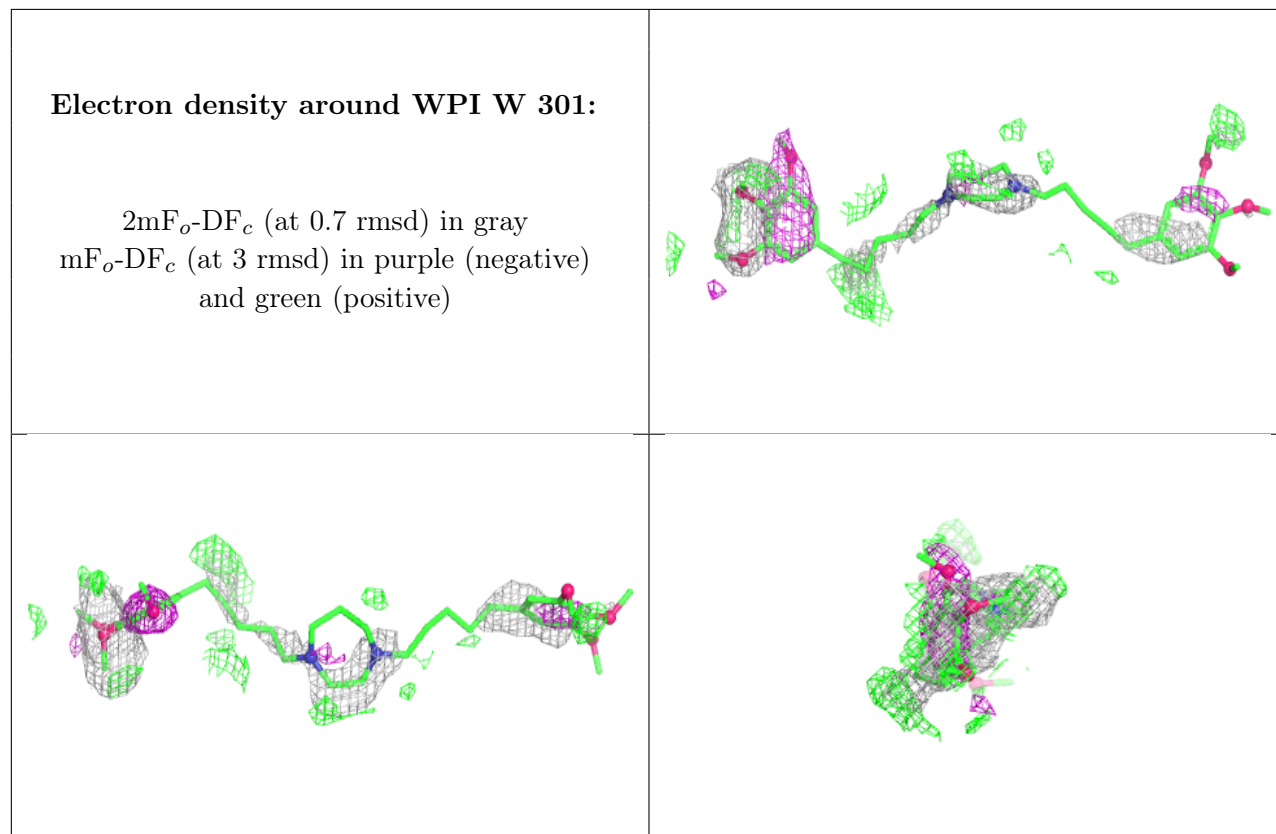
6.4 Ligands [i](#)

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	WPI	W	301	41/41	0.61	0.37	46,99,128,133	0
15	WPI	I	301	41/41	0.63	0.37	46,94,124,133	0
15	WPI	H	300	41/41	0.64	0.35	40,78,102,107	0
15	WPI	L	301	41/41	0.66	0.33	38,67,111,118	0
15	WPI	Z	301	41/41	0.67	0.31	36,76,123,131	0
15	WPI	V	201	41/41	0.69	0.27	38,67,81,90	0

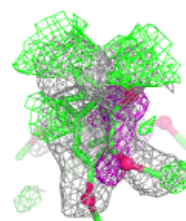
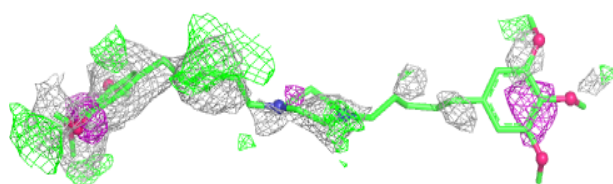
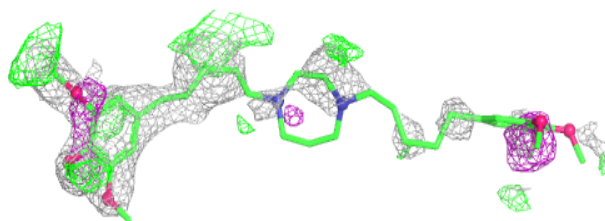
The following is a graphical depiction of the model fit to experimental electron density of all

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.

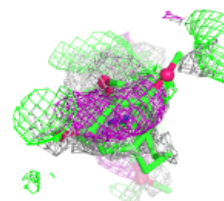
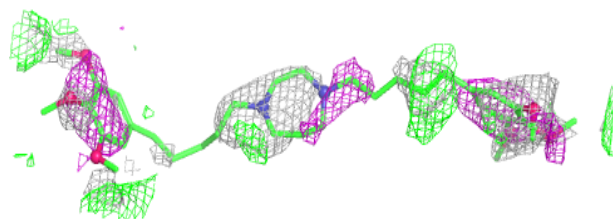
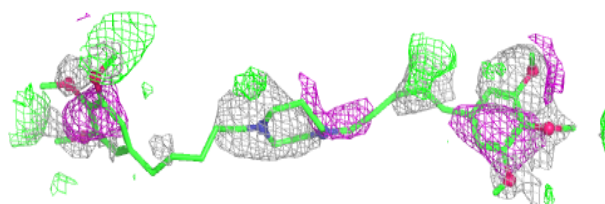


Electron density around WPI I 301:

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

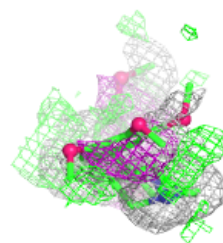
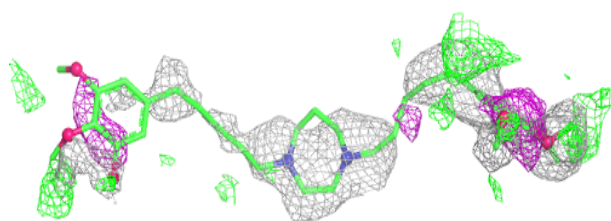
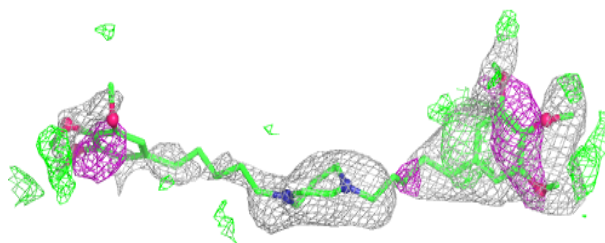
**Electron density around WPI H 300:**

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

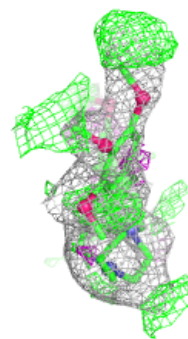
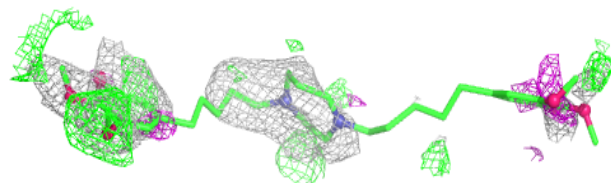
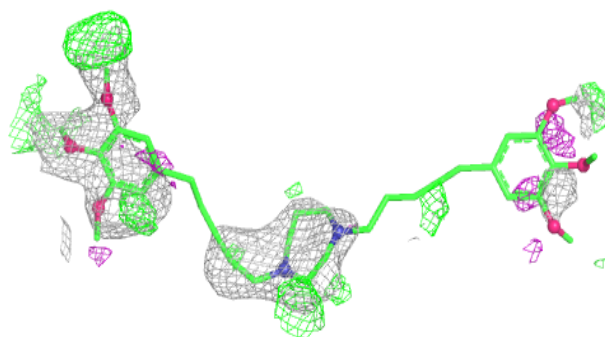


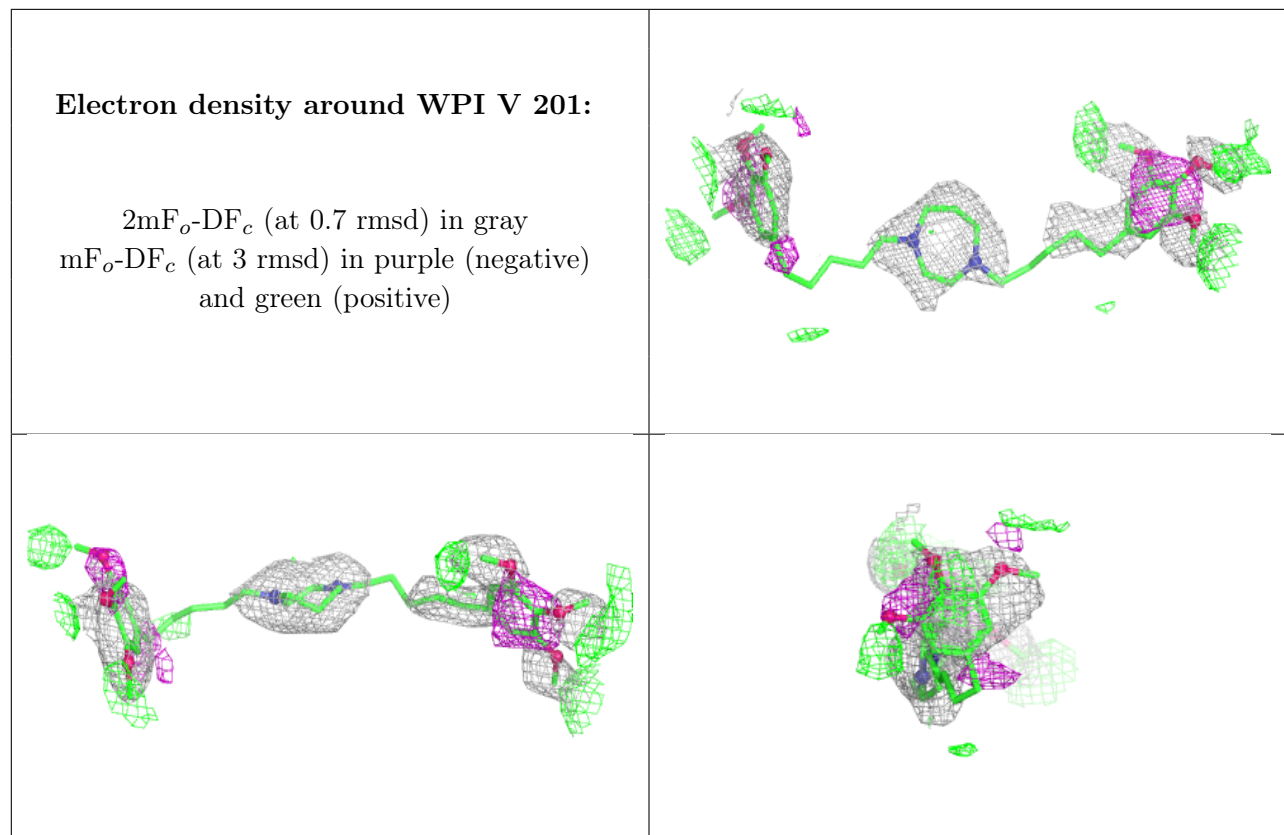
Electron density around WPI L 301:

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

**Electron density around WPI Z 301:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.