



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 2, 2024 – 12:25 pm GMT

PDB ID : 5BOU
Title : Yeast 20S proteasome in complex with a beta1 / beta2 specific non-peptidic sulfonamide Ligand
Authors : Beck, P.; Groll, M.
Deposited on : 2015-05-27
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

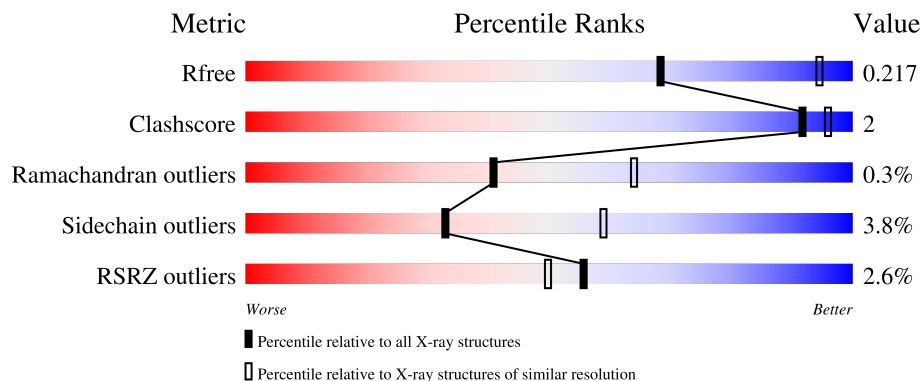
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	250	 3% 98%
1	O	250	 4% 96%
2	B	258	 3% 86% 8% • 5%
2	P	258	 5% 86% 8% • 5%
3	C	254	 8% 86% 7% • 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	7% 86% 7% • 6%
4	D	260	2% 85% • • 10%
4	R	260	2% 84% 5% • 10%
5	E	234	3% 92% 6% •
5	S	234	4% 91% 7% •
6	F	288	2% 80% 5% 16%
6	T	288	3% 80% • 16%
7	G	252	2% 90% 5% •
7	U	252	2% 90% 5% •
8	H	232	3% 89% 7% • •
8	V	232	3% 90% 6% • •
9	I	205	% 94% 5%
9	W	205	% 93% 6%
10	J	198	2% 91% 7% • •
10	X	198	2% 91% 7% • •
11	K	212	92% 6% •
11	Y	212	92% 6% •
12	L	222	95% • •
12	Z	222	% 95% •
13	M	246	% 87% 6% 7%
13	a	246	92% • 6%
14	N	196	% 92% 7% •
14	b	196	% 98% •

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 50207 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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
5	E	231	1773	1114	307	348	4	0	0	0
5	S	231	1773	1114	307	348	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	243	1892	1203	329	356	4	0	0	0
6	T	243	1892	1203	329	356	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	241	1907	1214	320	365	8	0	0	0
7	U	241	1907	1214	320	365	8	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	226	1719	1082	298	332	7	0	0	0
8	V	226	1719	1082	298	332	7	0	0	0

- Molecule 9 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	I	204	1581	1010	258	305	8	0	0	0
9	W	204	1581	1010	258	305	8	0	0	0

- Molecule 10 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	J	195	1561	992	264	299	6	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	195	Total	C	N	O	S	0	0	0
			1561	992	264	299	6			

- Molecule 11 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	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	229	Total	C	N	O	S	0	0	0
			1790	1133	306	344	7			
13	a	232	Total	C	N	O	S	0	0	0
			1815	1148	311	349	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
14	b	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	G	1	Total	Mg	0	0
			1	1		
15	I	2	Total	Mg	0	0
			2	2		

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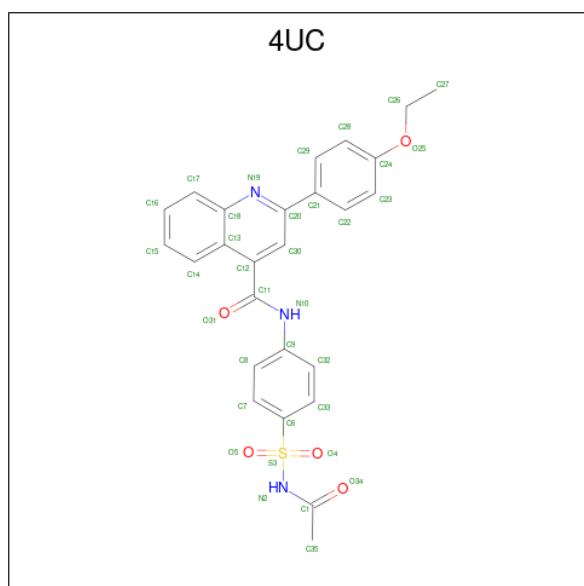
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	K	1	Total Mg 1 1	0	0
15	L	1	Total Mg 1 1	0	0
15	N	1	Total Mg 1 1	0	0
15	W	1	Total Mg 1 1	0	0
15	Z	1	Total Mg 1 1	0	0

- Molecule 16 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 17 is N-[4-(acetylsulfamoyl)phenyl]-2-(4-ethoxyphenyl)quinoline-4-carboxamide (three-letter code: 4UC) (formula: C₂₆H₂₃N₃O₅S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	H	1	Total C N O S 35 26 3 5 1	0	0
17	V	1	Total C N O S 35 26 3 5 1	0	0

- Molecule 18 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	33	Total O 33 33	0	0
18	B	32	Total O 32 32	0	0
18	C	30	Total O 30 30	0	0
18	D	16	Total O 16 16	0	0
18	E	12	Total O 12 12	0	0
18	F	26	Total O 26 26	0	0
18	G	27	Total O 27 27	0	0
18	H	36	Total O 36 36	0	0
18	I	37	Total O 37 37	0	0
18	J	31	Total O 31 31	0	0
18	K	38	Total O 38 38	0	0
18	L	34	Total O 34 34	0	0
18	M	43	Total O 43 43	0	0
18	N	29	Total O 29 29	0	0
18	O	17	Total O 17 17	0	0
18	P	19	Total O 19 19	0	0
18	Q	20	Total O 20 20	0	0
18	R	14	Total O 14 14	0	0
18	S	9	Total O 9 9	0	0
18	T	26	Total O 26 26	0	0
18	U	40	Total O 40 40	0	0

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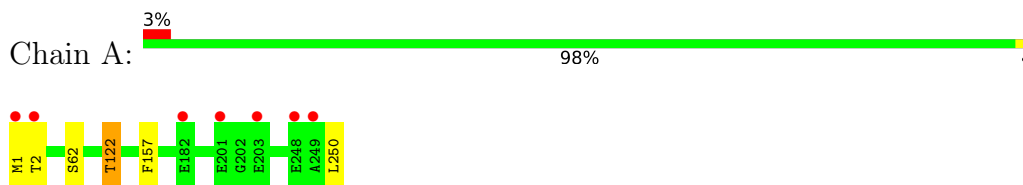
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	V	22	Total O 22 22	0	0
18	W	28	Total O 28 28	0	0
18	X	31	Total O 31 31	0	0
18	Y	36	Total O 36 36	0	0
18	Z	40	Total O 40 40	0	0
18	a	41	Total O 41 41	0	0
18	b	37	Total O 37 37	0	0

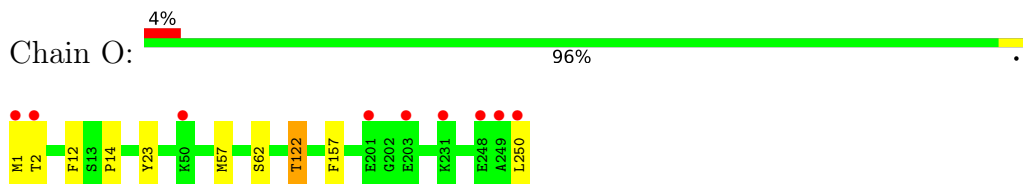
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

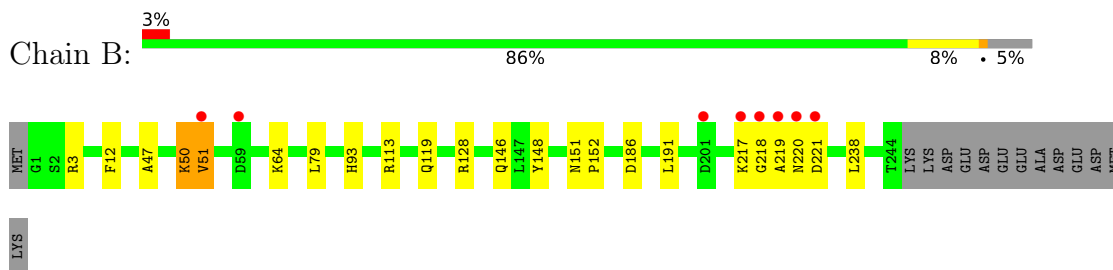
- Molecule 1: Proteasome subunit alpha type-2



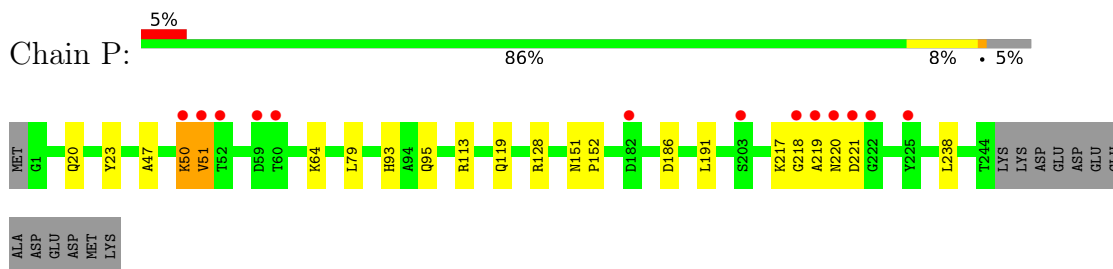
- Molecule 1: Proteasome subunit alpha type-2



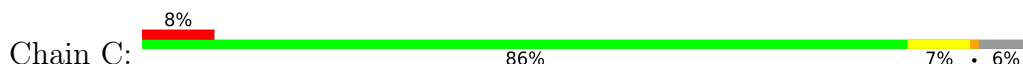
- Molecule 2: Proteasome subunit alpha type-3

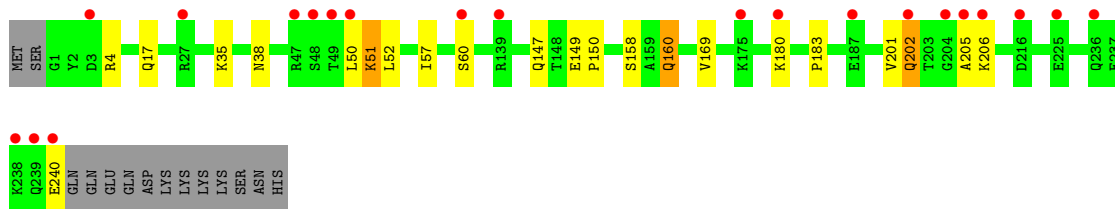


- Molecule 2: Proteasome subunit alpha type-3

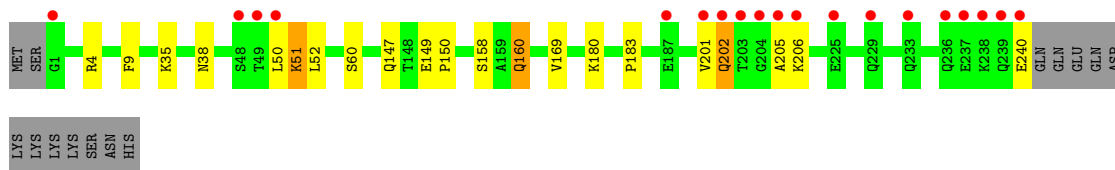
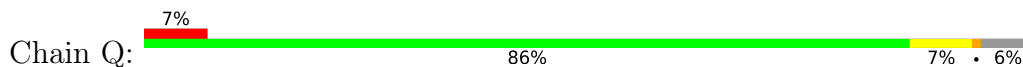


- Molecule 3: Proteasome subunit alpha type-4

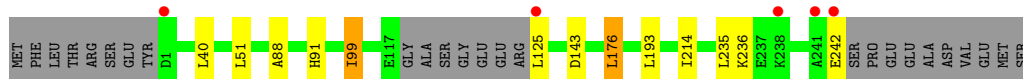
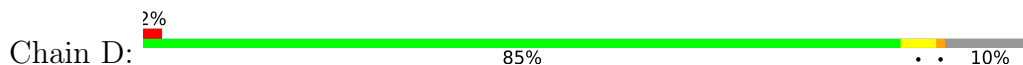




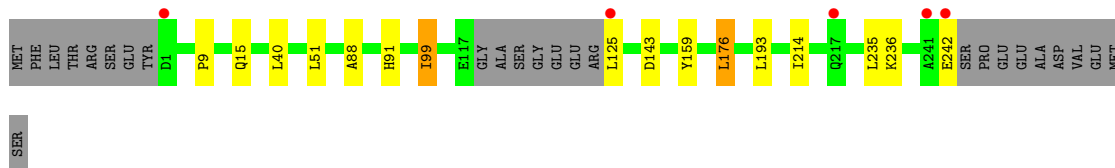
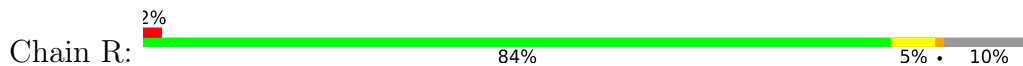
- Molecule 3: Proteasome subunit alpha type-4



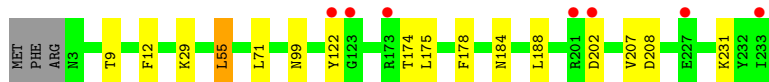
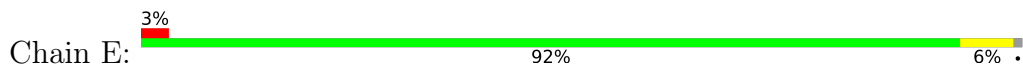
- Molecule 4: Proteasome subunit alpha type-5



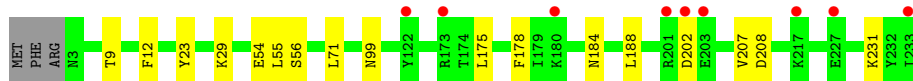
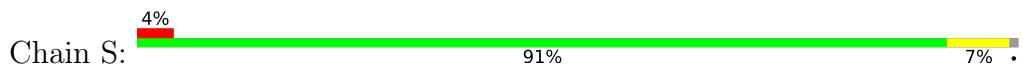
- Molecule 4: Proteasome subunit alpha type-5



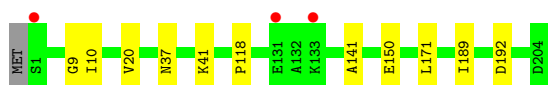
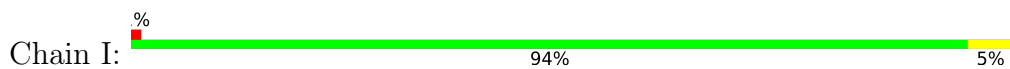
- Molecule 5: Proteasome subunit alpha type-6



- Molecule 5: Proteasome subunit alpha type-6



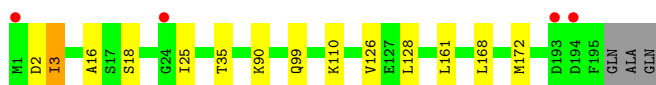
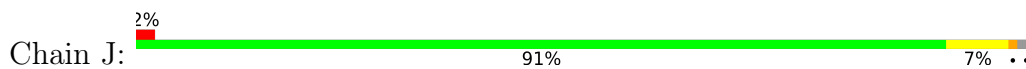
- Molecule 6: Probable proteasome subunit alpha type-7



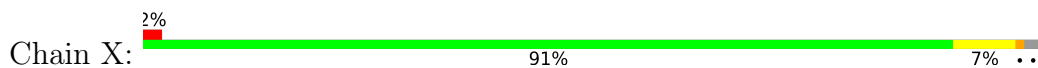
- Molecule 9: Proteasome subunit beta type-3



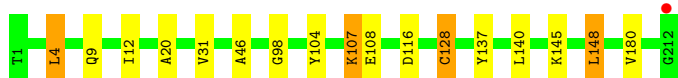
- Molecule 10: Proteasome subunit beta type-4



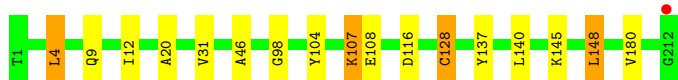
- Molecule 10: Proteasome subunit beta type-4



- Molecule 11: Proteasome subunit beta type-5



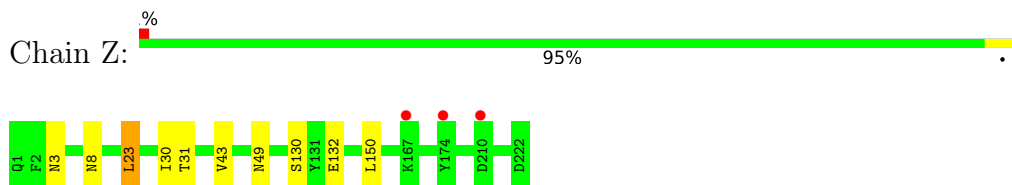
- Molecule 11: Proteasome subunit beta type-5



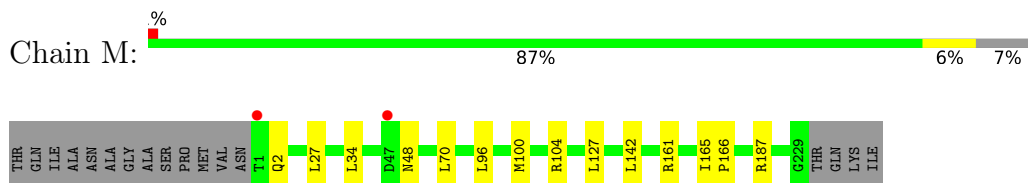
- Molecule 12: Proteasome subunit beta type-6



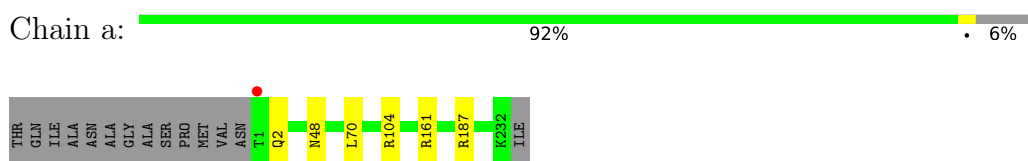
- Molecule 12: Proteasome subunit beta type-6



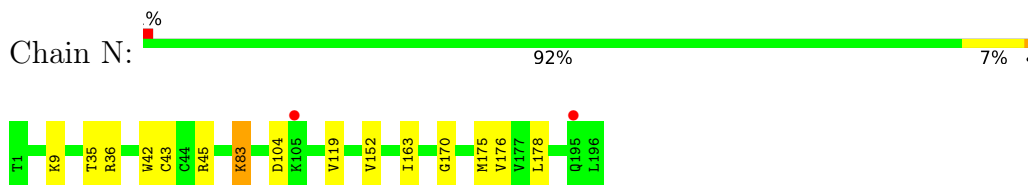
- Molecule 13: Proteasome subunit beta type-7



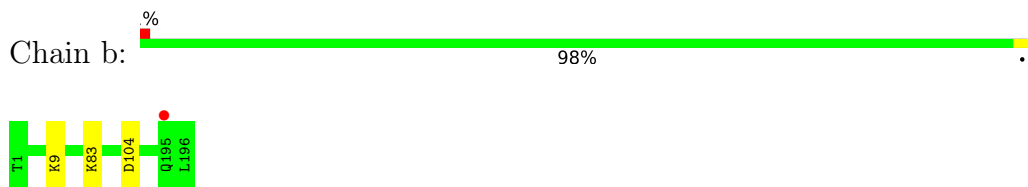
- Molecule 13: Proteasome subunit beta type-7



- Molecule 14: Proteasome subunit beta type-1



- Molecule 14: Proteasome subunit beta type-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.84Å 301.00Å 146.30Å 90.00° 113.27° 90.00°	Depositor
Resolution (Å)	15.00 – 2.60 15.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.5 (15.00-2.60) 95.6 (15.00-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.192 , 0.214 0.197 , 0.217	Depositor DCC
R_{free} test set	15663 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	52.6	Xtrriage
Anisotropy	0.069	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	50207	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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: 4UC, CL, MG

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	0.27	0/1952	0.46	0/2642
1	O	0.26	0/1952	0.46	0/2642
2	B	0.27	0/1934	0.50	0/2618
2	P	0.27	0/1934	0.50	0/2618
3	C	0.27	0/1910	0.51	0/2586
3	Q	0.27	0/1910	0.50	0/2586
4	D	0.26	0/1837	0.48	0/2475
4	R	0.26	0/1837	0.48	0/2475
5	E	0.27	0/1800	0.48	0/2433
5	S	0.26	0/1800	0.48	0/2433
6	F	0.27	0/1932	0.45	0/2609
6	T	0.27	0/1932	0.45	0/2609
7	G	0.27	0/1945	0.47	0/2634
7	U	0.27	0/1945	0.47	0/2634
8	H	0.31	0/1750	0.52	0/2373
8	V	0.29	0/1750	0.51	0/2373
9	I	0.27	0/1611	0.53	0/2174
9	W	0.27	0/1611	0.53	0/2174
10	J	0.25	0/1589	0.51	0/2142
10	X	0.25	0/1589	0.51	0/2142
11	K	0.25	0/1681	0.53	1/2274 (0.0%)
11	Y	0.25	0/1681	0.53	1/2274 (0.0%)
12	L	0.27	0/1795	0.53	0/2420
12	Z	0.27	0/1795	0.53	0/2420
13	M	0.26	0/1821	0.54	0/2470
13	a	0.26	0/1846	0.54	0/2503
14	N	0.25	0/1541	0.50	0/2087
14	b	0.25	0/1541	0.50	0/2087
All	All	0.27	0/50221	0.50	2/67907 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Y	4	LEU	CA-CB-CG	5.41	127.75	115.30
11	K	4	LEU	CA-CB-CG	5.40	127.72	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	2	0
1	O	1915	0	1929	6	0
2	B	1904	0	1904	11	0
2	P	1904	0	1904	10	0
3	C	1881	0	1895	8	0
3	Q	1881	0	1895	6	0
4	D	1813	0	1797	5	0
4	R	1813	0	1797	8	0
5	E	1773	0	1775	5	0
5	S	1773	0	1775	5	0
6	F	1892	0	1883	3	0
6	T	1892	0	1883	2	0
7	G	1907	0	1901	3	0
7	U	1907	0	1901	3	0
8	H	1719	0	1719	16	0
8	V	1719	0	1719	14	0
9	I	1581	0	1574	6	0
9	W	1581	0	1574	7	0
10	J	1561	0	1569	5	0
10	X	1561	0	1569	5	0
11	K	1644	0	1595	7	0
11	Y	1644	0	1595	7	0
12	L	1757	0	1711	4	0
12	Z	1757	0	1711	3	0
13	M	1790	0	1793	4	0
13	a	1815	0	1821	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	N	1512	0	1481	9	0
14	b	1512	0	1481	0	0
15	G	1	0	0	0	0
15	I	2	0	0	0	0
15	K	1	0	0	0	0
15	L	1	0	0	0	0
15	N	1	0	0	0	0
15	W	1	0	0	0	0
15	Z	1	0	0	0	0
16	G	1	0	0	0	0
16	U	1	0	0	0	0
17	H	35	0	23	3	0
17	V	35	0	23	4	0
18	A	33	0	0	0	0
18	B	32	0	0	1	0
18	C	30	0	0	0	0
18	D	16	0	0	0	0
18	E	12	0	0	1	0
18	F	26	0	0	0	0
18	G	27	0	0	0	0
18	H	36	0	0	0	0
18	I	37	0	0	0	0
18	J	31	0	0	0	0
18	K	38	0	0	0	0
18	L	34	0	0	0	0
18	M	43	0	0	0	0
18	N	29	0	0	0	0
18	O	17	0	0	0	0
18	P	19	0	0	1	0
18	Q	20	0	0	0	0
18	R	14	0	0	0	0
18	S	9	0	0	0	0
18	T	26	0	0	0	0
18	U	40	0	0	1	0
18	V	22	0	0	0	0
18	W	28	0	0	0	0
18	X	31	0	0	0	0
18	Y	36	0	0	0	0
18	Z	40	0	0	0	0
18	a	41	0	0	0	0
18	b	37	0	0	0	0
All	All	50207	0	49126	139	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 2.

All (139) 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)
8:H:126:SER:O	8:H:127:LEU:HD12	1.62	1.00
8:H:126:SER:O	8:H:127:LEU:CD1	2.27	0.82
8:H:80:LEU:HD12	8:H:113:ILE:CD1	2.18	0.73
8:H:80:LEU:HD12	8:H:113:ILE:HD11	1.78	0.64
8:V:1:THR:H1	17:V:301:4UC:H22	1.62	0.63
7:G:68:ARG:HH12	14:N:36:ARG:HH22	1.47	0.61
8:H:43:CYS:SG	8:H:56:THR:HG21	2.43	0.59
11:K:31:VAL:HA	12:L:132:GLU:OE1	2.03	0.58
8:V:43:CYS:SG	8:V:56:THR:HG21	2.44	0.58
11:Y:31:VAL:HA	12:Z:132:GLU:OE1	2.04	0.58
14:N:35:THR:HG21	14:N:45:ARG:HE	1.68	0.57
8:H:43:CYS:SG	8:H:56:THR:CG2	2.93	0.57
8:V:43:CYS:SG	8:V:56:THR:CG2	2.94	0.56
10:J:3:ILE:HG23	10:J:18:SER:HB3	1.88	0.56
10:X:3:ILE:HG23	10:X:18:SER:HB3	1.89	0.55
10:X:126:VAL:HG12	10:X:128:LEU:HG	1.89	0.55
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.41	0.55
11:K:145:LYS:HB2	11:K:148:LEU:HD13	1.88	0.55
17:H:301:4UC:O31	17:H:301:4UC:H16	2.07	0.55
10:J:126:VAL:HG12	10:J:128:LEU:HG	1.88	0.54
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.38	0.54
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	1.88	0.54
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.91	0.53
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.90	0.53
11:Y:107:LYS:HG3	11:Y:108:GLU:HG3	1.91	0.53
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.08	0.53
2:P:217:LYS:C	2:P:219:ALA:H	2.12	0.53
2:B:3:ARG:HB3	5:E:122:TYR:OH	2.09	0.52
3:C:51:LYS:O	3:C:52:LEU:HB2	2.08	0.52
8:H:80:LEU:HD12	8:H:113:ILE:HD13	1.91	0.52
3:C:201:VAL:O	3:C:202:GLN:CB	2.57	0.52
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.57	0.52
17:V:301:4UC:H16	17:V:301:4UC:O31	2.08	0.52
8:V:1:THR:N	17:V:301:4UC:H22	2.25	0.51
2:B:217:LYS:C	2:B:219:ALA:H	2.12	0.51
11:K:107:LYS:HG3	11:K:108:GLU:HG3	1.91	0.51
8:H:196:ARG:NH2	9:I:150:GLU:HG3	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:218:VAL:CG2	9:W:196:LYS:HB2	2.41	0.51
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.77	0.50
8:H:3:ILE:HG13	8:H:99:ILE:HD12	1.93	0.50
13:M:96:LEU:O	13:M:100:MET:HG2	2.12	0.50
2:B:12:PHE:H	3:C:17:GLN:HE22	1.58	0.50
12:L:23:LEU:HD13	12:L:43:VAL:HG13	1.93	0.50
7:G:23:PHE:O	7:G:26:THR:HB	2.12	0.50
8:V:99:ILE:HG13	8:V:127:LEU:HD22	1.93	0.50
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.94	0.50
10:X:168:LEU:O	10:X:172:MET:HB2	2.13	0.49
12:Z:23:LEU:HD13	12:Z:43:VAL:HG13	1.93	0.49
1:O:1:MET:HG3	6:T:122:TYR:CZ	2.47	0.49
8:V:126:SER:O	8:V:127:LEU:CD1	2.61	0.49
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.77	0.48
5:E:12:PHE:H	6:F:19:GLN:HE22	1.59	0.48
10:J:168:LEU:O	10:J:172:MET:HB2	2.12	0.48
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.49	0.48
7:U:23:PHE:O	7:U:26:THR:HB	2.13	0.48
8:V:126:SER:O	8:V:127:LEU:HD12	2.13	0.48
8:V:196:ARG:NH2	9:W:150:GLU:HG3	2.29	0.48
9:W:20:VAL:HG23	9:W:189:ILE:HB	1.96	0.48
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.95	0.48
8:H:113:ILE:HG23	8:H:119:THR:HG22	1.95	0.48
2:B:93:HIS:HB3	18:B:301:HOH:O	2.12	0.48
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.95	0.48
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.96	0.47
9:I:20:VAL:HG23	9:I:189:ILE:HB	1.96	0.47
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.97	0.47
14:N:35:THR:CG2	14:N:45:ARG:HE	2.28	0.47
8:H:196:ARG:NH2	9:I:150:GLU:O	2.47	0.47
11:K:46:ALA:HB3	11:K:98:GLY:O	2.15	0.47
11:Y:46:ALA:HB3	11:Y:98:GLY:O	2.14	0.47
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.78	0.47
2:P:47:ALA:HB1	2:P:64:LYS:HD2	1.97	0.47
4:R:91:HIS:HB3	4:R:99:ILE:HG22	1.97	0.47
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.96	0.47
8:V:1:THR:HB	17:V:301:4UC:O5	2.14	0.46
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.96	0.46
2:B:47:ALA:HB1	2:B:64:LYS:HD2	1.97	0.46
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.81	0.46
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:91:HIS:HB3	4:D:99:ILE:HG22	1.98	0.46
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.96	0.46
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.98	0.46
2:B:146:GLN:HG2	3:C:57:ILE:HG21	1.98	0.46
4:D:176:LEU:HD22	5:E:55:LEU:CD2	2.46	0.46
11:Y:128:CYS:HB2	11:Y:137:TYR:CZ	2.51	0.45
1:O:14:PRO:HA	2:P:23:TYR:CD1	2.51	0.45
5:S:12:PHE:H	6:T:19:GLN:HE22	1.63	0.45
8:H:104:ASP:HB2	8:H:105:PRO:CD	2.46	0.45
8:H:46:ALA:HB1	17:H:301:4UC:H19	1.98	0.45
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.99	0.45
11:K:128:CYS:HB2	11:K:137:TYR:CZ	2.52	0.45
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.47	0.45
14:N:152:VAL:HA	14:N:175:MET:HE1	1.99	0.45
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.17	0.45
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.47	0.45
3:C:35:LYS:HG2	3:C:158:SER:O	2.17	0.44
8:H:112:SER:HB3	8:H:125:LEU:HD13	1.98	0.44
2:P:93:HIS:HB3	18:P:301:HOH:O	2.17	0.44
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.47	0.44
14:N:35:THR:OG1	14:N:43:CYS:SG	2.75	0.44
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.99	0.44
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.00	0.44
5:E:174:THR:HG21	18:E:306:HOH:O	2.18	0.43
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.00	0.43
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.48	0.43
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.48	0.43
13:M:127:LEU:HG	13:M:142:LEU:HD12	2.01	0.43
7:G:78:ILE:N	7:G:79:PRO:CD	2.82	0.43
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.42
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.19	0.42
8:H:1:THR:HB	17:H:301:4UC:O5	2.20	0.42
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.54	0.42
2:P:95:GLN:HB3	9:W:68:TYR:CD2	2.55	0.42
4:D:88:ALA:HA	4:D:99:ILE:HG21	2.02	0.42
12:L:8:ASN:HA	12:L:30:ILE:O	2.20	0.42
2:B:148:TYR:OH	3:C:57:ILE:HB	2.20	0.42
4:R:91:HIS:CD2	4:R:99:ILE:HG22	2.55	0.42
13:M:27:LEU:HD21	13:M:34:LEU:HD22	2.01	0.42
10:J:25:ILE:O	10:X:139:TYR:OH	2.38	0.41
4:D:91:HIS:CD2	4:D:99:ILE:HG22	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:57:MET:HE1	18:U:406:HOH:O	2.20	0.41
4:R:9:PRO:HA	5:S:23:TYR:CD1	2.55	0.41
11:Y:12:ILE:HB	11:Y:180:VAL:HB	2.03	0.41
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.68	0.41
8:V:84:LYS:HA	8:V:113:ILE:HD11	2.03	0.41
1:O:12:PHE:H	2:P:20:GLN:HE22	1.69	0.41
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.03	0.41
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.03	0.41
2:P:50:LYS:O	2:P:51:VAL:C	2.59	0.41
2:B:50:LYS:O	2:B:51:VAL:C	2.59	0.40
14:N:163:ILE:HG23	14:N:170:GLY:HA2	2.03	0.40
11:K:12:ILE:HB	11:K:180:VAL:HB	2.03	0.40
4:R:176:LEU:HD11	5:S:54:GLU:HB2	2.02	0.40
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.57	0.40
6:F:198:LEU:HD12	6:F:243:ILE:HG22	2.03	0.40
1:A:1:MET:HG3	6:F:122:TYR:CZ	2.56	0.40
2:B:151:ASN:HB2	2:B:152:PRO:HD2	2.03	0.40
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.86	0.40
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.04	0.40
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.56	0.40

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%)	8 (3%)	1 (0%)	34 57
1	O	248/250 (99%)	238 (96%)	9 (4%)	1 (0%)	34 57
2	B	242/258 (94%)	235 (97%)	3 (1%)	4 (2%)	9 18
2	P	242/258 (94%)	236 (98%)	2 (1%)	4 (2%)	9 18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	238/254 (94%)	232 (98%)	3 (1%)	3 (1%)	12	24
3	Q	238/254 (94%)	232 (98%)	3 (1%)	3 (1%)	12	24
4	D	231/260 (89%)	229 (99%)	2 (1%)	0	100	100
4	R	231/260 (89%)	229 (99%)	2 (1%)	0	100	100
5	E	229/234 (98%)	225 (98%)	4 (2%)	0	100	100
5	S	229/234 (98%)	224 (98%)	5 (2%)	0	100	100
6	F	241/288 (84%)	238 (99%)	3 (1%)	0	100	100
6	T	241/288 (84%)	238 (99%)	3 (1%)	0	100	100
7	G	239/252 (95%)	238 (100%)	1 (0%)	0	100	100
7	U	239/252 (95%)	239 (100%)	0	0	100	100
8	H	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
8	V	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
10	J	193/198 (98%)	188 (97%)	5 (3%)	0	100	100
10	X	193/198 (98%)	188 (97%)	5 (3%)	0	100	100
11	K	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
11	Y	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
12	L	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
12	Z	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
13	M	227/246 (92%)	220 (97%)	7 (3%)	0	100	100
13	a	230/246 (94%)	222 (96%)	8 (4%)	0	100	100
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	b	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
All	All	6279/6614 (95%)	6137 (98%)	126 (2%)	16 (0%)	41	64

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
2	B	221	ASP
3	C	202	GLN
2	P	51	VAL
2	P	221	ASP

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Mol	Chain	Res	Type
3	Q	202	GLN
1	A	2	THR
2	B	218	GLY
2	B	220	ASN
1	O	2	THR
2	P	218	GLY
2	P	220	ASN
3	C	205	ALA
3	Q	205	ALA
3	C	183	PRO
3	Q	183	PRO

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	209/209 (100%)	205 (98%)	4 (2%)	57	79
1	O	209/209 (100%)	205 (98%)	4 (2%)	57	79
2	B	203/216 (94%)	196 (97%)	7 (3%)	37	63
2	P	203/216 (94%)	196 (97%)	7 (3%)	37	63
3	C	212/226 (94%)	201 (95%)	11 (5%)	23	46
3	Q	212/226 (94%)	201 (95%)	11 (5%)	23	46
4	D	194/215 (90%)	183 (94%)	11 (6%)	20	41
4	R	194/215 (90%)	183 (94%)	11 (6%)	20	41
5	E	190/193 (98%)	179 (94%)	11 (6%)	20	40
5	S	190/193 (98%)	179 (94%)	11 (6%)	20	40
6	F	201/239 (84%)	191 (95%)	10 (5%)	24	47
6	T	201/239 (84%)	191 (95%)	10 (5%)	24	47
7	G	206/210 (98%)	196 (95%)	10 (5%)	25	48
7	U	206/210 (98%)	196 (95%)	10 (5%)	25	48
8	H	185/190 (97%)	179 (97%)	6 (3%)	39	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	V	185/190 (97%)	180 (97%)	5 (3%)	44	71
9	I	172/173 (99%)	169 (98%)	3 (2%)	60	81
9	W	172/173 (99%)	169 (98%)	3 (2%)	60	81
10	J	173/175 (99%)	167 (96%)	6 (4%)	36	62
10	X	173/175 (99%)	167 (96%)	6 (4%)	36	62
11	K	169/169 (100%)	161 (95%)	8 (5%)	26	50
11	Y	169/169 (100%)	161 (95%)	8 (5%)	26	50
12	L	185/185 (100%)	179 (97%)	6 (3%)	39	65
12	Z	185/185 (100%)	179 (97%)	6 (3%)	39	65
13	M	195/208 (94%)	189 (97%)	6 (3%)	40	66
13	a	198/208 (95%)	192 (97%)	6 (3%)	41	67
14	N	162/162 (100%)	159 (98%)	3 (2%)	57	79
14	b	162/162 (100%)	159 (98%)	3 (2%)	57	79
All	All	5315/5540 (96%)	5112 (96%)	203 (4%)	33	59

All (203) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	SER
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
2	B	50	LYS
2	B	79	LEU
2	B	113	ARG
2	B	119	GLN
2	B	186	ASP
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	50	LEU
3	C	51	LYS
3	C	60	SER
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL

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Mol	Chain	Res	Type
3	C	180	LYS
3	C	206	LYS
3	C	240	GLU
4	D	40	LEU
4	D	51	LEU
4	D	99	ILE
4	D	125	LEU
4	D	143	ASP
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	29	LYS
5	E	55	LEU
5	E	71	LEU
5	E	99	ASN
5	E	184	ASN
5	E	188	LEU
5	E	202	ASP
5	E	207	VAL
5	E	208	ASP
5	E	231	LYS
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	172	LEU
6	F	181	GLU
6	F	201	GLU
6	F	202	ASP
6	F	207	ASP
6	F	214	TRP
6	F	240	GLN
7	G	26	THR
7	G	75	ASN
7	G	83	ASN
7	G	115	LEU
7	G	117	GLN
7	G	122	ARG
7	G	125	MET

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Mol	Chain	Res	Type
7	G	208	GLU
7	G	235	ARG
7	G	236	LEU
8	H	3	ILE
8	H	30	ASN
8	H	55	VAL
8	H	68	LEU
8	H	113	ILE
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
9	I	192	ASP
10	J	2	ASP
10	J	3	ILE
10	J	35	THR
10	J	90	LYS
10	J	99	GLN
10	J	110	LYS
11	K	4	LEU
11	K	9	GLN
11	K	104	TYR
11	K	107	LYS
11	K	116	ASP
11	K	128	CYS
11	K	140	LEU
11	K	148	LEU
12	L	3	ASN
12	L	23	LEU
12	L	31	THR
12	L	49	ASN
12	L	130	SER
12	L	150	LEU
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
14	N	9	LYS
14	N	83	LYS
14	N	104	ASP
1	O	62	SER

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Mol	Chain	Res	Type
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	50	LYS
2	P	79	LEU
2	P	113	ARG
2	P	119	GLN
2	P	186	ASP
2	P	191	LEU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	50	LEU
3	Q	51	LYS
3	Q	60	SER
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	206	LYS
3	Q	240	GLU
4	R	40	LEU
4	R	51	LEU
4	R	99	ILE
4	R	125	LEU
4	R	143	ASP
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	55	LEU
5	S	71	LEU
5	S	99	ASN
5	S	184	ASN
5	S	188	LEU
5	S	202	ASP
5	S	207	VAL
5	S	208	ASP

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Mol	Chain	Res	Type
5	S	231	LYS
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	172	LEU
6	T	181	GLU
6	T	201	GLU
6	T	202	ASP
6	T	207	ASP
6	T	214	TRP
6	T	240	GLN
7	U	26	THR
7	U	75	ASN
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN
7	U	122	ARG
7	U	125	MET
7	U	208	GLU
7	U	235	ARG
7	U	236	LEU
8	V	30	ASN
8	V	55	VAL
8	V	68	LEU
8	V	127	LEU
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
9	W	192	ASP
10	X	2	ASP
10	X	3	ILE
10	X	35	THR
10	X	90	LYS
10	X	99	GLN
10	X	110	LYS
11	Y	4	LEU
11	Y	9	GLN
11	Y	104	TYR
11	Y	107	LYS
11	Y	116	ASP
11	Y	128	CYS
11	Y	140	LEU

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Mol	Chain	Res	Type
11	Y	148	LEU
12	Z	3	ASN
12	Z	23	LEU
12	Z	31	THR
12	Z	49	ASN
12	Z	130	SER
12	Z	150	LEU
13	a	2	GLN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
14	b	9	LYS
14	b	83	LYS
14	b	104	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (115) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	20	GLN
2	B	58	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
3	C	17	GLN
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	100	ASN
4	D	146	GLN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN

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Mol	Chain	Res	Type
5	E	151	ASN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
6	F	240	GLN
7	G	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	167	GLN
8	H	22	GLN
8	H	30	ASN
8	H	35	HIS
8	H	66	HIS
8	H	165	ASN
8	H	172	ASN
8	H	189	ASN
9	I	37	ASN
10	J	55	GLN
11	K	85	ASN
11	K	176	ASN
11	K	208	ASN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
13	M	48	ASN
13	M	102	GLN
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
14	N	38	HIS
14	N	161	GLN
1	O	94	HIS
2	P	20	GLN
2	P	58	GLN
2	P	95	GLN
2	P	119	GLN

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Mol	Chain	Res	Type
2	P	123	GLN
2	P	176	GLN
3	Q	17	GLN
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	100	ASN
4	R	146	GLN
4	R	225	ASN
5	S	59	GLN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	151	ASN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
6	T	240	GLN
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
7	U	167	GLN
8	V	22	GLN
8	V	35	HIS
8	V	165	ASN
9	W	37	ASN
10	X	55	GLN
10	X	147	HIS
11	Y	85	ASN
11	Y	176	ASN
11	Y	208	ASN
12	Z	3	ASN

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Mol	Chain	Res	Type
12	Z	49	ASN
12	Z	70	ASN
12	Z	158	ASN
13	a	48	ASN
13	a	102	GLN
13	a	179	ASN
13	a	194	ASN
13	a	213	GLN
14	b	161	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 10 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
17	4UC	H	301	-	38,38,38	2.75	12 (31%)	53,54,54	2.26	8 (15%)
17	4UC	V	301	-	38,38,38	2.84	12 (31%)	53,54,54	2.24	9 (16%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	4UC	H	301	-	-	11/26/26/26	0/4/4/4
17	4UC	V	301	-	-	12/26/26/26	0/4/4/4

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	V	301	4UC	S3-N2	-9.81	1.43	1.64
17	H	301	4UC	S3-N2	-8.81	1.45	1.64
17	V	301	4UC	C12-C11	-6.88	1.38	1.50
17	V	301	4UC	C21-C20	-6.81	1.38	1.48
17	H	301	4UC	C6-S3	-6.34	1.66	1.76
17	H	301	4UC	C21-C20	-6.26	1.39	1.48
17	H	301	4UC	C12-C11	-5.97	1.40	1.50
17	V	301	4UC	C6-S3	-5.17	1.68	1.76
17	V	301	4UC	C9-N10	-5.01	1.31	1.41
17	H	301	4UC	C9-N10	-4.25	1.33	1.41
17	H	301	4UC	O4-S3	4.02	1.48	1.43
17	H	301	4UC	C1-N2	-3.63	1.34	1.38
17	V	301	4UC	O4-S3	3.61	1.47	1.43
17	H	301	4UC	C18-N19	-3.08	1.32	1.37
17	V	301	4UC	C18-N19	-3.08	1.32	1.37
17	H	301	4UC	C13-C18	-2.87	1.37	1.42
17	H	301	4UC	O5-S3	2.80	1.46	1.43
17	V	301	4UC	C1-N2	-2.75	1.35	1.38
17	V	301	4UC	C13-C18	-2.73	1.38	1.42
17	V	301	4UC	C12-C13	-2.33	1.38	1.43
17	H	301	4UC	C12-C13	-2.11	1.39	1.43
17	V	301	4UC	O5-S3	2.03	1.45	1.43
17	H	301	4UC	C17-C18	-2.02	1.38	1.41
17	V	301	4UC	C17-C18	-2.01	1.38	1.41

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	H	301	4UC	O5-S3-O4	-10.05	107.19	119.55
17	V	301	4UC	O5-S3-O4	-9.22	108.22	119.55
17	H	301	4UC	C35-C1-N2	7.95	121.33	114.89
17	V	301	4UC	C35-C1-N2	7.91	121.30	114.89
17	H	301	4UC	C20-N19-C18	5.33	122.03	118.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	V	301	4UC	C6-S3-N2	5.24	113.91	105.97
17	V	301	4UC	C20-N19-C18	4.55	121.45	118.06
17	H	301	4UC	O4-S3-C6	3.81	112.66	107.97
17	V	301	4UC	O4-S3-C6	3.44	112.20	107.97
17	H	301	4UC	C30-C20-N19	-3.09	119.41	122.23
17	H	301	4UC	C6-S3-N2	2.56	109.86	105.97
17	V	301	4UC	O34-C1-C35	-2.47	117.46	122.06
17	V	301	4UC	C30-C20-N19	-2.45	119.99	122.23
17	H	301	4UC	C9-N10-C11	-2.45	120.21	126.58
17	H	301	4UC	O34-C1-C35	-2.36	117.68	122.06
17	V	301	4UC	C9-N10-C11	-2.28	120.67	126.58
17	V	301	4UC	C21-C20-N19	2.27	120.24	117.09

There are no chirality outliers.

All (23) torsion outliers are listed below:

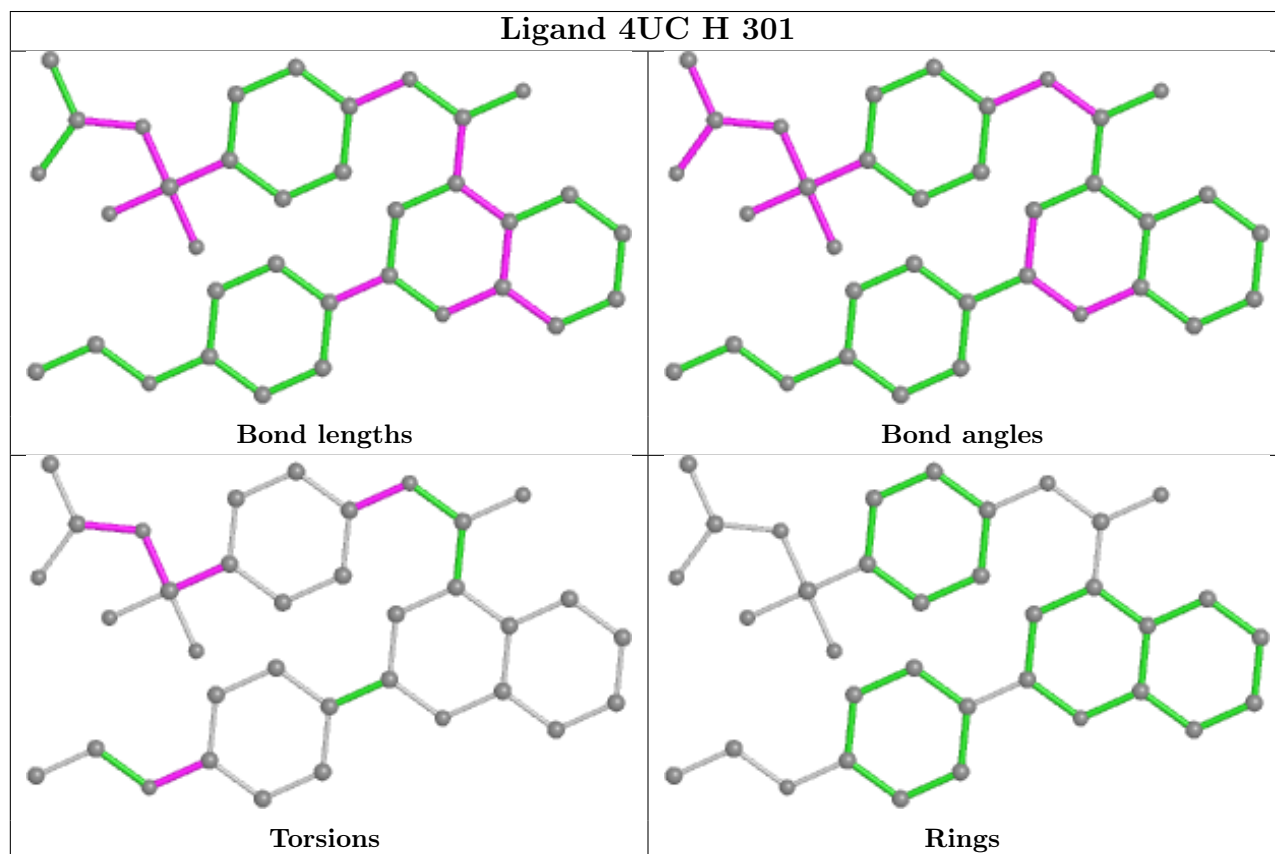
Mol	Chain	Res	Type	Atoms
17	H	301	4UC	O34-C1-N2-S3
17	H	301	4UC	C35-C1-N2-S3
17	V	301	4UC	O34-C1-N2-S3
17	V	301	4UC	C35-C1-N2-S3
17	H	301	4UC	C7-C6-S3-N2
17	H	301	4UC	C33-C6-S3-N2
17	H	301	4UC	C1-N2-S3-C6
17	V	301	4UC	C1-N2-S3-C6
17	V	301	4UC	C27-C26-O25-C24
17	V	301	4UC	C7-C6-S3-N2
17	V	301	4UC	C33-C6-S3-N2
17	V	301	4UC	C8-C9-N10-C11
17	V	301	4UC	C33-C6-S3-O5
17	V	301	4UC	C32-C9-N10-C11
17	V	301	4UC	C7-C6-S3-O5
17	H	301	4UC	C23-C24-O25-C26
17	H	301	4UC	C28-C24-O25-C26
17	H	301	4UC	C7-C6-S3-O5
17	H	301	4UC	C33-C6-S3-O5
17	H	301	4UC	C8-C9-N10-C11
17	V	301	4UC	C23-C24-O25-C26
17	V	301	4UC	C28-C24-O25-C26
17	H	301	4UC	C32-C9-N10-C11

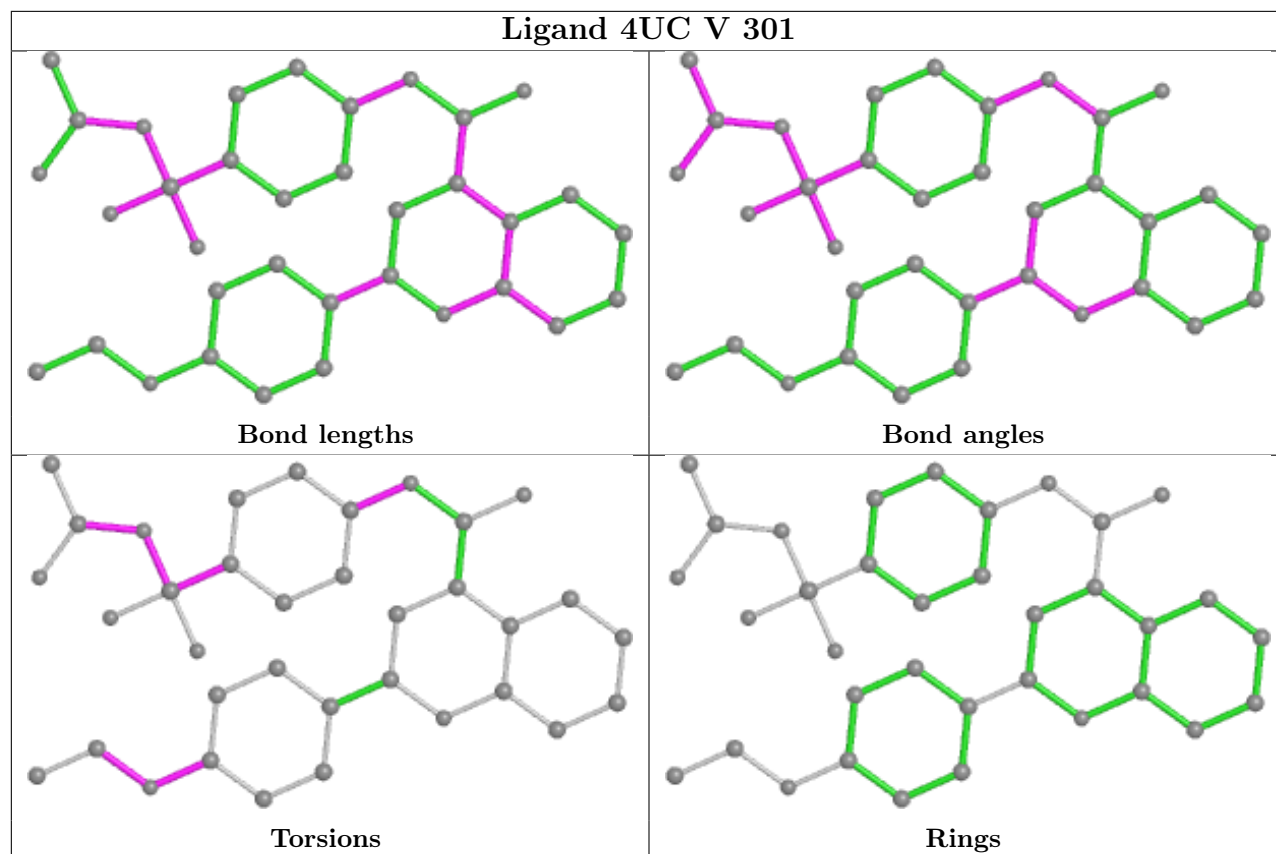
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	H	301	4UC	3	0
17	V	301	4UC	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 [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	250/250 (100%)	-0.40	7 (2%) 53 46	36, 49, 82, 120	0
1	O	250/250 (100%)	-0.27	9 (3%) 42 35	41, 57, 100, 130	0
2	B	244/258 (94%)	-0.25	8 (3%) 46 39	36, 54, 95, 142	0
2	P	244/258 (94%)	-0.17	13 (5%) 26 20	42, 58, 102, 147	0
3	C	240/254 (94%)	-0.01	21 (8%) 10 7	36, 60, 123, 153	0
3	Q	240/254 (94%)	0.17	19 (7%) 12 9	43, 70, 152, 183	0
4	D	235/260 (90%)	-0.31	5 (2%) 63 58	41, 61, 94, 137	0
4	R	235/260 (90%)	-0.23	5 (2%) 63 58	43, 64, 103, 138	0
5	E	231/234 (98%)	-0.19	7 (3%) 50 43	45, 63, 101, 145	0
5	S	231/234 (98%)	-0.04	9 (3%) 39 32	48, 72, 110, 155	0
6	F	243/288 (84%)	-0.36	5 (2%) 63 58	38, 55, 105, 137	0
6	T	243/288 (84%)	-0.15	10 (4%) 37 30	41, 66, 123, 156	0
7	G	241/252 (95%)	-0.42	5 (2%) 63 58	31, 51, 85, 135	0
7	U	241/252 (95%)	-0.34	4 (1%) 70 66	40, 55, 87, 131	0
8	H	226/232 (97%)	-0.36	6 (2%) 54 48	33, 49, 81, 143	0
8	V	226/232 (97%)	-0.29	7 (3%) 49 42	40, 52, 84, 159	0
9	I	204/205 (99%)	-0.62	3 (1%) 73 70	34, 45, 74, 95	0
9	W	204/205 (99%)	-0.57	2 (0%) 82 80	37, 48, 78, 102	0
10	J	195/198 (98%)	-0.50	4 (2%) 63 58	34, 49, 74, 127	0
10	X	195/198 (98%)	-0.48	3 (1%) 73 70	35, 50, 73, 135	0
11	K	212/212 (100%)	-0.52	1 (0%) 91 89	32, 48, 69, 89	0
11	Y	212/212 (100%)	-0.56	1 (0%) 91 89	36, 48, 71, 92	0
12	L	222/222 (100%)	-0.55	1 (0%) 91 89	36, 51, 81, 114	0
12	Z	222/222 (100%)	-0.51	3 (1%) 75 71	37, 50, 82, 117	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	229/246 (93%)	-0.56	2 (0%) 84 82	34, 51, 74, 90	0
13	a	232/246 (94%)	-0.58	1 (0%) 92 91	33, 49, 70, 89	0
14	N	196/196 (100%)	-0.59	2 (1%) 82 80	34, 45, 72, 100	0
14	b	196/196 (100%)	-0.56	1 (0%) 91 89	35, 47, 74, 105	0
All	All	6339/6614 (95%)	-0.36	164 (2%) 56 50	31, 54, 98, 183	0

All (164) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	50	LEU	7.5
2	B	219	ALA	7.0
3	Q	49	THR	6.9
10	X	1	MET	6.6
3	C	205	ALA	6.6
2	B	218	GLY	6.4
3	Q	206	LYS	6.3
2	P	51	VAL	6.2
2	B	221	ASP	6.2
8	V	224	GLN	5.8
3	C	236	GLN	5.7
10	J	1	MET	5.5
8	H	226	GLU	5.5
2	B	51	VAL	5.5
8	V	226	GLU	5.2
2	P	221	ASP	5.2
1	A	1	MET	5.1
8	H	221	CYS	5.1
3	Q	236	GLN	5.1
9	W	1	SER	4.8
8	V	221	CYS	4.7
3	Q	202	GLN	4.7
3	C	50	LEU	4.7
2	P	59	ASP	4.7
3	Q	239	GLN	4.7
2	P	220	ASN	4.7
10	X	194	ASP	4.7
3	C	49	THR	4.6
1	O	1	MET	4.6
8	V	222	ASP	4.5
2	P	218	GLY	4.4
7	U	242	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	249	ALA	4.1
1	O	249	ALA	4.1
12	L	174	TYR	3.9
3	Q	240	GLU	3.9
4	D	242	GLU	3.9
5	S	202	ASP	3.7
6	F	244	ASN	3.7
7	G	3	TYR	3.7
2	B	217	LYS	3.7
3	C	238	LYS	3.6
5	E	202	ASP	3.6
6	T	178	HIS	3.5
8	V	223	ILE	3.5
13	a	1	THR	3.5
3	C	239	GLN	3.5
10	J	194	ASP	3.4
3	C	240	GLU	3.4
9	I	1	SER	3.4
3	Q	204	GLY	3.4
2	P	219	ALA	3.3
3	Q	238	LYS	3.3
6	T	244	ASN	3.3
6	T	243	ILE	3.3
2	B	59	ASP	3.2
8	H	222	ASP	3.1
4	R	1	ASP	3.1
12	Z	174	TYR	3.1
3	Q	205	ALA	3.1
14	b	195	GLN	3.1
7	U	2	GLY	3.0
2	P	52	THR	3.0
3	C	206	LYS	3.0
5	S	233	ILE	3.0
8	H	223	ILE	3.0
5	E	122	TYR	3.0
4	R	217	GLN	2.9
1	O	201	GLU	2.9
3	Q	225	GLU	2.9
5	S	122	TYR	2.9
6	F	178	HIS	2.9
4	R	125	LEU	2.9
3	Q	48	SER	2.9

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Mol	Chain	Res	Type	RSRZ
3	Q	203	THR	2.9
9	I	133	LYS	2.9
5	E	233	ILE	2.8
1	O	250	LEU	2.8
7	U	206	GLY	2.8
5	S	173	ARG	2.8
4	D	241	ALA	2.8
6	T	241	LYS	2.8
10	X	193	ASP	2.7
2	B	220	ASN	2.7
14	N	195	GLN	2.7
3	Q	233	GLN	2.7
8	H	224	GLN	2.7
1	A	2	THR	2.7
3	Q	187	GLU	2.7
6	T	230	ASP	2.7
3	C	216	ASP	2.6
10	J	24	GLY	2.6
4	R	242	GLU	2.6
1	O	2	THR	2.6
6	F	181	GLU	2.6
3	Q	229	GLN	2.5
3	C	225	GLU	2.5
7	G	241	GLU	2.5
3	Q	201	VAL	2.5
3	Q	237	GLU	2.5
4	R	241	ALA	2.5
10	J	193	ASP	2.5
6	T	215	CYS	2.5
9	W	192	ASP	2.5
2	P	222	GLY	2.5
3	C	27	ARG	2.4
5	E	123	GLY	2.4
11	Y	212	GLY	2.4
1	A	182	GLU	2.4
2	P	182	ASP	2.4
6	T	182	GLY	2.4
3	C	47	ARG	2.4
8	V	215	GLU	2.4
3	C	3	ASP	2.4
3	C	202	GLN	2.4
3	C	187	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
5	E	173	ARG	2.4
2	B	201	ASP	2.4
5	S	203	GLU	2.4
6	T	180	PRO	2.3
2	P	50	LYS	2.3
5	E	227	GLU	2.3
13	M	1	THR	2.3
5	S	180	LYS	2.3
7	G	240	ALA	2.3
13	M	47	ASP	2.3
7	U	51	PRO	2.3
8	H	198	GLU	2.3
3	C	180	LYS	2.3
1	A	203	GLU	2.3
3	C	204	GLY	2.2
8	V	145	ASP	2.2
6	F	205	GLU	2.2
5	S	201	ARG	2.2
4	D	1	ASP	2.2
4	D	125	LEU	2.2
3	C	60	SER	2.2
4	D	238	LYS	2.2
14	N	105	LYS	2.2
7	G	51	PRO	2.1
6	T	205	GLU	2.1
5	E	201	ARG	2.1
6	F	241	LYS	2.1
2	P	225	TYR	2.1
7	G	2	GLY	2.1
1	O	231	LYS	2.1
11	K	212	GLY	2.1
2	P	60	THR	2.1
3	C	175	LYS	2.1
5	S	227	GLU	2.1
6	T	201	GLU	2.1
12	Z	167	LYS	2.1
2	P	203	SER	2.1
3	C	48	SER	2.1
1	A	201	GLU	2.1
1	O	203	GLU	2.1
1	A	248	GLU	2.1
9	I	131	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
5	S	217	LYS	2.0
3	C	139	ARG	2.0
1	O	248	GLU	2.0
3	Q	1	GLY	2.0
12	Z	210	ASP	2.0
1	O	50	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

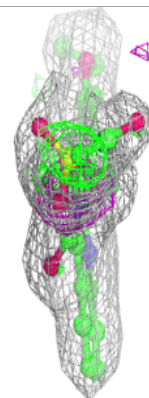
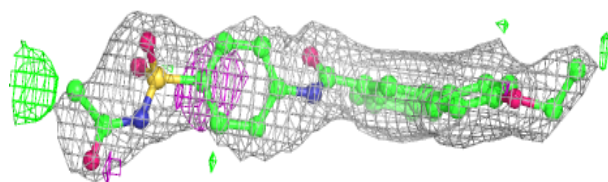
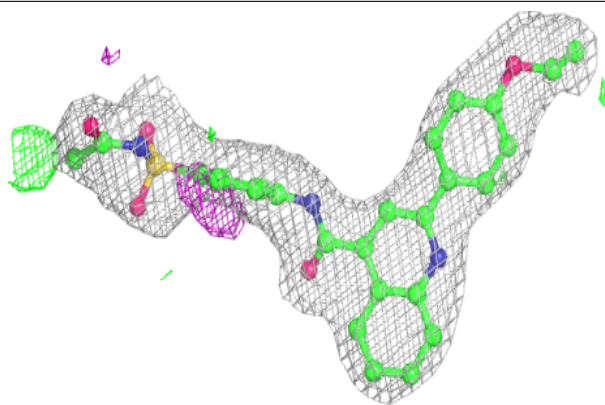
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	MG	G	301	1/1	0.92	0.06	47,47,47,47	0
15	MG	I	301	1/1	0.92	0.15	54,54,54,54	0
15	MG	Z	301	1/1	0.92	0.18	55,55,55,55	0
17	4UC	V	301	35/35	0.93	0.25	61,69,73,76	0
17	4UC	H	301	35/35	0.94	0.25	60,68,74,74	0
15	MG	W	301	1/1	0.95	0.17	56,56,56,56	0
15	MG	I	302	1/1	0.96	0.12	44,44,44,44	0
15	MG	L	301	1/1	0.97	0.06	59,59,59,59	0
15	MG	N	201	1/1	0.97	0.11	50,50,50,50	0
15	MG	K	301	1/1	0.98	0.08	44,44,44,44	0
16	CL	G	302	1/1	0.99	0.09	43,43,43,43	0
16	CL	U	301	1/1	0.99	0.17	44,44,44,44	0

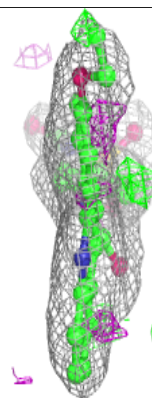
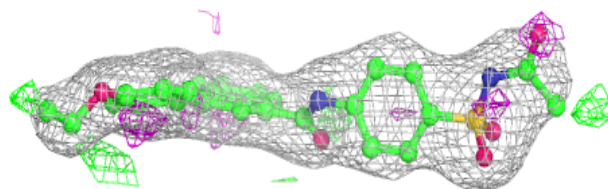
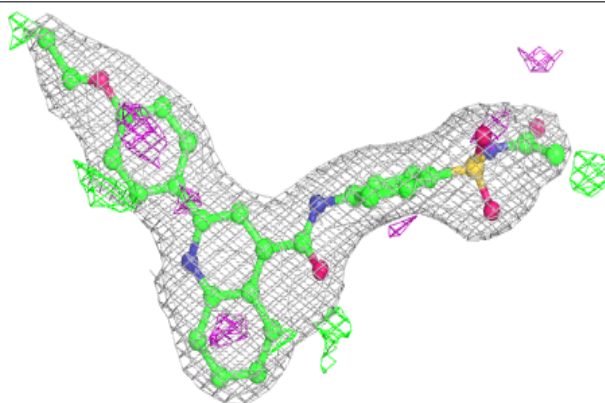
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 4UC V 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 4UC H 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.