



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 03:00 am BST

PDB ID : 6HW7
Title : Yeast 20S proteasome in complex with 29
Authors : Huber, E.M.; Groll, M.
Deposited on : 2018-10-11
Resolution : 2.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

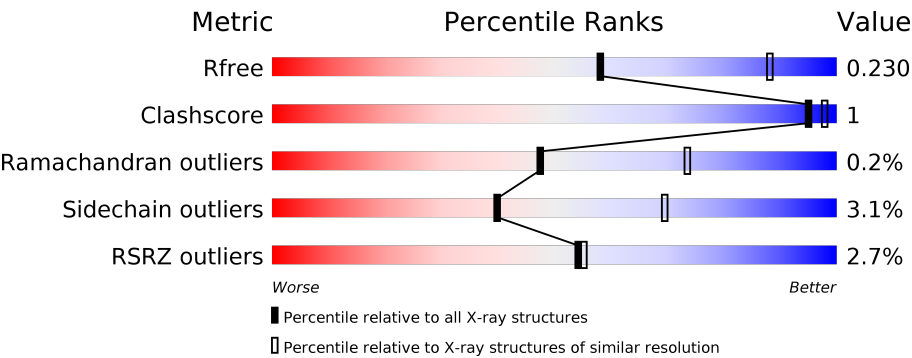
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 on 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	<div><div>6%</div><div>98%</div><div>•</div></div>
1	O	250	<div><div>4%</div><div>97%</div><div>•</div></div>
2	B	258	<div><div>5%</div><div>90%</div><div>• • 5%</div></div>
2	P	258	<div><div>5%</div><div>89%</div><div>5% • 5%</div></div>
3	C	254	<div><div>6%</div><div>90%</div><div>• • 6%</div></div>
3	Q	254	<div><div>8%</div><div>89%</div><div>• • 6%</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	196	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 49775 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
1	O	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

- Molecule 2 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			
2	P	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	240	Total	C	N	O	S	0	0	0
			1881	1176	329	372	4			
3	Q	240	Total	C	N	O	S	0	0	0
			1881	1176	329	372	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	235	Total	C	N	O	S	0	0	0
			1813	1136	304	366	7			
4	R	235	Total	C	N	O	S	0	0	0
			1813	1136	304	366	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	231	Total	C	N	O	S	0	0	0
			1773	1114	307	348	4			
5	S	231	Total	C	N	O	S	0	0	0
			1773	1114	307	348	4			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			
8	V	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			

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

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

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

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

Continued on next page...

Continued from previous page...

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	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	a	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	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	K	2	Total	Mg	0	0
			2	2		

Continued on next page...

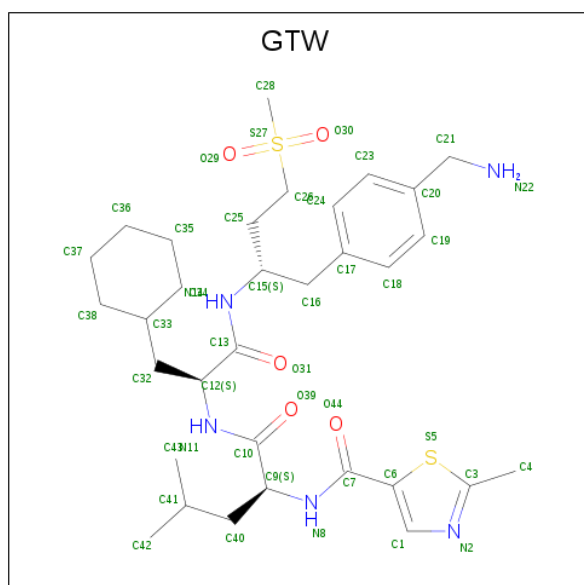
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	I	1	Total Mg 1 1	0	0
15	V	1	Total Mg 1 1	0	0
15	Z	1	Total Mg 1 1	0	0
15	N	1	Total Mg 1 1	0	0
15	X	1	Total Mg 1 1	0	0
15	Y	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}-[(2 {S})-1-[(2 {S})-1-[(2 {S})-1-[4-(aminomethyl)phenyl]-4-methylsulfonyl-butan-2-yl]amino]-3-cyclohexyl-1-oxidanylidene-propan-2-yl]amino]-4-methyl-1-oxidanylidene-pentan-2-yl]-2-methyl-1,3-thiazole-5-carboxamide (three-letter code: GTW) (formula: C₃₂H₄₉N₅O₅S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	H	1	Total	C	N	O	S	0	0
			44	32	5	5	2		
17	K	1	Total	C	N	O	S	0	0
			44	32	5	5	2		
17	V	1	Total	C	N	O	S	0	0
			44	32	5	5	2		
17	Y	1	Total	C	N	O	S	0	0
			44	32	5	5	2		

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	9	Total	O	0	0
			9	9		
18	B	10	Total	O	0	0
			10	10		
18	C	14	Total	O	0	0
			14	14		
18	D	10	Total	O	0	0
			10	10		
18	F	7	Total	O	0	0
			7	7		
18	G	15	Total	O	0	0
			15	15		
18	H	7	Total	O	0	0
			7	7		
18	I	14	Total	O	0	0
			14	14		
18	J	25	Total	O	0	0
			25	25		
18	K	15	Total	O	0	0
			15	15		
18	L	11	Total	O	0	0
			11	11		
18	M	12	Total	O	0	0
			12	12		
18	N	11	Total	O	0	0
			11	11		
18	O	5	Total	O	0	0
			5	5		
18	P	9	Total	O	0	0
			9	9		
18	Q	10	Total	O	0	0
			10	10		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	R	2	Total 2	O 2	0	0
18	S	7	Total 7	O 7	0	0
18	T	9	Total 9	O 9	0	0
18	U	15	Total 15	O 15	0	0
18	V	6	Total 6	O 6	0	0
18	W	12	Total 12	O 12	0	0
18	X	16	Total 16	O 16	0	0
18	Y	9	Total 9	O 9	0	0
18	Z	13	Total 13	O 13	0	0
18	a	12	Total 12	O 12	0	0
18	b	7	Total 7	O 7	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

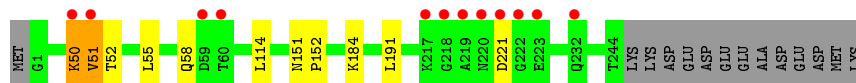
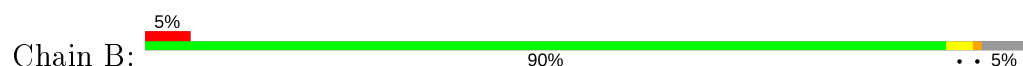
- Molecule 1: Proteasome subunit alpha type-2



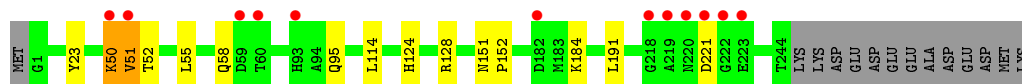
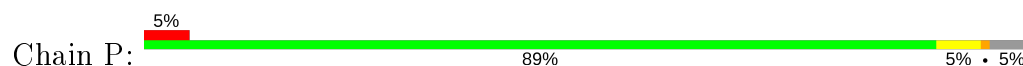
- Molecule 1: Proteasome subunit alpha type-2



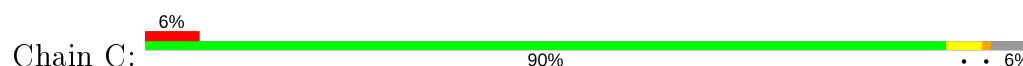
- Molecule 2: Proteasome subunit alpha type-3



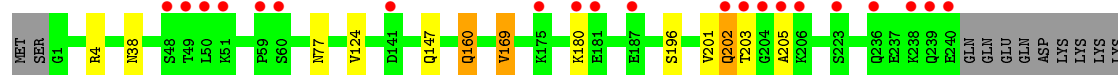
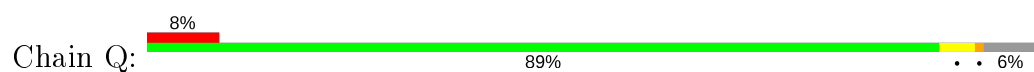
- Molecule 2: Proteasome subunit alpha type-3



- Molecule 3: Proteasome subunit alpha type-4

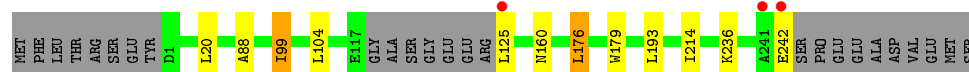
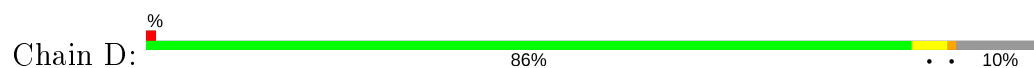


- Molecule 3: Proteasome subunit alpha type-4

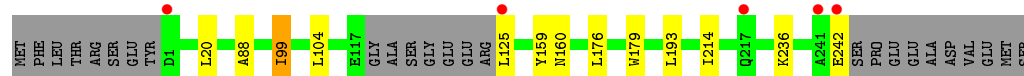
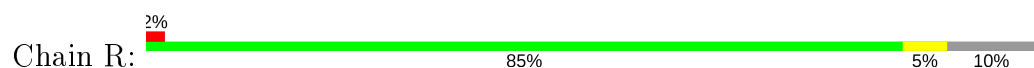


SER
ASN
HIS

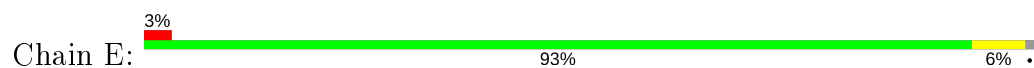
- Molecule 4: Proteasome subunit alpha type-5



- Molecule 4: Proteasome subunit alpha type-5



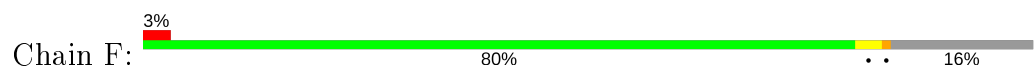
- Molecule 5: Proteasome subunit alpha type-6



- Molecule 5: Proteasome subunit alpha type-6

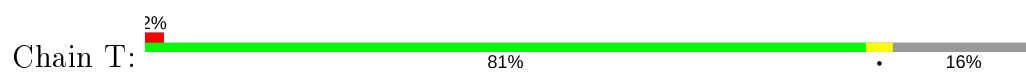


- Molecule 6: Probable proteasome subunit alpha type-7

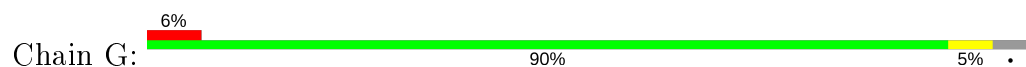


ASN
ALA
PRO
VAL
ALA
THR
ASN
ALA
ASN
THR
THR
ASP
GLN
GLY
ASP
ILE
HIS
LEU
GLU

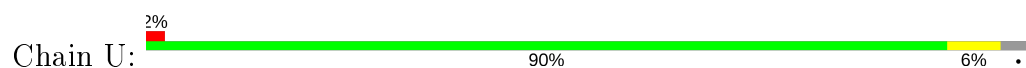
- Molecule 6: Probable proteasome subunit alpha type-7



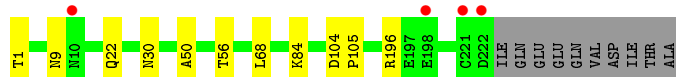
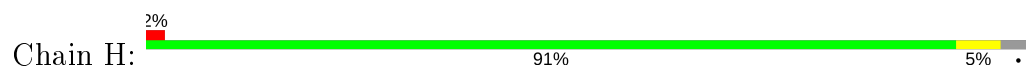
- Molecule 7: Proteasome subunit alpha type-1



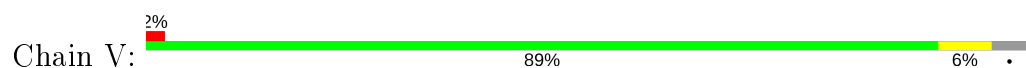
- Molecule 7: Proteasome subunit alpha type-1



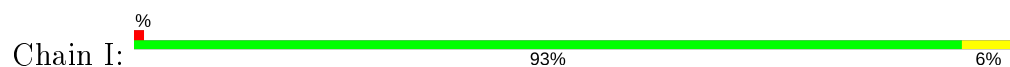
- Molecule 8: Proteasome subunit beta type-2



- Molecule 8: Proteasome subunit beta type-2



- Molecule 9: Proteasome subunit beta type-3

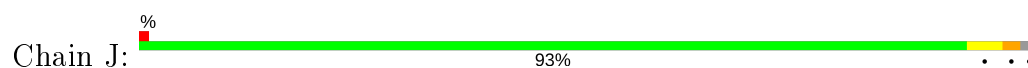


- Molecule 9: Proteasome subunit beta type-3

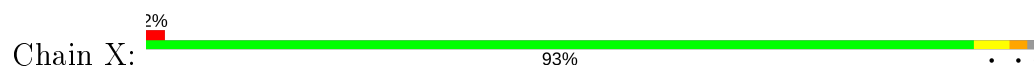




- Molecule 10: Proteasome subunit beta type-4



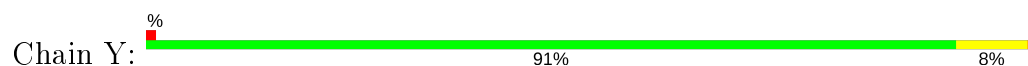
- Molecule 10: Proteasome subunit beta type-4



- Molecule 11: Proteasome subunit beta type-5



- Molecule 11: Proteasome subunit beta type-5



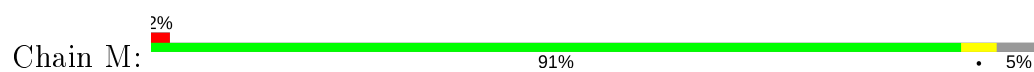
- Molecule 12: Proteasome subunit beta type-6



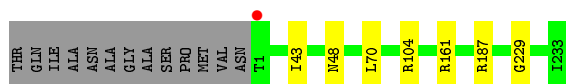
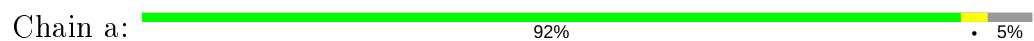
- Molecule 12: Proteasome subunit beta type-6



- Molecule 13: Proteasome subunit beta type-7



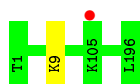
- Molecule 13: Proteasome subunit beta type-7



- Molecule 14: Proteasome subunit beta type-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	136.35Å 299.45Å 144.96Å 90.00° 112.68° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.1 (15.00-2.70) 99.1 (15.00-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.202 , 0.225 0.207 , 0.230	Depositor DCC
R_{free} test set	14416 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	62.9	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 39.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	49775	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.47	0/2642
1	O	0.27	0/1952	0.47	0/2642
2	B	0.27	0/1934	0.49	0/2618
2	P	0.27	0/1934	0.48	0/2618
3	C	0.28	0/1910	0.51	0/2586
3	Q	0.27	0/1910	0.51	0/2586
4	D	0.26	0/1837	0.47	0/2475
4	R	0.27	0/1837	0.47	0/2475
5	E	0.27	0/1800	0.46	0/2433
5	S	0.27	0/1800	0.46	0/2433
6	F	0.27	0/1932	0.45	0/2609
6	T	0.27	0/1932	0.44	0/2609
7	G	0.27	0/1945	0.46	0/2634
7	U	0.27	0/1945	0.47	0/2634
8	H	0.25	0/1715	0.51	1/2326 (0.0%)
8	V	0.26	0/1715	0.51	1/2326 (0.0%)
9	I	0.27	0/1611	0.52	0/2174
9	W	0.28	0/1611	0.53	0/2174
10	J	0.27	0/1589	0.49	0/2142
10	X	0.27	0/1589	0.49	0/2142
11	K	0.26	0/1681	0.51	0/2274
11	Y	0.27	0/1681	0.51	0/2274
12	L	0.28	0/1795	0.51	0/2420
12	Z	0.33	0/1795	0.52	0/2420
13	M	0.27	0/1855	0.51	0/2514
13	a	0.26	0/1855	0.51	0/2514
14	N	0.25	0/1541	0.47	0/2087
14	b	0.25	0/1541	0.47	0/2087
All	All	0.27	0/50194	0.49	2/67868 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	V	1	THR	CA-CB-OG1	6.24	122.11	109.00
8	H	1	THR	CA-CB-OG1	5.83	121.24	109.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	2	0
1	O	1915	0	1929	4	0
2	B	1904	0	1904	2	0
2	P	1904	0	1904	6	0
3	C	1881	0	1895	4	0
3	Q	1881	0	1895	5	0
4	D	1813	0	1797	4	0
4	R	1813	0	1797	4	0
5	E	1773	0	1775	4	0
5	S	1773	0	1775	3	0
6	F	1892	0	1883	4	0
6	T	1892	0	1883	1	0
7	G	1907	0	1901	3	0
7	U	1907	0	1901	3	0
8	H	1684	0	1687	3	0
8	V	1684	0	1687	6	0
9	I	1581	0	1574	8	0
9	W	1581	0	1574	8	0
10	J	1561	0	1569	7	0
10	X	1561	0	1569	5	0
11	K	1644	0	1594	9	0
11	Y	1644	0	1594	10	0
12	L	1757	0	1711	7	0
12	Z	1757	0	1711	6	0
13	M	1824	0	1832	1	0
13	a	1824	0	1832	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	N	1512	0	1481	2	0
14	b	1512	0	1481	0	0
15	G	1	0	0	0	0
15	I	1	0	0	0	0
15	K	2	0	0	0	0
15	N	1	0	0	0	0
15	V	1	0	0	0	0
15	X	1	0	0	0	0
15	Y	1	0	0	0	0
15	Z	1	0	0	0	0
16	G	1	0	0	0	0
16	U	1	0	0	0	0
17	H	44	0	0	1	0
17	K	44	0	0	0	0
17	V	44	0	0	0	0
17	Y	44	0	0	0	0
18	A	9	0	0	0	0
18	B	10	0	0	0	0
18	C	14	0	0	0	0
18	D	10	0	0	0	0
18	F	7	0	0	0	0
18	G	15	0	0	1	0
18	H	7	0	0	0	0
18	I	14	0	0	0	0
18	J	25	0	0	1	0
18	K	15	0	0	0	0
18	L	11	0	0	0	0
18	M	12	0	0	0	0
18	N	11	0	0	0	0
18	O	5	0	0	0	0
18	P	9	0	0	0	0
18	Q	10	0	0	0	0
18	R	2	0	0	0	0
18	S	7	0	0	0	0
18	T	9	0	0	0	0
18	U	15	0	0	0	0
18	V	6	0	0	0	0
18	W	12	0	0	0	0
18	X	16	0	0	0	0
18	Y	9	0	0	0	0
18	Z	13	0	0	0	0
18	a	12	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	b	7	0	0	0	0
All	All	49775	0	49064	105	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 1.

All (105) 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:V:35:HIS:NE2	8:V:53:GLU:OE1	2.16	0.79
10:J:1:MET:O	10:J:2:ASP:HB2	1.88	0.74
10:X:1:MET:O	10:X:2:ASP:HB2	1.88	0.72
8:H:22:GLN:HG2	17:H:301:GTW:O44	1.93	0.68
8:V:22:GLN:HG3	8:V:27:ALA:HB2	1.80	0.64
11:Y:5:ALA:HB3	11:Y:100:MET:HE2	1.80	0.64
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.81	0.63
11:K:5:ALA:HB3	11:K:100:MET:HE2	1.82	0.62
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.81	0.62
11:Y:53:GLN:O	11:Y:57:THR:OG1	2.19	0.60
14:N:152:VAL:HA	14:N:175:MET:HE1	1.84	0.58
11:K:53:GLN:O	11:K:57:THR:OG1	2.23	0.56
11:K:100:MET:HE3	11:K:127:PHE:HB2	1.88	0.56
14:N:49:ALA:O	14:N:53:GLN:HB2	2.06	0.55
11:Y:99:THR:HG22	11:Y:115:VAL:HB	1.89	0.55
11:Y:100:MET:HE3	11:Y:127:PHE:HB2	1.89	0.55
11:K:99:THR:HG22	11:K:115:VAL:HB	1.89	0.54
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.43	0.54
10:X:67:TYR:CE1	10:X:75:LEU:HD13	2.44	0.53
8:V:50:ALA:HB2	9:W:128:CYS:HB2	1.91	0.52
7:U:23:PHE:O	7:U:26:THR:HB	2.10	0.52
10:J:174:MET:HA	10:X:174:MET:HA	1.94	0.50
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.60	0.49
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.94	0.49
3:C:201:VAL:O	3:C:202:GLN:CB	2.60	0.49
7:G:23:PHE:O	7:G:26:THR:HB	2.12	0.49
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.94	0.49
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.93	0.49
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.96	0.48
9:I:37:ASN:ND2	11:Y:209:ASN:O	2.47	0.48
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.96	0.48
4:D:176:LEU:HD22	5:E:55:LEU:HD13	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.96	0.48
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.14	0.48
12:L:8:ASN:HA	12:L:30:ILE:O	2.15	0.47
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.79	0.47
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.97	0.47
1:O:14:PRO:HA	2:P:23:TYR:CD1	2.51	0.46
10:J:23:ARG:HG3	18:J:215:HOH:O	2.15	0.46
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.98	0.46
8:H:50:ALA:HB2	9:I:128:CYS:HB2	1.98	0.46
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.98	0.46
11:Y:100:MET:CE	11:Y:127:PHE:HB2	2.47	0.45
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.46	0.45
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.98	0.45
11:K:100:MET:CE	11:K:127:PHE:HB2	2.46	0.45
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.32	0.45
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.51	0.44
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.99	0.44
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.46	0.44
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.99	0.44
3:C:201:VAL:HG13	3:C:202:GLN:N	2.32	0.44
9:I:10:ILE:HG21	9:I:141:ALA:HB3	2.00	0.44
11:K:5:ALA:HB3	11:K:100:MET:CE	2.47	0.44
8:V:50:ALA:HB3	9:W:126:ILE:HD12	1.99	0.44
11:K:37:ILE:HG23	11:K:60:GLY:HA2	1.99	0.43
13:M:97:ALA:HA	13:M:130:VAL:HG21	2.00	0.43
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.99	0.43
7:G:78:ILE:N	7:G:79:PRO:CD	2.81	0.43
11:Y:37:ILE:HG23	11:Y:60:GLY:HA2	2.00	0.43
11:Y:5:ALA:HB3	11:Y:100:MET:CE	2.47	0.43
6:F:172:LEU:CD1	6:F:195:ILE:HD13	2.49	0.43
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.99	0.43
1:O:115:ALA:HB1	1:O:154:GLY:O	2.19	0.43
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.54	0.43
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.54	0.43
6:T:172:LEU:CD1	6:T:195:ILE:HD13	2.49	0.43
8:V:218:VAL:CG2	9:W:196:LYS:HB2	2.48	0.43
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	2.00	0.43
12:L:100:LYS:HD3	12:L:105:TYR:CZ	2.55	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.42
4:D:88:ALA:HA	4:D:99:ILE:HG21	2.01	0.42
9:W:20:VAL:HG23	9:W:189:ILE:HB	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:147:MET:N	12:L:148:PRO:HD2	2.34	0.42
9:I:98:ARG:O	9:I:126:ILE:HD11	2.20	0.42
12:Z:147:MET:N	12:Z:148:PRO:HD2	2.34	0.42
1:A:115:ALA:HB1	1:A:154:GLY:O	2.20	0.42
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.01	0.42
5:E:77:ALA:N	5:E:78:PRO:CD	2.83	0.42
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.55	0.42
6:F:13:PRO:HA	7:G:21:TYR:CD1	2.55	0.42
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.54	0.42
11:K:145:LYS:HB2	11:K:148:LEU:HD13	2.01	0.42
11:K:16:VAL:HG21	11:K:34:VAL:HG23	2.01	0.42
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.54	0.42
6:F:14:ASP:N	6:F:14:ASP:OD2	2.52	0.41
2:P:50:LYS:O	2:P:51:VAL:C	2.59	0.41
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	2.02	0.41
5:S:77:ALA:N	5:S:78:PRO:CD	2.83	0.41
1:A:78:MET:HE2	18:G:407:HOH:O	2.20	0.41
5:E:18:LEU:HD21	6:F:126:ARG:HD2	2.03	0.41
10:X:1:MET:HA	10:X:34:LYS:CE	2.50	0.41
11:Y:16:VAL:HG21	11:Y:34:VAL:HG23	2.01	0.41
4:D:99:ILE:HD11	4:D:104:LEU:HB2	2.02	0.41
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.51	0.41
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.50	0.41
10:J:1:MET:O	10:J:2:ASP:CB	2.65	0.41
2:B:50:LYS:O	2:B:51:VAL:C	2.59	0.40
2:P:95:GLN:HB3	9:W:68:TYR:CD2	2.57	0.40
9:I:20:VAL:HG23	9:I:189:ILE:HB	2.02	0.40
12:L:100:LYS:O	12:L:104:PRO:HA	2.20	0.40
12:Z:100:LYS:HD3	12:Z:105:TYR:CZ	2.57	0.40
3:C:160:GLN:HA	3:C:160:GLN:HE21	1.86	0.40
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.86	0.40
4:R:99:ILE:HD11	4:R:104:LEU:HB2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	241 (97%)	7 (3%)	0	100	100
1	O	248/250 (99%)	241 (97%)	7 (3%)	0	100	100
2	B	242/258 (94%)	233 (96%)	7 (3%)	2 (1%)	19	43
2	P	242/258 (94%)	232 (96%)	8 (3%)	2 (1%)	19	43
3	C	238/254 (94%)	230 (97%)	6 (2%)	2 (1%)	19	43
3	Q	238/254 (94%)	230 (97%)	6 (2%)	2 (1%)	19	43
4	D	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
4	R	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
5	E	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
5	S	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
6	F	241/288 (84%)	235 (98%)	6 (2%)	0	100	100
6	T	241/288 (84%)	235 (98%)	6 (2%)	0	100	100
7	G	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
7	U	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
8	H	220/232 (95%)	214 (97%)	5 (2%)	1 (0%)	29	54
8	V	220/232 (95%)	215 (98%)	4 (2%)	1 (0%)	29	54
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	29	54
10	X	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	29	54
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%)	215 (98%)	5 (2%)	0	100	100
12	Z	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
13	M	231/246 (94%)	222 (96%)	8 (4%)	1 (0%)	34	60
13	a	231/246 (94%)	223 (96%)	7 (3%)	1 (0%)	34	60
14	N	194/196 (99%)	186 (96%)	8 (4%)	0	100	100
14	b	194/196 (99%)	186 (96%)	8 (4%)	0	100	100
All	All	6276/6614 (95%)	6099 (97%)	163 (3%)	14 (0%)	47	73

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN
10	J	2	ASP
2	P	51	VAL
3	Q	202	GLN
10	X	2	ASP
3	C	205	ALA
3	Q	205	ALA
2	B	221	ASP
8	H	9	ASN
2	P	221	ASP
8	V	9	ASN
13	M	229	GLY
13	a	229	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	206 (99%)	3 (1%)	67	86
1	O	209/209 (100%)	206 (99%)	3 (1%)	67	86
2	B	203/216 (94%)	196 (97%)	7 (3%)	37	66
2	P	203/216 (94%)	196 (97%)	7 (3%)	37	66
3	C	212/226 (94%)	204 (96%)	8 (4%)	33	62
3	Q	212/226 (94%)	204 (96%)	8 (4%)	33	62
4	D	194/215 (90%)	186 (96%)	8 (4%)	30	59
4	R	194/215 (90%)	186 (96%)	8 (4%)	30	59
5	E	190/193 (98%)	183 (96%)	7 (4%)	34	63
5	S	190/193 (98%)	183 (96%)	7 (4%)	34	63
6	F	201/239 (84%)	192 (96%)	9 (4%)	27	55
6	T	201/239 (84%)	192 (96%)	9 (4%)	27	55

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	206/210 (98%)	198 (96%)	8 (4%)	32	61
7	U	206/210 (98%)	197 (96%)	9 (4%)	28	56
8	H	181/190 (95%)	176 (97%)	5 (3%)	43	73
8	V	181/190 (95%)	176 (97%)	5 (3%)	43	73
9	I	172/173 (99%)	169 (98%)	3 (2%)	60	84
9	W	172/173 (99%)	169 (98%)	3 (2%)	60	84
10	J	173/175 (99%)	168 (97%)	5 (3%)	42	71
10	X	173/175 (99%)	168 (97%)	5 (3%)	42	71
11	K	169/169 (100%)	161 (95%)	8 (5%)	26	54
11	Y	169/169 (100%)	161 (95%)	8 (5%)	26	54
12	L	185/185 (100%)	180 (97%)	5 (3%)	44	74
12	Z	185/185 (100%)	180 (97%)	5 (3%)	44	74
13	M	199/208 (96%)	193 (97%)	6 (3%)	41	70
13	a	199/208 (96%)	193 (97%)	6 (3%)	41	70
14	N	162/162 (100%)	161 (99%)	1 (1%)	86	95
14	b	162/162 (100%)	161 (99%)	1 (1%)	86	95
All	All	5312/5540 (96%)	5145 (97%)	167 (3%)	40	69

All (167) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	61	LEU
1	A	157	PHE
2	B	50	LYS
2	B	52	THR
2	B	55	LEU
2	B	58	GLN
2	B	114	LEU
2	B	184	LYS
2	B	191	LEU
3	C	4	ARG
3	C	38	ASN
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	169	VAL
3	C	180	LYS
3	C	203	THR
4	D	20	LEU
4	D	99	ILE
4	D	125	LEU
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	29	LYS
5	E	54	GLU
5	E	71	LEU
5	E	184	ASN
5	E	188	LEU
5	E	202	ASP
6	F	14	ASP
6	F	117	GLN
6	F	123	ASN
6	F	172	LEU
6	F	181	GLU
6	F	203	ASN
6	F	206	LYS
6	F	214	TRP
6	F	221	ASN
7	G	115	LEU
7	G	117	GLN
7	G	125	MET
7	G	154	TYR
7	G	166	GLN
7	G	181	LYS
7	G	235	ARG
7	G	236	LEU
8	H	30	ASN
8	H	56	THR
8	H	68	LEU
8	H	84	LYS
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	I	182	TRP
10	J	23	ARG
10	J	75	LEU
10	J	78	GLN
10	J	144	LEU
10	J	174	MET
11	K	4	LEU
11	K	7	ARG
11	K	9	GLN
11	K	35	ILE
11	K	57	THR
11	K	99	THR
11	K	106	ARG
11	K	118	ASP
12	L	1	GLN
12	L	23	LEU
12	L	49	ASN
12	L	136	CYS
12	L	167	LYS
13	M	43	ILE
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
14	N	9	LYS
1	O	17	LYS
1	O	61	LEU
1	O	157	PHE
2	P	50	LYS
2	P	52	THR
2	P	55	LEU
2	P	58	GLN
2	P	114	LEU
2	P	184	LYS
2	P	191	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	Q	180	LYS
3	Q	203	THR
4	R	20	LEU
4	R	99	ILE
4	R	125	LEU
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	54	GLU
5	S	71	LEU
5	S	184	ASN
5	S	188	LEU
5	S	202	ASP
6	T	14	ASP
6	T	117	GLN
6	T	123	ASN
6	T	172	LEU
6	T	181	GLU
6	T	203	ASN
6	T	206	LYS
6	T	214	TRP
6	T	221	ASN
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN
7	U	125	MET
7	U	154	TYR
7	U	166	GLN
7	U	181	LYS
7	U	235	ARG
7	U	236	LEU
8	V	30	ASN
8	V	56	THR
8	V	68	LEU
8	V	84	LYS
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	W	182	TRP
10	X	23	ARG
10	X	75	LEU
10	X	78	GLN
10	X	144	LEU
10	X	174	MET
11	Y	4	LEU
11	Y	7	ARG
11	Y	9	GLN
11	Y	35	ILE
11	Y	57	THR
11	Y	99	THR
11	Y	106	ARG
11	Y	118	ASP
12	Z	1	GLN
12	Z	23	LEU
12	Z	49	ASN
12	Z	136	CYS
12	Z	167	LYS
13	a	43	ILE
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
14	b	9	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
3	C	38	ASN
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	91	HIS
4	D	146	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
5	E	184	ASN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
6	F	240	GLN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
8	H	66	HIS
10	J	55	GLN
11	K	85	ASN
11	K	176	ASN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	158	ASN
13	M	48	ASN
13	M	102	GLN
13	M	194	ASN
13	M	213	GLN
14	N	161	GLN
1	O	94	HIS
2	P	20	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	176	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
4	R	91	HIS
4	R	100	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	R	225	ASN
5	S	68	HIS
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	184	ASN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
6	T	240	GLN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
10	X	55	GLN
11	Y	85	ASN
11	Y	176	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	158	ASN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	194	ASN
13	a	213	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 15 ligands modelled in this entry, 11 are monoatomic - leaving 4 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	GTW	K	301	11	43,46,46	2.34	7 (16%)	55,63,63	1.70	9 (16%)
17	GTW	H	301	8	43,46,46	2.54	6 (13%)	55,63,63	2.92	15 (27%)
17	GTW	Y	301	11	43,46,46	2.15	6 (13%)	55,63,63	2.01	12 (21%)
17	GTW	V	301	8	43,46,46	2.20	6 (13%)	55,63,63	3.91	14 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	GTW	K	301	11	-	5/40/52/52	0/3/3/3
17	GTW	H	301	8	-	5/40/52/52	0/3/3/3
17	GTW	Y	301	11	-	4/40/52/52	0/3/3/3
17	GTW	V	301	8	-	7/40/52/52	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	H	301	GTW	C3-S5	-12.96	1.33	1.73
17	K	301	GTW	C3-S5	-11.44	1.38	1.73
17	V	301	GTW	C3-S5	-10.07	1.42	1.73
17	Y	301	GTW	C3-S5	-9.94	1.43	1.73
17	H	301	GTW	C16-C17	-5.41	1.38	1.51
17	V	301	GTW	C16-C17	-5.19	1.38	1.51
17	Y	301	GTW	C16-C17	-5.08	1.39	1.51
17	K	301	GTW	C16-C17	-5.00	1.39	1.51
17	Y	301	GTW	C21-C20	-4.25	1.36	1.51
17	K	301	GTW	C21-C20	-4.16	1.36	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	H	301	GTW	C1-C6	-3.96	1.31	1.37
17	V	301	GTW	C21-C20	-3.95	1.37	1.51
17	H	301	GTW	C21-C20	-3.94	1.37	1.51
17	V	301	GTW	C1-N2	-3.89	1.30	1.36
17	Y	301	GTW	C1-N2	-3.76	1.30	1.36
17	V	301	GTW	C1-C6	-3.72	1.31	1.37
17	K	301	GTW	C1-C6	-3.63	1.31	1.37
17	K	301	GTW	C1-N2	-3.59	1.30	1.36
17	Y	301	GTW	C1-C6	-3.05	1.32	1.37
17	H	301	GTW	C25-C26	-2.85	1.49	1.52
17	H	301	GTW	C1-N2	-2.75	1.32	1.36
17	V	301	GTW	C25-C26	-2.16	1.50	1.52
17	K	301	GTW	C34-C33	-2.03	1.46	1.52
17	Y	301	GTW	C34-C33	-2.00	1.46	1.52
17	K	301	GTW	C35-C34	-2.00	1.47	1.53

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	V	301	GTW	O30-S27-C26	19.74	122.17	108.34
17	V	301	GTW	O29-S27-C26	-15.61	97.42	108.34
17	H	301	GTW	O30-S27-C26	14.78	118.69	108.34
17	H	301	GTW	O29-S27-C26	-7.49	103.10	108.34
17	K	301	GTW	O29-S27-C26	-6.65	103.69	108.34
17	V	301	GTW	C15-N14-C13	5.98	132.72	123.20
17	Y	301	GTW	O30-S27-C26	5.98	112.53	108.34
17	Y	301	GTW	C4-C3-S5	5.73	127.82	120.12
17	H	301	GTW	O29-S27-O30	-5.69	104.93	117.09
17	Y	301	GTW	O29-S27-O30	-5.60	105.12	117.09
17	H	301	GTW	C15-N14-C13	5.54	132.03	123.20
17	V	301	GTW	O29-S27-O30	-5.52	105.30	117.09
17	Y	301	GTW	O29-S27-C26	-5.51	104.48	108.34
17	V	301	GTW	O30-S27-C28	4.88	113.81	108.91
17	K	301	GTW	C4-C3-S5	4.30	125.90	120.12
17	H	301	GTW	O30-S27-C28	4.12	113.05	108.91
17	K	301	GTW	O29-S27-O30	-4.04	108.46	117.09
17	V	301	GTW	C16-C15-N14	3.72	117.54	110.39
17	V	301	GTW	C32-C12-C13	-3.71	101.72	110.57
17	H	301	GTW	C40-C9-N8	-3.70	102.06	110.58
17	Y	301	GTW	C6-C7-N8	3.62	121.92	115.21
17	H	301	GTW	C32-C12-C13	-3.61	101.98	110.57
17	V	301	GTW	C4-C3-S5	3.53	124.86	120.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	H	301	GTW	C16-C15-N14	3.39	116.89	110.39
17	Y	301	GTW	C25-C15-C16	-3.29	105.79	111.14
17	K	301	GTW	C6-C7-N8	3.28	121.29	115.21
17	Y	301	GTW	C40-C9-C10	-3.15	103.07	110.57
17	K	301	GTW	C28-S27-C26	2.99	116.75	105.21
17	H	301	GTW	C25-C15-N14	-2.91	106.44	110.54
17	V	301	GTW	C25-C15-N14	-2.78	106.63	110.54
17	V	301	GTW	C40-C9-N8	-2.72	104.32	110.58
17	V	301	GTW	C25-C15-C16	2.65	115.45	111.14
17	K	301	GTW	C25-C15-C16	-2.54	107.01	111.14
17	V	301	GTW	C33-C32-C12	2.53	117.93	114.52
17	H	301	GTW	C12-C13-N14	-2.49	111.24	116.70
17	H	301	GTW	O29-S27-C28	2.43	111.35	108.91
17	Y	301	GTW	C16-C17-C18	-2.40	116.13	120.91
17	K	301	GTW	C32-C12-C13	-2.37	104.92	110.57
17	K	301	GTW	C40-C9-C10	-2.33	105.02	110.57
17	H	301	GTW	C25-C15-C16	2.33	114.92	111.14
17	Y	301	GTW	C6-C1-N2	2.22	113.55	109.09
17	Y	301	GTW	C28-S27-C26	2.21	113.71	105.21
17	Y	301	GTW	C16-C17-C24	2.20	125.27	120.91
17	H	301	GTW	C4-C3-N2	2.20	127.64	121.87
17	H	301	GTW	C32-C12-N11	-2.13	105.68	110.58
17	Y	301	GTW	C32-C33-C38	-2.08	107.22	111.73
17	V	301	GTW	C12-C13-N14	-2.07	112.17	116.70
17	H	301	GTW	C10-C9-N8	-2.06	105.55	111.16
17	K	301	GTW	C16-C17-C24	2.05	124.97	120.91
17	V	301	GTW	C40-C9-C10	2.01	115.36	110.57

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	K	301	GTW	C15-C25-C26-S27
17	V	301	GTW	C25-C26-S27-O30
17	V	301	GTW	C25-C26-S27-O29
17	Y	301	GTW	C15-C25-C26-S27
17	K	301	GTW	C15-C16-C17-C24
17	Y	301	GTW	C15-C16-C17-C24
17	K	301	GTW	C15-C16-C17-C18
17	Y	301	GTW	C15-C16-C17-C18
17	H	301	GTW	C15-C16-C17-C18
17	V	301	GTW	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

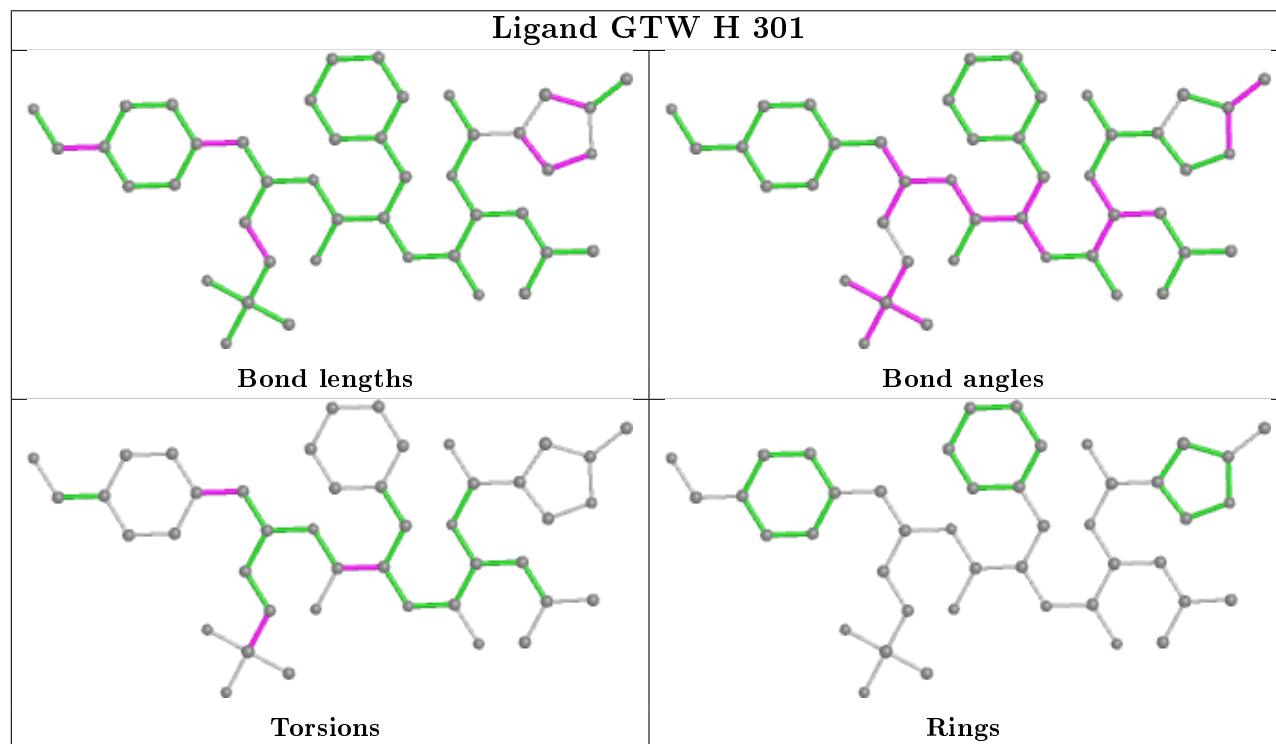
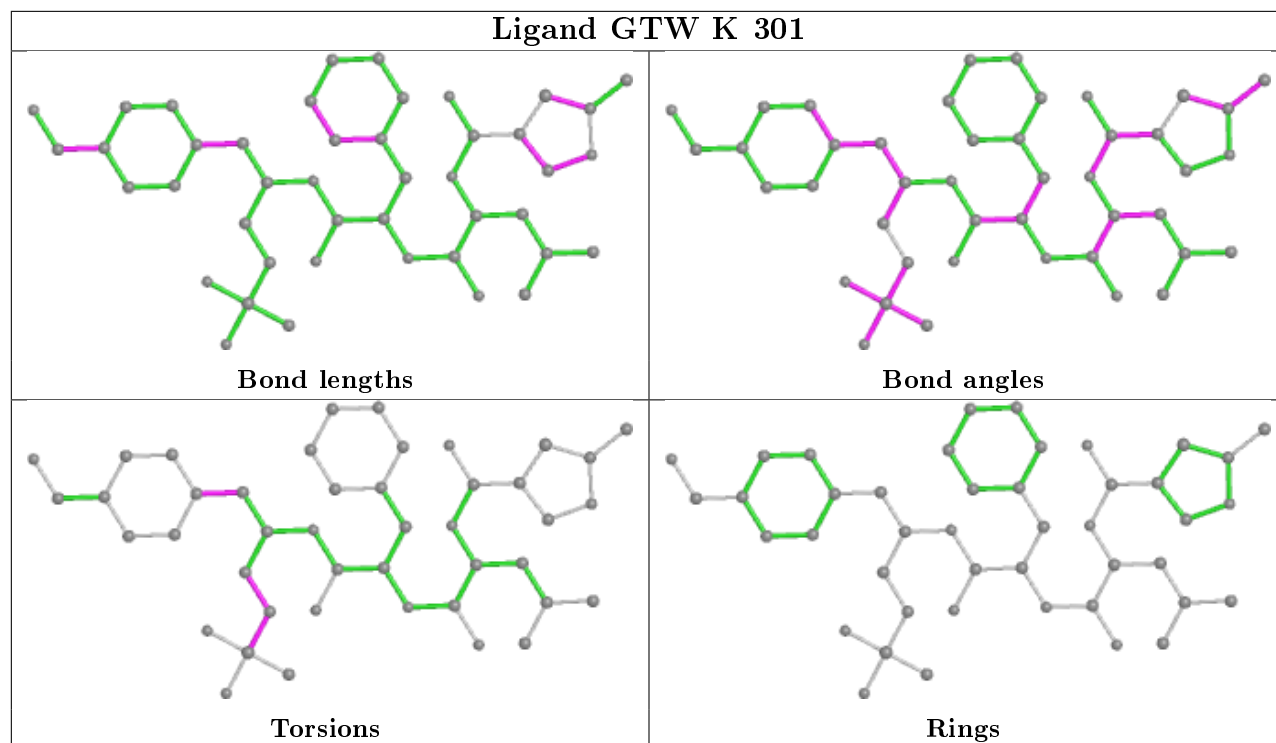
Mol	Chain	Res	Type	Atoms
17	V	301	GTW	C15-C16-C17-C24
17	H	301	GTW	C15-C16-C17-C24
17	K	301	GTW	C25-C26-S27-C28
17	V	301	GTW	C25-C26-S27-C28
17	K	301	GTW	C25-C26-S27-O30
17	H	301	GTW	C25-C26-S27-C28
17	H	301	GTW	N11-C12-C13-O31
17	V	301	GTW	C16-C15-C25-C26
17	H	301	GTW	N11-C12-C13-N14
17	Y	301	GTW	C25-C26-S27-C28
17	V	301	GTW	N11-C12-C13-O31

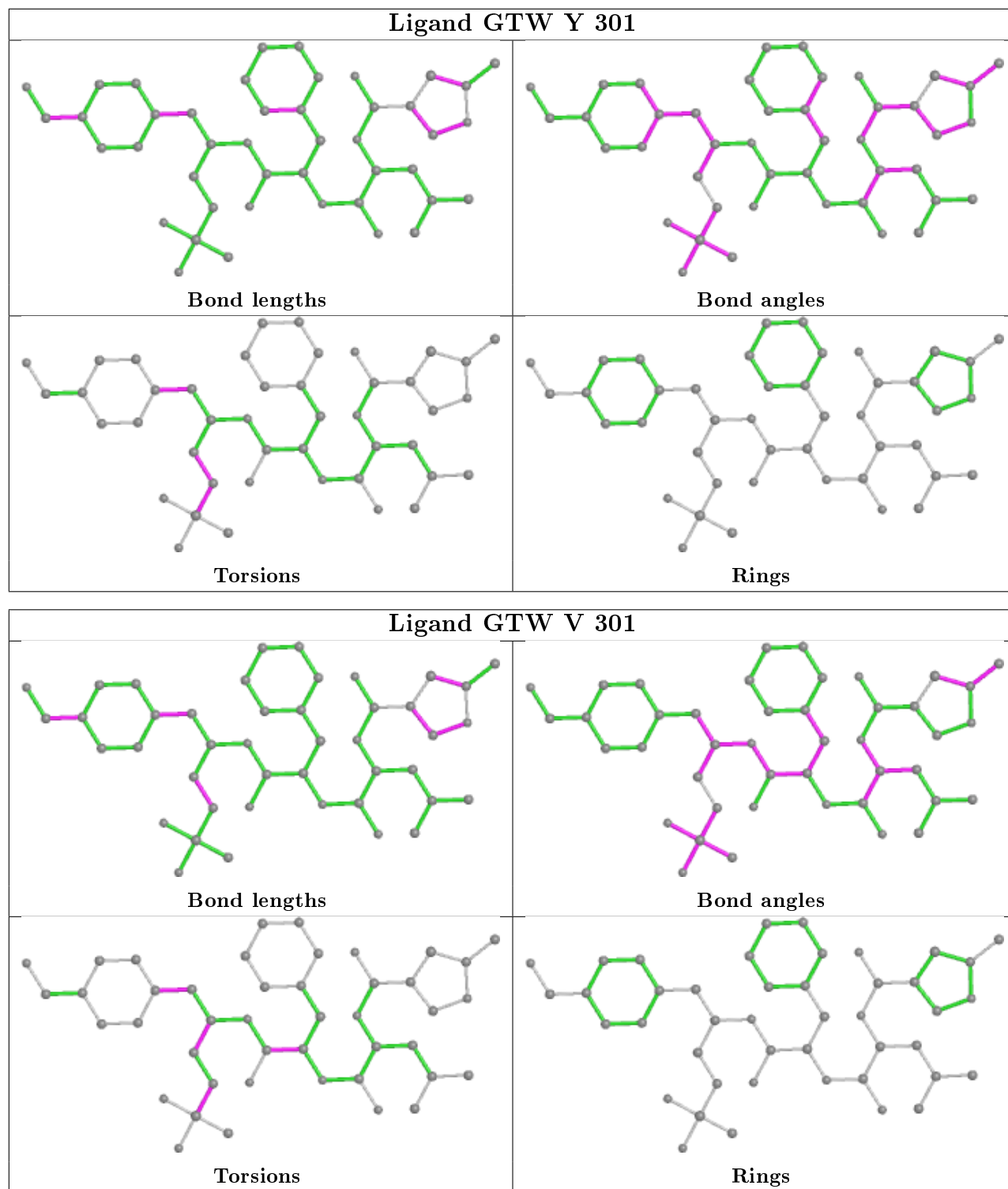
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	H	301	GTW	1	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	-0.04	15 (6%) 21 20	45, 73, 126, 170	0
1	O	250/250 (100%)	-0.22	9 (3%) 42 42	46, 66, 108, 152	0
2	B	244/258 (94%)	-0.10	12 (4%) 29 28	44, 66, 119, 169	0
2	P	244/258 (94%)	-0.12	12 (4%) 29 28	45, 71, 116, 162	0
3	C	240/254 (94%)	-0.06	14 (5%) 23 22	41, 68, 134, 164	0
3	Q	240/254 (94%)	0.28	21 (8%) 10 8	54, 90, 178, 209	0
4	D	235/260 (90%)	-0.19	3 (1%) 77 78	50, 77, 112, 155	0
4	R	235/260 (90%)	-0.19	5 (2%) 63 65	54, 80, 124, 177	0
5	E	231/234 (98%)	0.04	7 (3%) 50 51	62, 95, 136, 178	0
5	S	231/234 (98%)	0.07	10 (4%) 35 33	57, 86, 139, 175	0
6	F	243/288 (84%)	-0.04	8 (3%) 46 46	61, 94, 152, 180	0
6	T	243/288 (84%)	-0.06	5 (2%) 63 65	51, 83, 145, 178	0
7	G	241/252 (95%)	0.03	14 (5%) 23 22	57, 92, 150, 207	0
7	U	241/252 (95%)	-0.22	6 (2%) 57 59	46, 68, 107, 152	0
8	H	222/232 (95%)	-0.06	4 (1%) 68 70	54, 78, 111, 127	0
8	V	222/232 (95%)	-0.19	5 (2%) 60 62	51, 68, 107, 140	0
9	I	204/205 (99%)	-0.61	2 (0%) 82 83	38, 57, 92, 118	0
9	W	204/205 (99%)	-0.56	2 (0%) 82 83	38, 57, 91, 122	0
10	J	195/198 (98%)	-0.51	2 (1%) 82 83	35, 54, 87, 129	0
10	X	195/198 (98%)	-0.47	3 (1%) 73 76	43, 59, 92, 143	0
11	K	212/212 (100%)	-0.40	0 100 100	40, 60, 90, 107	0
11	Y	212/212 (100%)	-0.47	3 (1%) 75 77	39, 60, 92, 126	0
12	L	222/222 (100%)	-0.38	1 (0%) 91 92	41, 68, 104, 126	0
12	Z	222/222 (100%)	-0.42	0 100 100	39, 65, 102, 116	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.32	5 (2%) 63 65	43, 72, 104, 114	0
13	a	233/246 (94%)	-0.37	1 (0%) 92 93	40, 67, 98, 131	0
14	N	196/196 (100%)	-0.34	2 (1%) 82 83	40, 69, 104, 136	0
14	b	196/196 (100%)	-0.41	1 (0%) 91 92	39, 64, 102, 125	0
All	All	6336/6614 (95%)	-0.21	172 (2%) 54 55	35, 72, 127, 209	0

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	49	THR	10.3
3	Q	206	LYS	9.1
1	A	1	MET	9.0
3	Q	50	LEU	7.7
3	C	206	LYS	7.6
2	B	218	GLY	7.1
3	C	49	THR	7.1
1	O	1	MET	6.3
2	P	218	GLY	6.2
10	X	1	MET	6.0
2	P	51	VAL	5.9
2	P	222	GLY	5.9
3	Q	48	SER	5.8
2	B	219	ALA	5.7
1	O	249	ALA	5.6
2	P	219	ALA	5.6
2	P	59	ASP	5.4
5	S	202	ASP	5.3
2	B	220	ASN	5.2
2	P	220	ASN	5.2
13	M	1	THR	5.2
3	Q	236	GLN	5.0
8	V	222	ASP	4.8
5	E	202	ASP	4.6
3	Q	204	GLY	4.5
3	Q	238	LYS	4.4
8	V	221	CYS	4.4
7	G	153	TYR	4.1
3	Q	240	GLU	4.1
2	B	221	ASP	4.0
3	Q	205	ALA	4.0
6	F	53	LYS	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	G	2	GLY	4.0
5	S	54	GLU	3.9
3	C	225	GLU	3.9
3	C	240	GLU	3.8
8	H	221	CYS	3.8
6	T	244	ASN	3.7
3	C	238	LYS	3.7
1	A	58	SER	3.6
1	O	50	LYS	3.6
10	X	194	ASP	3.6
7	U	2	GLY	3.6
2	B	51	VAL	3.5
4	D	242	GLU	3.5
1	A	62	SER	3.4
6	F	215	CYS	3.4
3	C	50	LEU	3.4
1	A	249	ALA	3.3
7	G	179	LYS	3.3
9	I	1	SER	3.3
7	G	242	GLN	3.3
13	a	1	THR	3.2
9	I	133	LYS	3.2
4	D	241	ALA	3.2
1	A	248	GLU	3.2
9	W	1	SER	3.2
2	P	221	ASP	3.2
6	F	241	LYS	3.2
3	C	205	ALA	3.2
4	R	125	LEU	3.2
1	O	231	LYS	3.1
10	J	194	ASP	3.1
9	W	133	LYS	3.1
8	H	222	ASP	3.1
3	C	239	GLN	3.1
5	E	233	ILE	3.1
10	J	1	MET	3.1
3	Q	239	GLN	3.1
6	F	181	GLU	3.1
1	A	250	LEU	3.0
14	N	181	ALA	3.0
13	M	233	ILE	3.0
1	A	202	GLY	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	S	180	LYS	2.9
2	B	60	THR	2.9
7	U	241	GLU	2.9
7	U	242	GLN	2.9
6	T	205	GLU	2.9
7	G	183	ASP	2.9
7	U	222	ASP	2.9
7	G	241	GLU	2.8
3	Q	202	GLN	2.8
2	P	60	THR	2.8
6	T	53	LYS	2.8
5	S	122	TYR	2.8
2	B	217	LYS	2.8
3	Q	51	LYS	2.8
7	G	208	GLU	2.8
3	Q	203	THR	2.7
14	N	195	GLN	2.7
5	E	201	ARG	2.7
1	A	60	THR	2.7
1	O	248	GLU	2.7
1	O	250	LEU	2.6
7	G	68	ARG	2.6
5	S	233	ILE	2.6
11	Y	212	GLY	2.6
13	M	216	ASN	2.6
3	Q	175	LYS	2.5
3	Q	181	GLU	2.5
13	M	47	ASP	2.5
1	O	201	GLU	2.5
4	R	242	GLU	2.5
6	F	201	GLU	2.5
2	P	50	LYS	2.5
6	T	215	CYS	2.5
3	C	202	GLN	2.5
2	P	182	ASP	2.5
2	B	222	GLY	2.5
3	C	59	PRO	2.5
5	E	194	GLU	2.5
3	C	180	LYS	2.5
1	O	52	SER	2.5
8	H	10	ASN	2.5
3	Q	141	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	59	ASP	2.4
2	B	50	LYS	2.4
6	T	182	GLY	2.4
3	Q	180	LYS	2.4
4	R	241	ALA	2.4
10	X	193	ASP	2.3
5	S	123	GLY	2.3
5	S	30	GLN	2.3
1	A	203	GLU	2.3
1	A	245	ASP	2.3
5	S	218	ASP	2.3
1	A	50	LYS	2.3
1	A	229	THR	2.3
4	D	125	LEU	2.3
6	F	221	ASN	2.3
7	G	240	ALA	2.3
8	H	198	GLU	2.3
3	C	175	LYS	2.3
8	V	145	ASP	2.2
4	R	217	GLN	2.2
4	R	1	ASP	2.2
5	S	225	ASP	2.2
12	L	174	TYR	2.2
1	A	201	GLU	2.2
11	Y	106	ARG	2.2
5	E	124	GLY	2.2
13	M	82	ASP	2.2
7	G	3	TYR	2.2
2	B	232	GLN	2.2
8	V	196	ARG	2.2
3	Q	60	SER	2.2
6	F	243	ILE	2.2
7	G	230	GLU	2.2
14	b	105	LYS	2.2
2	P	223	GLU	2.1
7	U	179	LYS	2.1
7	G	188	GLU	2.1
3	Q	223	SER	2.1
3	C	236	GLN	2.1
3	Q	187	GLU	2.1
7	U	181	LYS	2.1
5	E	218	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	G	40	ASP	2.1
3	C	48	SER	2.1
1	A	182	GLU	2.1
2	B	223	GLU	2.1
6	F	193	ALA	2.0
7	G	181	LYS	2.0
3	Q	59	PRO	2.0
1	O	178	ARG	2.0
5	S	163	ARG	2.0
11	Y	202	GLU	2.0
5	E	123	GLY	2.0
1	A	241	GLN	2.0
2	P	93	HIS	2.0
8	V	217	ILE	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 carbohydrates 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.

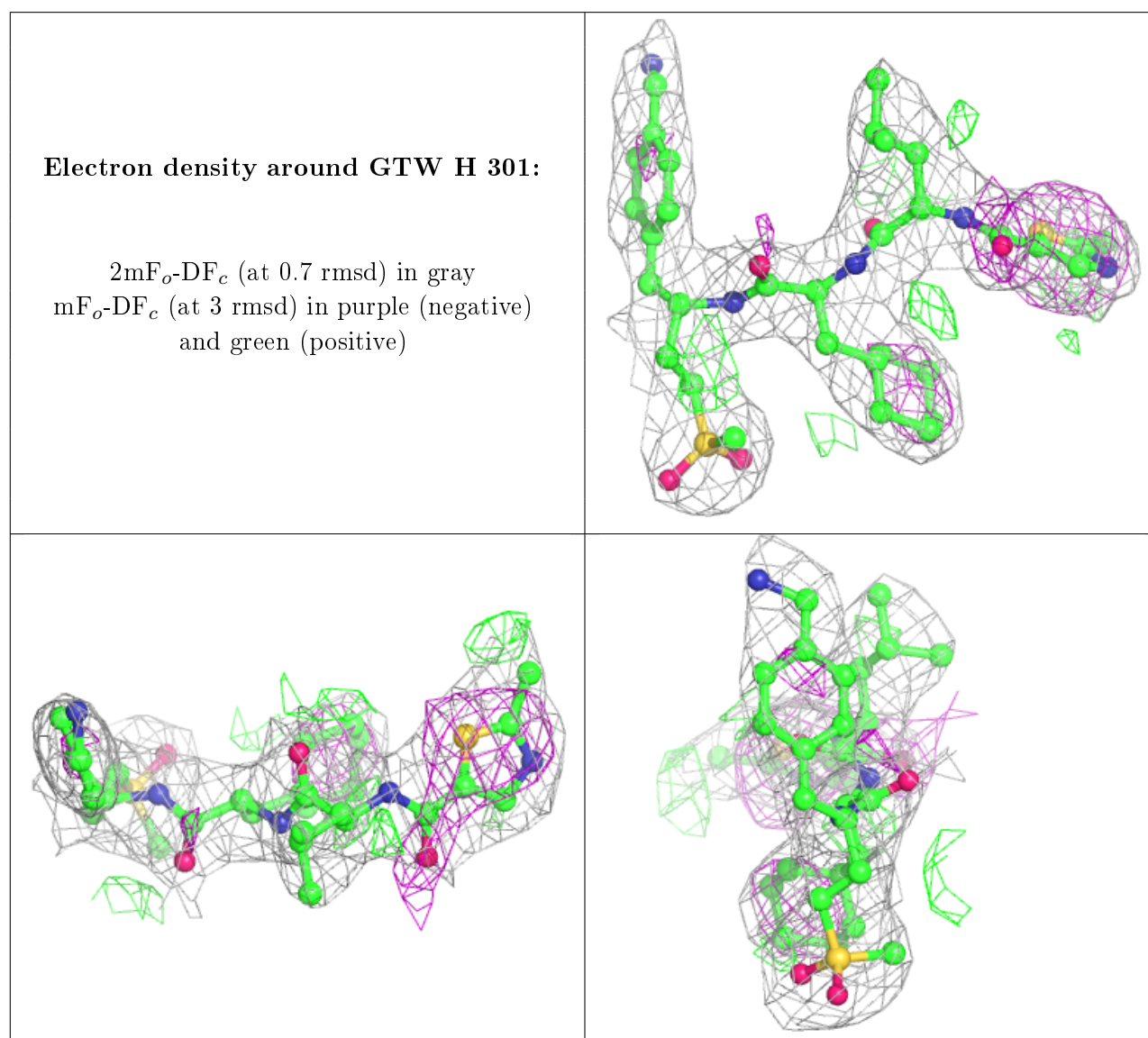
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
15	MG	K	303	1/1	0.86	0.16	81,81,81,81	0
17	GTW	H	301	44/44	0.88	0.20	39,61,65,71	0
17	GTW	V	301	44/44	0.89	0.20	34,55,59,67	0
15	MG	G	301	1/1	0.91	0.07	64,64,64,64	0
17	GTW	K	301	44/44	0.92	0.16	28,48,52,64	0
17	GTW	Y	301	44/44	0.93	0.17	30,48,52,60	0
15	MG	N	201	1/1	0.93	0.12	54,54,54,54	0
16	CL	G	302	1/1	0.95	0.14	59,59,59,59	0
15	MG	V	302	1/1	0.96	0.06	71,71,71,71	0

Continued on next page...

Continued from previous page...

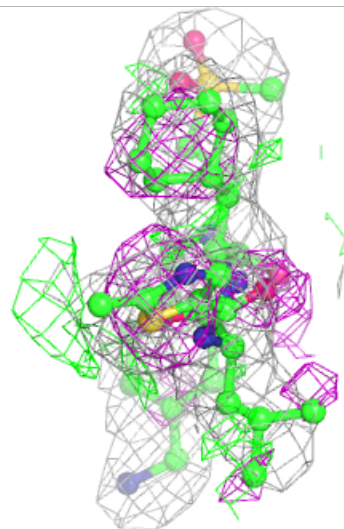
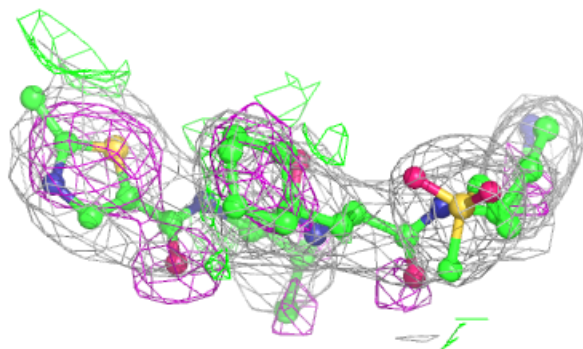
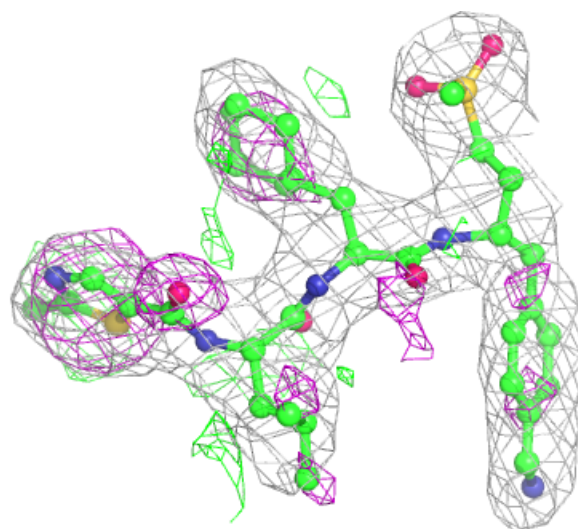
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
15	MG	Y	302	1/1	0.97	0.05	61,61,61,61	0
15	MG	Z	301	1/1	0.97	0.24	75,75,75,75	0
15	MG	X	201	1/1	0.98	0.29	48,48,48,48	0
15	MG	K	302	1/1	0.98	0.08	63,63,63,63	0
16	CL	U	301	1/1	0.99	0.20	52,52,52,52	0
15	MG	I	301	1/1	0.99	0.07	66,66,66,66	0

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.



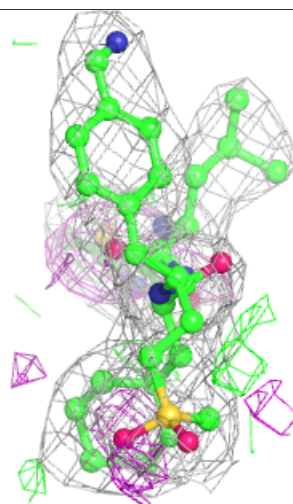
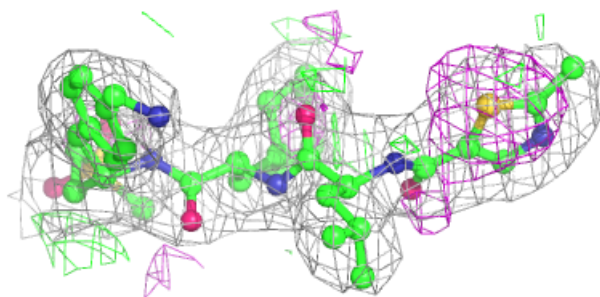
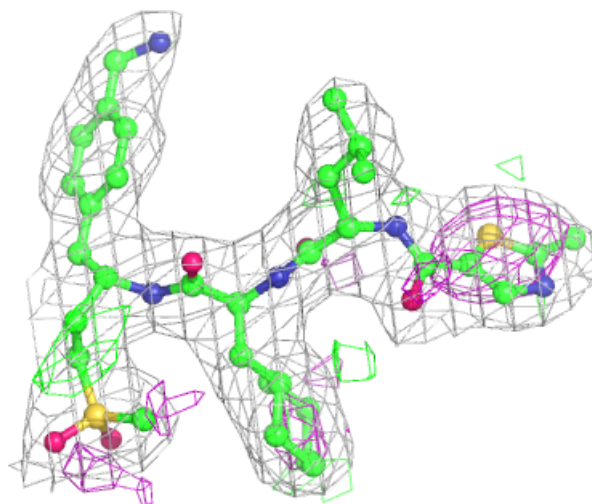
Electron density around GTW V 301:

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



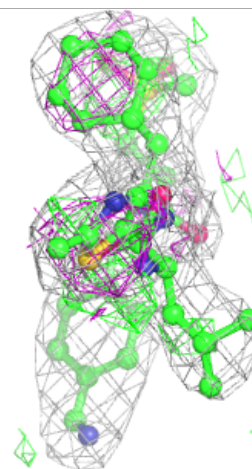
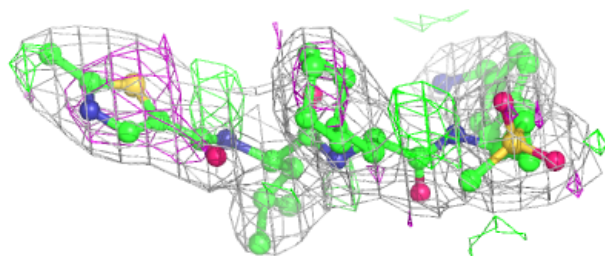
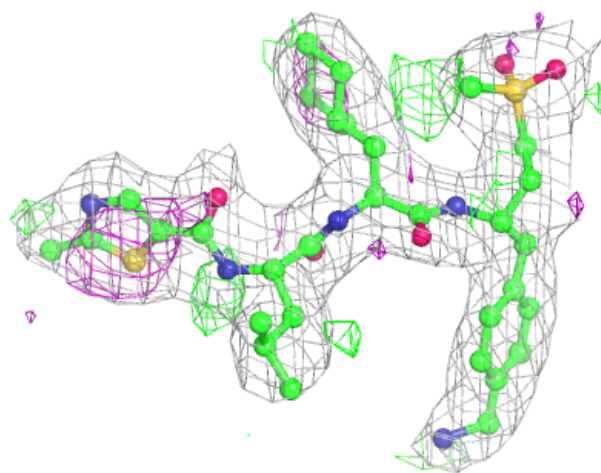
Electron density around GTW K 301:

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



Electron density around GTW Y 301:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.