



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 11:13 pm BST

PDB ID : 6HVT
Title : Yeast 20S proteasome with human beta2i (1-53) in complex with 20
Authors : Huber, E.M.; Groll, M.
Deposited on : 2018-10-11
Resolution : 2.90 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

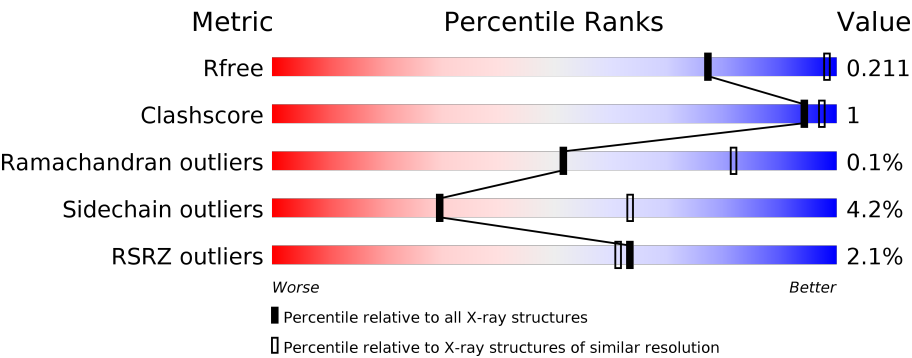
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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.





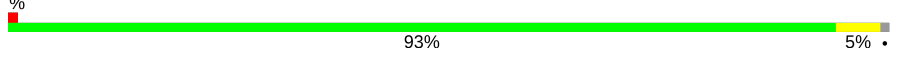
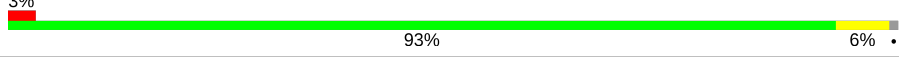

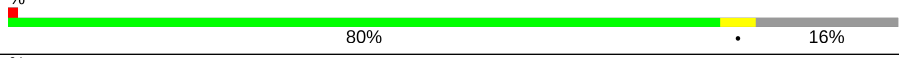
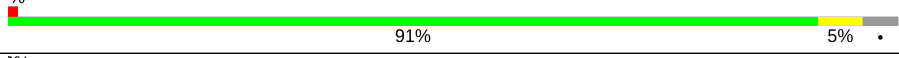
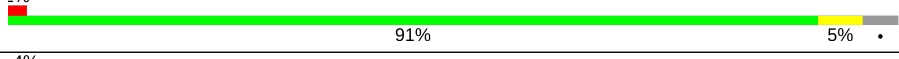
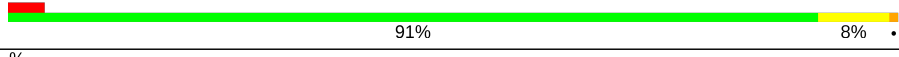
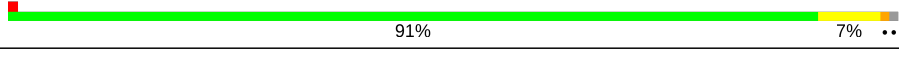
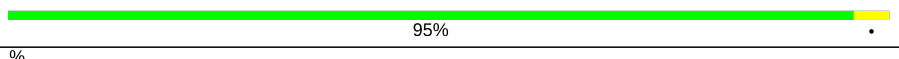
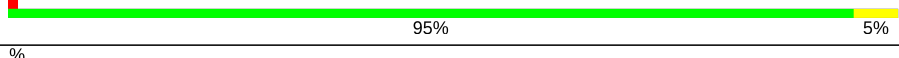
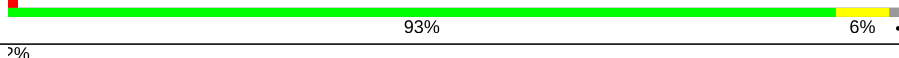
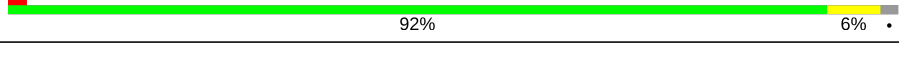
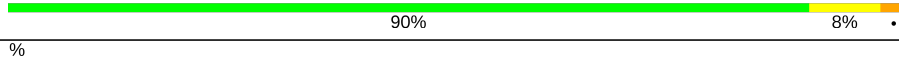
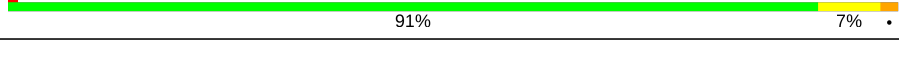
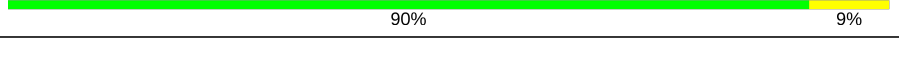
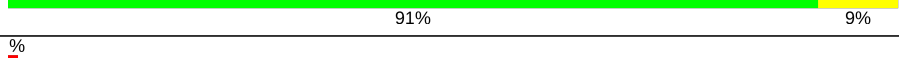
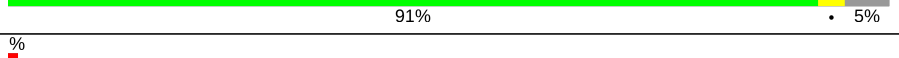
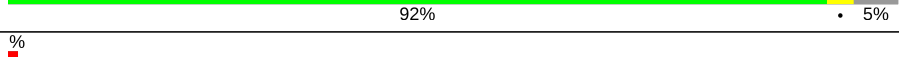
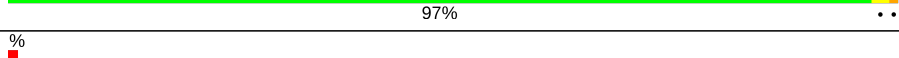
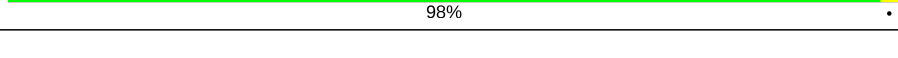
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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>3%</div><div>98%</div><div>•</div></div>
1	O	250	<div><div>3%</div><div>98%</div><div>•</div></div>
2	B	258	<div><div>3%</div><div>87%</div><div>7% • 5%</div></div>
2	P	258	<div><div>5%</div><div>87%</div><div>7% 5%</div></div>
3	C	254	<div><div>6%</div><div>87%</div><div>6% • 6%</div></div>
3	Q	254	<div><div>6%</div><div>88%</div><div>6% 6%</div></div>

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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	226	
8	V	226	
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 49836 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-10, Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	226	Total	C	N	O	S	0	0	0
			1716	1081	291	336	8			
8	V	223	Total	C	N	O	S	0	0	0
			1688	1066	287	327	8			

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	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	1	Total	Mg	0	0
			1	1		

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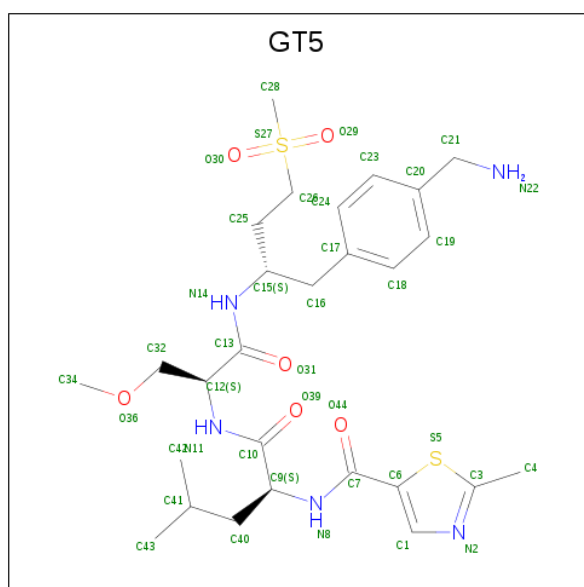
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	I	2	Total	Mg	0	0
			2	2		
15	W	1	Total	Mg	0	0
			1	1		
15	Z	1	Total	Mg	0	0
			1	1		
15	N	1	Total	Mg	0	0
			1	1		
15	L	1	Total	Mg	0	0
			1	1		

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

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

- Molecule 17 is {N}-[(2 {S})-1-[(2 {S})-1-[(2 {S})-1-[4-(aminomethyl)phenyl]-4-methylsulfonyl-butan-2-yl]amino]-3-methoxy-1-oxidanylidene-propan-2-yl]amino]-4-methyl-1-oxidanylidene-pentan-2-yl]-2-methyl-1,3-thiazole-5-carboxamide (three-letter code: GT5) (formula: C₂₇H₄₁N₅O₆S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	H	1	Total	C	N	O	S	0	0
			40	27	5	6	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	K	1	Total 40	C 27	N 5	O 6	S 2	0	0
17	V	1	Total 40	C 27	N 5	O 6	S 2	0	0
17	Y	1	Total 40	C 27	N 5	O 6	S 2	0	0

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	9	Total 9	O 9	0	0
18	B	15	Total 15	O 15	0	0
18	C	13	Total 13	O 13	0	0
18	D	6	Total 6	O 6	0	0
18	E	5	Total 5	O 5	0	0
18	F	9	Total 9	O 9	0	0
18	G	17	Total 17	O 17	0	0
18	H	16	Total 16	O 16	0	0
18	I	7	Total 7	O 7	0	0
18	J	19	Total 19	O 19	0	0
18	K	16	Total 16	O 16	0	0
18	L	24	Total 24	O 24	0	0
18	M	19	Total 19	O 19	0	0
18	N	12	Total 12	O 12	0	0
18	O	3	Total 3	O 3	0	0
18	P	9	Total 9	O 9	0	0

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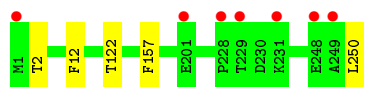
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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18	R	5	Total 5	O 5	0	0
18	S	5	Total 5	O 5	0	0
18	T	10	Total 10	O 10	0	0
18	U	15	Total 15	O 15	0	0
18	V	13	Total 13	O 13	0	0
18	W	8	Total 8	O 8	0	0
18	X	16	Total 16	O 16	0	0
18	Y	19	Total 19	O 19	0	0
18	Z	13	Total 13	O 13	0	0
18	a	11	Total 11	O 11	0	0
18	b	12	Total 12	O 12	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.

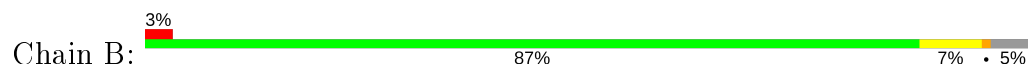
- Molecule 1: Proteasome subunit alpha type-2



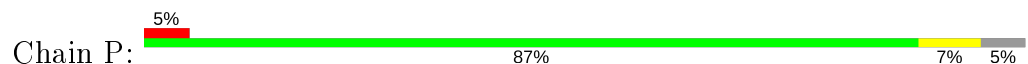
- Molecule 1: Proteasome subunit alpha type-2



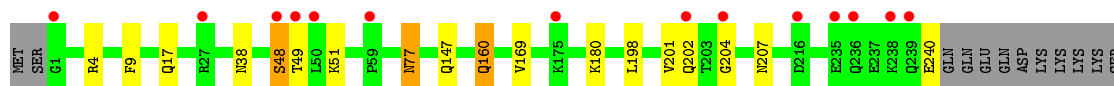
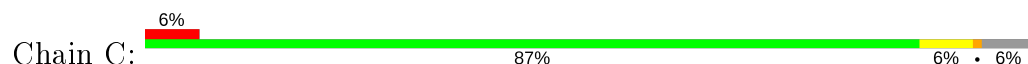
- Molecule 2: Proteasome subunit alpha type-3



- Molecule 2: Proteasome subunit alpha type-3

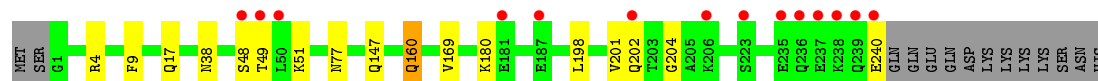
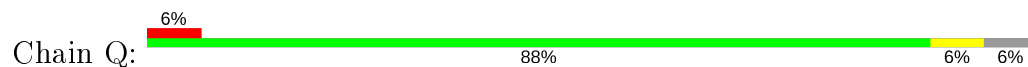


- Molecule 3: Proteasome subunit alpha type-4

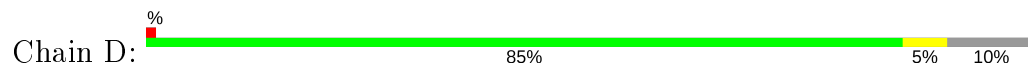


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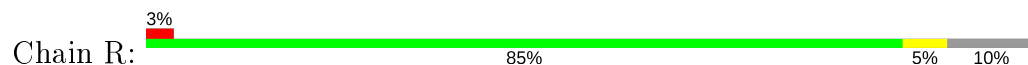
- Molecule 3: Proteasome subunit alpha type-4



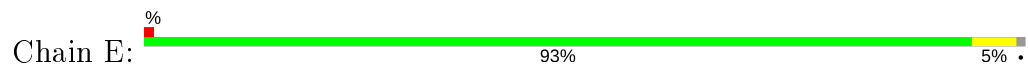
- Molecule 4: Proteasome subunit alpha type-5



- Molecule 4: Proteasome subunit alpha type-5



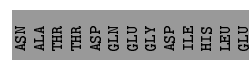
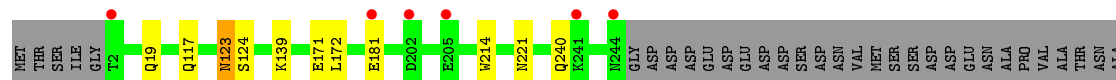
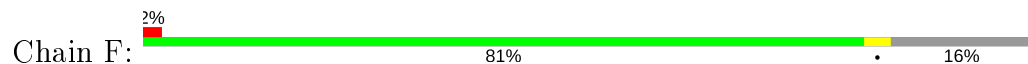
- Molecule 5: Proteasome subunit alpha type-6



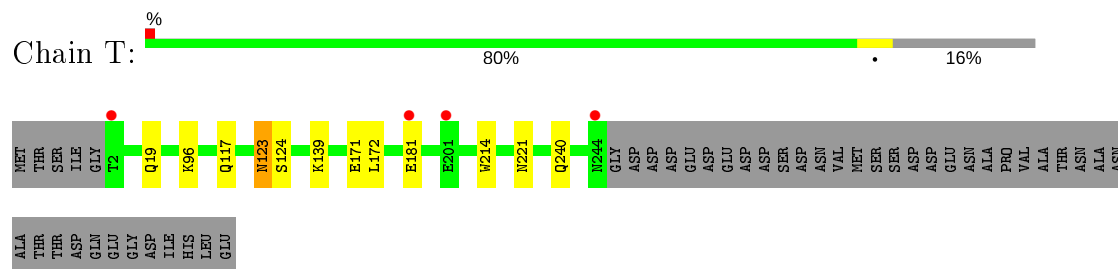
- Molecule 5: Proteasome subunit alpha type-6



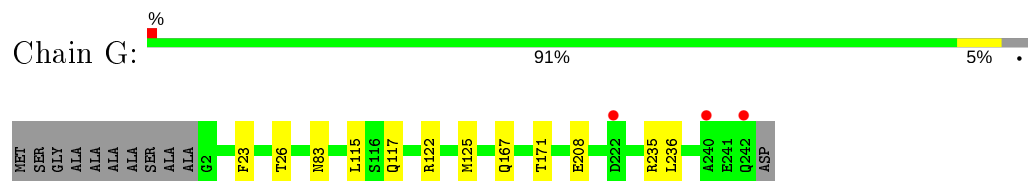
- Molecule 6: Probable proteasome subunit alpha type-7



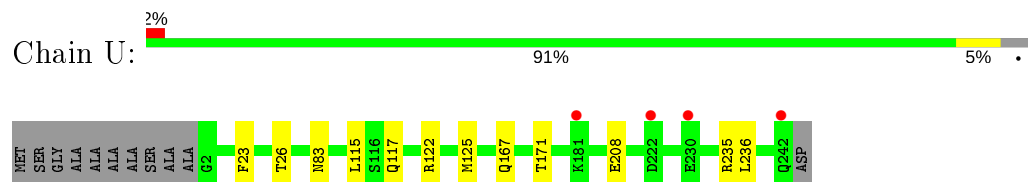
- Molecule 6: Probable proteasome subunit alpha type-7



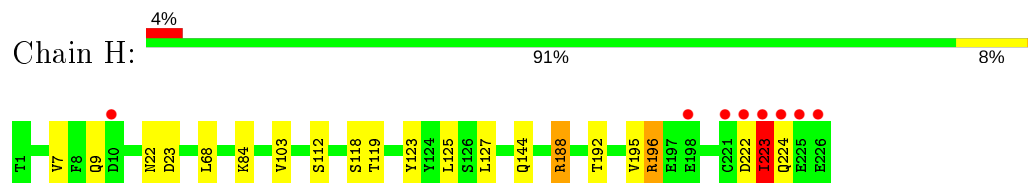
- Molecule 7: Proteasome subunit alpha type-1



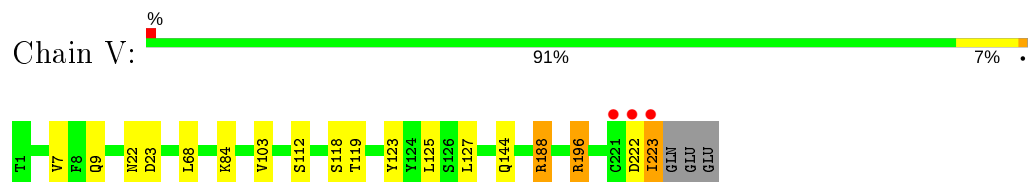
- Molecule 7: Proteasome subunit alpha type-1



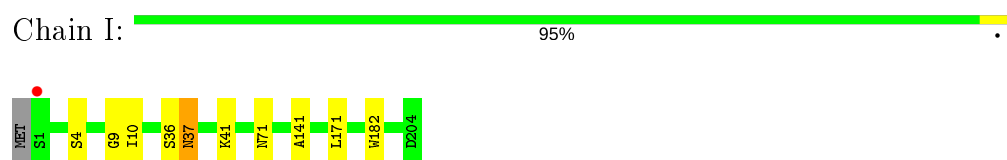
- Molecule 8: Proteasome subunit beta type-10, Proteasome subunit beta type-2



- Molecule 8: Proteasome subunit beta type-10, Proteasome subunit beta type-2



- Molecule 9: Proteasome subunit beta type-3

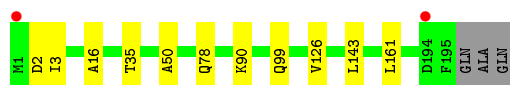
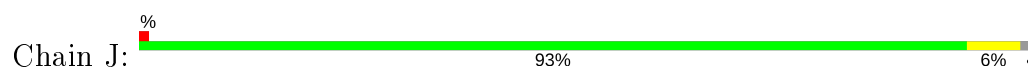


- Molecule 9: Proteasome subunit beta type-3

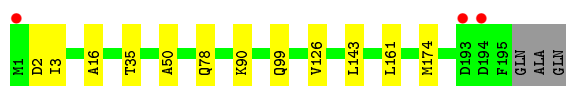




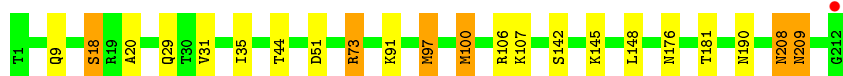
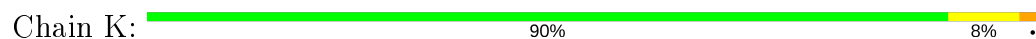
- Molecule 10: Proteasome subunit beta type-4



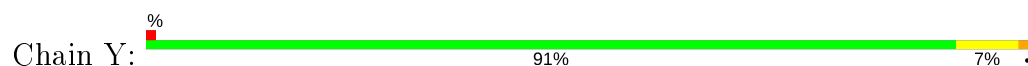
- Molecule 10: Proteasome subunit beta type-4



- Molecule 11: Proteasome subunit beta type-5



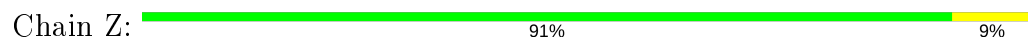
- Molecule 11: Proteasome subunit beta type-5



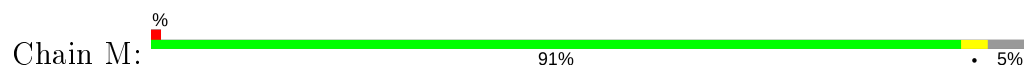
- Molecule 12: Proteasome subunit beta type-6



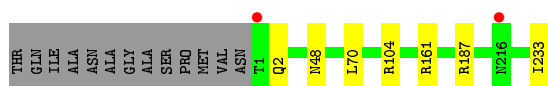
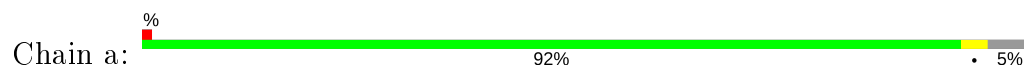
- Molecule 12: Proteasome subunit beta type-6



- 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	135.56Å 300.05Å 144.50Å 90.00° 112.92° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 15.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.2 (15.00-2.90) 97.9 (15.00-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.179 , 0.206 0.185 , 0.211	Depositor DCC
R_{free} test set	11374 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	59.6	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	49836	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% 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, GT5, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.37	0/1952	0.57	0/2642
1	O	0.36	0/1952	0.57	0/2642
2	B	0.39	0/1934	0.65	1/2618 (0.0%)
2	P	0.39	0/1934	0.67	3/2618 (0.1%)
3	C	0.37	0/1910	0.63	0/2586
3	Q	0.37	0/1910	0.63	0/2586
4	D	0.36	0/1837	0.59	0/2475
4	R	0.35	0/1837	0.59	0/2475
5	E	0.36	0/1800	0.58	1/2433 (0.0%)
5	S	0.35	0/1800	0.58	0/2433
6	F	0.36	0/1932	0.56	0/2609
6	T	0.35	0/1932	0.56	0/2609
7	G	0.37	0/1945	0.58	0/2634
7	U	0.37	0/1945	0.58	0/2634
8	H	0.34	0/1746	0.83	5/2365 (0.2%)
8	V	0.33	0/1718	0.84	4/2329 (0.2%)
9	I	0.36	0/1611	0.59	0/2174
9	W	0.35	0/1611	0.59	0/2174
10	J	0.36	0/1589	0.62	0/2142
10	X	0.36	0/1589	0.62	0/2142
11	K	0.36	0/1681	0.82	5/2274 (0.2%)
11	Y	0.36	0/1681	0.87	3/2274 (0.1%)
12	L	0.37	0/1795	0.62	0/2420
12	Z	0.37	0/1795	0.61	0/2420
13	M	0.38	0/1855	0.64	0/2514
13	a	0.37	0/1855	0.64	0/2514
14	N	0.34	0/1541	0.58	0/2087
14	b	0.34	0/1541	0.59	0/2087
All	All	0.36	0/50228	0.64	22/67910 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
8	H	0	1
8	V	0	1
11	K	0	1
11	Y	0	1
All	All	0	4

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	V	188	ARG	NE-CZ-NH2	-21.00	109.80	120.30
11	Y	73	ARG	NE-CZ-NH1	-20.75	109.92	120.30
8	H	188	ARG	NE-CZ-NH1	-18.72	110.94	120.30
11	K	73	ARG	NE-CZ-NH2	-17.68	111.46	120.30
11	Y	73	ARG	NE-CZ-NH2	17.20	128.90	120.30
8	H	188	ARG	NE-CZ-NH2	14.93	127.76	120.30
8	V	188	ARG	NE-CZ-NH1	14.84	127.72	120.30
11	K	73	ARG	NE-CZ-NH1	13.73	127.16	120.30
8	V	188	ARG	CD-NE-CZ	10.11	137.75	123.60
11	Y	73	ARG	CD-NE-CZ	9.46	136.84	123.60
11	K	73	ARG	CD-NE-CZ	9.37	136.72	123.60
8	H	188	ARG	CD-NE-CZ	8.91	136.07	123.60
8	H	223	ILE	CB-CA-C	-6.89	97.83	111.60
2	P	51	VAL	CB-CA-C	-6.03	99.94	111.40
2	P	224	VAL	CG1-CB-CG2	5.82	120.21	110.90
11	K	97	MET	CG-SD-CE	5.56	109.10	100.20
2	B	224	VAL	CG1-CB-CG2	5.51	119.71	110.90
8	V	196	ARG	NE-CZ-NH1	5.40	123.00	120.30
11	K	97	MET	CB-CG-SD	5.36	128.47	112.40
2	P	51	VAL	CG1-CB-CG2	5.22	119.25	110.90
8	H	196	ARG	NE-CZ-NH1	5.07	122.84	120.30
5	E	71	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	H	188	ARG	Sidechain

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Mol	Chain	Res	Type	Group
11	K	73	ARG	Sidechain
8	V	188	ARG	Sidechain
11	Y	73	ARG	Sidechain

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	1	0
1	O	1915	0	1929	1	0
2	B	1904	0	1904	13	0
2	P	1904	0	1904	12	0
3	C	1881	0	1895	8	0
3	Q	1881	0	1895	6	0
4	D	1813	0	1797	3	0
4	R	1813	0	1797	3	0
5	E	1773	0	1775	6	0
5	S	1773	0	1775	6	0
6	F	1892	0	1883	3	0
6	T	1892	0	1883	4	0
7	G	1907	0	1901	2	0
7	U	1907	0	1901	2	0
8	H	1716	0	1702	8	0
8	V	1688	0	1682	7	0
9	I	1581	0	1574	5	0
9	W	1581	0	1574	4	0
10	J	1561	0	1569	5	0
10	X	1561	0	1569	6	0
11	K	1644	0	1594	14	0
11	Y	1644	0	1594	14	0
12	L	1757	0	1711	10	0
12	Z	1757	0	1711	9	0
13	M	1824	0	1832	0	0
13	a	1824	0	1832	0	0
14	N	1512	0	1481	1	0
14	b	1512	0	1481	0	0
15	G	1	0	0	0	0
15	I	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	40	0	0	0	0
17	K	40	0	0	1	0
17	V	40	0	0	0	0
17	Y	40	0	0	1	0
18	A	9	0	0	0	0
18	B	15	0	0	2	0
18	C	13	0	0	0	0
18	D	6	0	0	0	0
18	E	5	0	0	0	0
18	F	9	0	0	0	0
18	G	17	0	0	0	0
18	H	16	0	0	0	0
18	I	7	0	0	0	0
18	J	19	0	0	0	0
18	K	16	0	0	0	0
18	L	24	0	0	0	0
18	M	19	0	0	0	0
18	N	12	0	0	0	0
18	O	3	0	0	0	0
18	P	9	0	0	2	0
18	Q	8	0	0	0	0
18	R	5	0	0	0	0
18	S	5	0	0	0	0
18	T	10	0	0	1	0
18	U	15	0	0	0	0
18	V	13	0	0	0	0
18	W	8	0	0	0	0
18	X	16	0	0	1	0
18	Y	19	0	0	0	0
18	Z	13	0	0	0	0
18	a	11	0	0	0	0
18	b	12	0	0	0	0
All	All	49836	0	49074	122	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 (122) 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)
11:K:142:SER:OG	10:X:143:LEU:HD21	1.75	0.86
10:J:143:LEU:HD21	11:Y:142:SER:OG	1.77	0.84
2:B:51:VAL:HG22	2:B:51:VAL:O	1.85	0.75
5:E:92:ASN:HD21	12:L:70:ASN:HD21	1.36	0.74
2:P:225:TYR:CD1	8:V:223:ILE:HG13	2.24	0.71
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.55	0.71
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.57	0.69
5:S:92:ASN:HD21	12:Z:70:ASN:HD21	1.41	0.69
2:B:145:TYR:OH	2:B:217:LYS:N	2.27	0.67
2:P:145:TYR:OH	2:P:217:LYS:N	2.27	0.67
3:C:160:GLN:HA	3:C:160:GLN:HE21	1.60	0.65
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.61	0.64
2:P:93:HIS:HB3	18:P:301:HOH:O	1.98	0.64
3:Q:202:GLN:O	3:Q:202:GLN:HG3	1.97	0.63
5:S:12:PHE:H	6:T:19:GLN:HE22	1.46	0.62
2:B:93:HIS:HB3	18:B:301:HOH:O	2.02	0.59
3:C:202:GLN:CG	3:C:202:GLN:O	2.50	0.59
12:Z:42:LYS:HD2	12:Z:55:ASN:HD22	1.67	0.59
2:B:51:VAL:CG2	2:B:51:VAL:O	2.51	0.58
3:Q:202:GLN:O	3:Q:202:GLN:CG	2.50	0.58
5:E:92:ASN:ND2	12:L:70:ASN:HD21	2.01	0.58
3:C:202:GLN:HG3	3:C:202:GLN:O	2.02	0.58
12:L:42:LYS:HD2	12:L:55:ASN:HD22	1.68	0.58
11:K:142:SER:HG	10:X:143:LEU:HD21	1.69	0.58
5:S:92:ASN:HD21	12:Z:70:ASN:ND2	2.01	0.57
5:E:92:ASN:HD21	12:L:70:ASN:ND2	2.00	0.57
2:B:12:PHE:H	3:C:17:GLN:HE22	1.53	0.57
7:G:23:PHE:O	7:G:26:THR:HB	2.05	0.56
6:F:123:ASN:HD22	6:F:124:SER:N	2.04	0.56
5:S:92:ASN:ND2	12:Z:70:ASN:HD21	2.04	0.56
6:T:123:ASN:HD22	6:T:124:SER:N	2.04	0.55
1:O:12:PHE:H	2:P:20:GLN:HE22	1.53	0.55
7:U:23:PHE:O	7:U:26:THR:HB	2.06	0.55
5:E:12:PHE:H	6:F:19:GLN:HE22	1.53	0.55
12:Z:31:THR:CG2	12:Z:36:ASN:HD21	2.21	0.54
11:K:176:ASN:ND2	11:K:190:ASN:HD22	2.06	0.54
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.89	0.53
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.91	0.53
3:Q:198:LEU:HA	3:Q:201:VAL:HG12	1.91	0.53
3:C:198:LEU:HA	3:C:201:VAL:HG12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:223:ILE:H	8:H:223:ILE:HD13	1.75	0.52
11:Y:31:VAL:HG11	17:Y:301:GT5:C23	2.40	0.52
11:K:31:VAL:HG11	17:K:301:GT5:C23	2.40	0.52
10:J:143:LEU:HD21	11:Y:142:SER:HG	1.75	0.52
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.91	0.52
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.91	0.52
11:K:44:THR:HG21	11:K:100:MET:HE3	1.91	0.51
6:T:123:ASN:C	6:T:123:ASN:HD22	2.14	0.51
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.59	0.51
12:L:31:THR:CG2	12:L:36:ASN:HD21	2.23	0.51
2:P:51:VAL:HG12	2:P:51:VAL:O	2.11	0.51
10:X:174:MET:HB2	18:X:209:HOH:O	2.11	0.51
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.41	0.50
11:Y:44:THR:HG21	11:Y:100:MET:HE3	1.92	0.50
11:K:51:ASP:HB3	11:K:97:MET:SD	2.51	0.50
8:V:223:ILE:H	8:V:223:ILE:HD13	1.75	0.50
11:Y:176:ASN:ND2	11:Y:190:ASN:HD22	2.09	0.50
6:F:123:ASN:C	6:F:123:ASN:HD22	2.14	0.50
8:V:223:ILE:HD13	8:V:223:ILE:N	2.27	0.50
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.42	0.50
8:H:223:ILE:N	8:H:223:ILE:HD13	2.28	0.49
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.93	0.49
10:J:50:ALA:O	11:K:91:LYS:NZ	2.46	0.48
2:B:225:TYR:CD1	8:H:223:ILE:HG13	2.48	0.48
11:K:208:ASN:HD22	11:K:208:ASN:N	2.11	0.48
2:B:220:ASN:HB2	8:H:224:GLN:O	2.13	0.48
2:P:95:GLN:HE22	9:W:71:ASN:HD22	1.61	0.47
11:Y:208:ASN:HD22	11:Y:208:ASN:N	2.11	0.47
2:P:145:TYR:HH	2:P:217:LYS:N	2.12	0.47
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.95	0.47
11:K:18:SER:OG	11:K:29:GLN:O	2.32	0.47
2:B:145:TYR:HH	2:B:217:LYS:N	2.12	0.47
8:H:112:SER:HB3	8:H:125:LEU:HD13	1.96	0.47
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.97	0.47
11:K:176:ASN:HD21	11:K:190:ASN:HD22	1.62	0.46
2:P:225:TYR:HD1	8:V:223:ILE:HG13	1.73	0.46
11:Y:145:LYS:HB2	11:Y:148:LEU:CD1	2.46	0.46
10:X:50:ALA:O	11:Y:91:LYS:NZ	2.48	0.46
1:A:12:PHE:H	2:B:20:GLN:HE22	1.63	0.45
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.62	0.45
8:V:84:LYS:HE2	8:V:119:THR:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:9:PHE:H	4:D:15:GLN:HE22	1.62	0.45
2:P:145:TYR:OH	2:P:217:LYS:HB2	2.17	0.45
9:I:37:ASN:ND2	11:Y:209:ASN:O	2.49	0.45
11:Y:18:SER:OG	11:Y:29:GLN:O	2.35	0.45
7:G:167:GLN:HE21	7:G:171:THR:HG23	1.82	0.45
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.98	0.44
6:T:96:LYS:NZ	18:T:301:HOH:O	2.49	0.44
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.98	0.44
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.99	0.44
2:B:113:ARG:NE	18:B:301:HOH:O	2.37	0.44
11:Y:176:ASN:HD21	11:Y:190:ASN:HD22	1.65	0.44
8:H:84:LYS:HE2	8:H:119:THR:HG23	2.00	0.44
2:P:88:ASN:HB3	18:P:308:HOH:O	2.17	0.44
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.99	0.43
11:K:145:LYS:HB2	11:K:148:LEU:CD1	2.47	0.43
2:B:145:TYR:OH	2:B:217:LYS:HB2	2.17	0.43
8:H:7:VAL:HG21	8:H:123:TYR:HD1	1.83	0.43
11:K:100:MET:HB2	11:K:100:MET:HE3	1.87	0.43
8:V:7:VAL:HG21	8:V:123:TYR:HD1	1.84	0.43
9:I:9:GLY:HA3	9:I:41:LYS:HE2	2.01	0.43
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.54	0.43
11:K:209:ASN:N	11:K:209:ASN:HD22	2.16	0.42
11:Y:209:ASN:N	11:Y:209:ASN:HD22	2.17	0.42
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.19	0.42
9:W:36:SER:HB2	10:X:126:VAL:HG11	2.02	0.42
2:B:3:ARG:CZ	5:E:122:TYR:OH	2.67	0.42
9:I:10:ILE:HG21	9:I:141:ALA:HB3	2.02	0.42
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.55	0.42
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.50	0.42
7:U:167:GLN:HE21	7:U:171:THR:HG23	1.85	0.42
9:W:9:GLY:HA3	9:W:41:LYS:HE2	2.02	0.41
3:C:48:SER:HB2	3:C:207:ASN:HD21	1.86	0.41
12:L:8:ASN:HA	12:L:30:ILE:O	2.20	0.41
2:P:3:ARG:CZ	5:S:122:TYR:OH	2.68	0.41
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.69	0.41
9:W:10:ILE:HG21	9:W:141:ALA:HB3	2.02	0.41
12:L:3:ASN:HD22	12:L:4:PRO:HD2	1.86	0.41
11:Y:100:MET:HE3	11:Y:100:MET:HB2	1.93	0.41
8:H:192:THR:HG22	8:H:195:VAL:HG13	2.02	0.41
9:I:36:SER:HB2	10:J:126:VAL:HG11	2.03	0.41
3:C:77:ASN:N	3:C:77:ASN:HD22	2.19	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%)	242 (98%)	6 (2%)	0	100	100
1	O	248/250 (99%)	242 (98%)	6 (2%)	0	100	100
2	B	242/258 (94%)	232 (96%)	10 (4%)	0	100	100
2	P	242/258 (94%)	232 (96%)	10 (4%)	0	100	100
3	C	238/254 (94%)	234 (98%)	3 (1%)	1 (0%)	34	66
3	Q	238/254 (94%)	235 (99%)	2 (1%)	1 (0%)	34	66
4	D	231/260 (89%)	225 (97%)	6 (3%)	0	100	100
4	R	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
5	E	229/234 (98%)	221 (96%)	8 (4%)	0	100	100
5	S	229/234 (98%)	221 (96%)	8 (4%)	0	100	100
6	F	241/288 (84%)	239 (99%)	2 (1%)	0	100	100
6	T	241/288 (84%)	239 (99%)	2 (1%)	0	100	100
7	G	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
7	U	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
8	H	224/226 (99%)	218 (97%)	5 (2%)	1 (0%)	34	66
8	V	221/226 (98%)	216 (98%)	5 (2%)	0	100	100
9	I	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
9	W	202/205 (98%)	194 (96%)	8 (4%)	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%)	207 (99%)	3 (1%)	0	100	100
11	Y	210/212 (99%)	207 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	L	220/222 (99%)	214 (97%)	5 (2%)	1 (0%)	29	61
12	Z	220/222 (99%)	214 (97%)	5 (2%)	1 (0%)	29	61
13	M	231/246 (94%)	223 (96%)	8 (4%)	0	100	100
13	a	231/246 (94%)	224 (97%)	7 (3%)	0	100	100
14	N	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
14	b	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
All	All	6281/6602 (95%)	6128 (98%)	148 (2%)	5 (0%)	51	82

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	223	ILE
3	C	204	GLY
3	Q	204	GLY
12	L	166	GLY
12	Z	166	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%)	205 (98%)	4 (2%)	57	84
1	O	209/209 (100%)	205 (98%)	4 (2%)	57	84
2	B	203/216 (94%)	193 (95%)	10 (5%)	25	57
2	P	203/216 (94%)	194 (96%)	9 (4%)	28	61
3	C	212/226 (94%)	201 (95%)	11 (5%)	23	55
3	Q	212/226 (94%)	201 (95%)	11 (5%)	23	55
4	D	194/215 (90%)	185 (95%)	9 (5%)	27	60
4	R	194/215 (90%)	185 (95%)	9 (5%)	27	60
5	E	190/193 (98%)	182 (96%)	8 (4%)	30	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	S	190/193 (98%)	182 (96%)	8 (4%)	30	63
6	F	201/239 (84%)	192 (96%)	9 (4%)	27	61
6	T	201/239 (84%)	192 (96%)	9 (4%)	27	61
7	G	206/210 (98%)	198 (96%)	8 (4%)	32	66
7	U	206/210 (98%)	198 (96%)	8 (4%)	32	66
8	H	184/184 (100%)	173 (94%)	11 (6%)	19	49
8	V	181/184 (98%)	170 (94%)	11 (6%)	18	48
9	I	172/173 (99%)	168 (98%)	4 (2%)	50	80
9	W	172/173 (99%)	168 (98%)	4 (2%)	50	80
10	J	173/175 (99%)	167 (96%)	6 (4%)	36	70
10	X	173/175 (99%)	167 (96%)	6 (4%)	36	70
11	K	169/169 (100%)	160 (95%)	9 (5%)	22	54
11	Y	169/169 (100%)	160 (95%)	9 (5%)	22	54
12	L	185/185 (100%)	174 (94%)	11 (6%)	19	49
12	Z	185/185 (100%)	174 (94%)	11 (6%)	19	49
13	M	199/208 (96%)	191 (96%)	8 (4%)	31	65
13	a	199/208 (96%)	192 (96%)	7 (4%)	36	70
14	N	162/162 (100%)	158 (98%)	4 (2%)	47	78
14	b	162/162 (100%)	158 (98%)	4 (2%)	47	78
All	All	5315/5528 (96%)	5093 (96%)	222 (4%)	30	63

All (222) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
2	B	50	LYS
2	B	51	VAL
2	B	52	THR
2	B	55	LEU
2	B	102	ASN
2	B	113	ARG
2	B	119	GLN

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Mol	Chain	Res	Type
2	B	191	LEU
2	B	223	GLU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	48	SER
3	C	49	THR
3	C	51	LYS
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	240	GLU
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	8	ASP
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
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	171	GLU
6	F	172	LEU
6	F	181	GLU
6	F	214	TRP
6	F	221	ASN
6	F	240	GLN
7	G	83	ASN
7	G	115	LEU

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Mol	Chain	Res	Type
7	G	117	GLN
7	G	122	ARG
7	G	125	MET
7	G	208	GLU
7	G	235	ARG
7	G	236	LEU
8	H	9	GLN
8	H	22	ASN
8	H	23	ASP
8	H	68	LEU
8	H	103	VAL
8	H	118	SER
8	H	127	LEU
8	H	144	GLN
8	H	196	ARG
8	H	222	ASP
8	H	223	ILE
9	I	4	SER
9	I	37	ASN
9	I	171	LEU
9	I	182	TRP
10	J	2	ASP
10	J	3	ILE
10	J	35	THR
10	J	78	GLN
10	J	90	LYS
10	J	99	GLN
11	K	9	GLN
11	K	18	SER
11	K	35	ILE
11	K	100	MET
11	K	106	ARG
11	K	107	LYS
11	K	181	THR
11	K	208	ASN
11	K	209	ASN
12	L	18	GLU
12	L	23	LEU
12	L	49	ASN
12	L	106	TYR
12	L	130	SER
12	L	135	GLN

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Mol	Chain	Res	Type
12	L	136	CYS
12	L	144	SER
12	L	150	LEU
12	L	172	LEU
12	L	179	GLU
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	85	GLU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
13	M	233	ILE
14	N	9	LYS
14	N	83	LYS
14	N	104	ASP
14	N	107	LYS
1	O	2	THR
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	50	LYS
2	P	52	THR
2	P	55	LEU
2	P	102	ASN
2	P	113	ARG
2	P	119	GLN
2	P	191	LEU
2	P	223	GLU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	48	SER
3	Q	49	THR
3	Q	51	LYS
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	240	GLU
4	R	99	ILE

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Mol	Chain	Res	Type
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	8	ASP
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
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	171	GLU
6	T	172	LEU
6	T	181	GLU
6	T	214	TRP
6	T	221	ASN
6	T	240	GLN
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	9	GLN
8	V	22	ASN
8	V	23	ASP
8	V	68	LEU
8	V	103	VAL
8	V	118	SER
8	V	127	LEU
8	V	144	GLN
8	V	196	ARG

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Mol	Chain	Res	Type
8	V	222	ASP
8	V	223	ILE
9	W	4	SER
9	W	37	ASN
9	W	171	LEU
9	W	182	TRP
10	X	2	ASP
10	X	3	ILE
10	X	35	THR
10	X	78	GLN
10	X	90	LYS
10	X	99	GLN
11	Y	9	GLN
11	Y	18	SER
11	Y	35	ILE
11	Y	73	ARG
11	Y	100	MET
11	Y	106	ARG
11	Y	107	LYS
11	Y	208	ASN
11	Y	209	ASN
12	Z	18	GLU
12	Z	23	LEU
12	Z	49	ASN
12	Z	106	TYR
12	Z	130	SER
12	Z	135	GLN
12	Z	136	CYS
12	Z	144	SER
12	Z	150	LEU
12	Z	172	LEU
12	Z	179	GLU
13	a	2	GLN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
13	a	233	ILE
14	b	9	LYS
14	b	83	LYS
14	b	104	ASP

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Mol	Chain	Res	Type
14	b	107	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (125) such sidechains are listed below:

Mol	Chain	Res	Type
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	38	ASN
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	91	HIS
4	D	100	ASN
4	D	146	GLN
4	D	160	ASN
4	D	225	ASN
5	E	68	HIS
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
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

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Mol	Chain	Res	Type
7	G	167	GLN
7	G	175	ASN
8	H	22	ASN
8	H	165	ASN
8	H	172	ASN
10	J	55	GLN
11	K	9	GLN
11	K	85	ASN
11	K	176	ASN
11	K	209	ASN
12	L	3	ASN
12	L	49	ASN
12	L	55	ASN
12	L	70	ASN
12	L	79	HIS
12	L	152	ASN
12	L	153	GLN
12	L	158	ASN
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
14	N	161	GLN
2	P	20	GLN
2	P	58	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	155	ASN
2	P	176	GLN
3	Q	17	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
4	R	146	GLN
4	R	225	ASN

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Mol	Chain	Res	Type
5	S	59	GLN
5	S	68	HIS
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
7	U	175	ASN
8	V	22	ASN
8	V	165	ASN
10	X	55	GLN
10	X	78	GLN
10	X	86	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	176	ASN
11	Y	209	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	55	ASN
12	Z	70	ASN
12	Z	152	ASN
12	Z	153	GLN
12	Z	158	ASN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN

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Mol	Chain	Res	Type
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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 10 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	GT5	Y	301	11	38,41,41	1.62	7 (18%)	48,56,56	1.61	11 (22%)
17	GT5	V	301	8	38,41,41	1.56	7 (18%)	48,56,56	1.53	11 (22%)
17	GT5	K	301	11	38,41,41	1.58	6 (15%)	48,56,56	1.57	11 (22%)
17	GT5	H	301	8	38,41,41	1.57	7 (18%)	48,56,56	1.47	9 (18%)

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	GT5	Y	301	11	-	5/39/43/43	0/2/2/2
17	GT5	V	301	8	-	6/39/43/43	0/2/2/2
17	GT5	K	301	11	-	4/39/43/43	0/2/2/2
17	GT5	H	301	8	-	6/39/43/43	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Y	301	GT5	C16-C17	-4.61	1.40	1.51
17	H	301	GT5	C16-C17	-4.36	1.40	1.51
17	K	301	GT5	C16-C17	-4.34	1.40	1.51
17	V	301	GT5	C16-C17	-4.23	1.41	1.51
17	Y	301	GT5	O30-S27	4.12	1.53	1.44
17	Y	301	GT5	O29-S27	4.05	1.53	1.44
17	K	301	GT5	O30-S27	3.94	1.53	1.44
17	K	301	GT5	O29-S27	3.67	1.52	1.44
17	H	301	GT5	C3-S5	-3.64	1.62	1.73
17	K	301	GT5	C3-S5	-3.62	1.62	1.73
17	H	301	GT5	O29-S27	3.60	1.52	1.44
17	V	301	GT5	O30-S27	3.60	1.52	1.44
17	V	301	GT5	O29-S27	3.47	1.52	1.44
17	Y	301	GT5	C26-S27	3.32	1.82	1.78
17	V	301	GT5	C26-S27	3.31	1.82	1.78
17	H	301	GT5	O30-S27	3.22	1.51	1.44
17	V	301	GT5	C3-S5	-3.22	1.63	1.73
17	H	301	GT5	C26-S27	3.22	1.82	1.78
17	H	301	GT5	C21-C20	-3.11	1.40	1.51
17	V	301	GT5	C21-C20	-3.00	1.40	1.51
17	K	301	GT5	C26-S27	2.94	1.82	1.78
17	K	301	GT5	C21-C20	-2.79	1.41	1.51
17	Y	301	GT5	C21-C20	-2.76	1.41	1.51
17	V	301	GT5	C4-C3	2.66	1.54	1.49
17	Y	301	GT5	C3-S5	-2.65	1.65	1.73
17	Y	301	GT5	C25-C26	2.48	1.55	1.52
17	H	301	GT5	C4-C3	2.25	1.53	1.49

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	H	301	GT5	O30-S27-O29	-4.42	107.66	117.09
17	V	301	GT5	O30-S27-O29	-4.24	108.02	117.09
17	Y	301	GT5	O29-S27-C26	-4.03	105.52	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	K	301	GT5	C32-C12-C13	-3.69	101.66	110.32
17	Y	301	GT5	C32-C12-C13	-3.49	102.13	110.32
17	K	301	GT5	O30-S27-O29	-3.37	109.89	117.09
17	V	301	GT5	O29-S27-C28	-3.31	105.58	108.91
17	K	301	GT5	O29-S27-C26	-3.23	106.08	108.34
17	H	301	GT5	O30-S27-C26	3.09	110.51	108.34
17	Y	301	GT5	O30-S27-C26	3.04	110.47	108.34
17	V	301	GT5	C32-C12-N11	-2.97	104.50	111.40
17	Y	301	GT5	C40-C9-C10	-2.90	103.65	110.57
17	H	301	GT5	C32-C12-N11	-2.90	104.64	111.40
17	K	301	GT5	C40-C9-C10	-2.80	103.90	110.57
17	Y	301	GT5	C4-C3-S5	2.79	123.86	120.12
17	Y	301	GT5	O30-S27-O29	-2.76	111.20	117.09
17	K	301	GT5	O30-S27-C26	2.70	110.24	108.34
17	K	301	GT5	C25-C15-N14	-2.65	106.82	110.54
17	Y	301	GT5	C25-C15-N14	-2.62	106.85	110.54
17	V	301	GT5	O30-S27-C28	2.57	111.49	108.91
17	K	301	GT5	C4-C3-S5	2.53	123.52	120.12
17	H	301	GT5	O29-S27-C26	-2.50	106.59	108.34
17	V	301	GT5	O30-S27-C26	2.48	110.08	108.34
17	H	301	GT5	C40-C9-N8	-2.44	104.96	110.58
17	V	301	GT5	C40-C9-N8	-2.42	105.01	110.58
17	Y	301	GT5	C6-C1-N2	2.42	113.94	109.09
17	V	301	GT5	C28-S27-C26	2.40	114.47	105.21
17	Y	301	GT5	C40-C9-N8	2.35	115.99	110.58
17	K	301	GT5	C40-C9-N8	2.31	115.90	110.58
17	H	301	GT5	C28-S27-C26	2.29	114.03	105.21
17	V	301	GT5	C10-C9-N8	-2.25	105.02	111.16
17	H	301	GT5	C10-C9-N8	-2.23	105.10	111.16
17	Y	301	GT5	C9-C10-N11	-2.22	111.82	116.70
17	V	301	GT5	O29-S27-C26	-2.21	106.80	108.34
17	K	301	GT5	C28-S27-C26	2.12	113.40	105.21
17	V	301	GT5	C4-C3-N2	2.10	127.38	121.87
17	K	301	GT5	C6-C1-N2	2.08	113.27	109.09
17	Y	301	GT5	C28-S27-C26	2.07	113.18	105.21
17	K	301	GT5	C9-C10-N11	-2.04	112.22	116.70
17	H	301	GT5	C4-C3-N2	2.04	127.24	121.87
17	V	301	GT5	C16-C15-N14	-2.02	106.51	110.39
17	H	301	GT5	C16-C15-N14	-2.01	106.52	110.39

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	K	301	GT5	C25-C26-S27-O29
17	K	301	GT5	C25-C26-S27-O30
17	Y	301	GT5	C25-C26-S27-O29
17	Y	301	GT5	C25-C26-S27-O30
17	Y	301	GT5	C15-C16-C17-C24
17	K	301	GT5	C15-C16-C17-C24
17	V	301	GT5	C15-C16-C17-C24
17	H	301	GT5	C15-C16-C17-C24
17	K	301	GT5	C15-C16-C17-C18
17	Y	301	GT5	C15-C16-C17-C18
17	V	301	GT5	C15-C16-C17-C18
17	H	301	GT5	C15-C16-C17-C18
17	H	301	GT5	C25-C26-S27-C28
17	V	301	GT5	C25-C26-S27-C28
17	H	301	GT5	C41-C40-C9-C10
17	V	301	GT5	C41-C40-C9-C10
17	H	301	GT5	C25-C26-S27-O30
17	V	301	GT5	C25-C26-S27-O30
17	H	301	GT5	C12-C32-O36-C34
17	V	301	GT5	C12-C32-O36-C34
17	Y	301	GT5	C25-C26-S27-C28

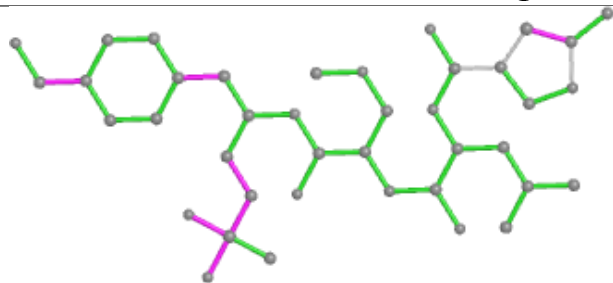
There are no ring outliers.

2 monomers are involved in 2 short contacts:

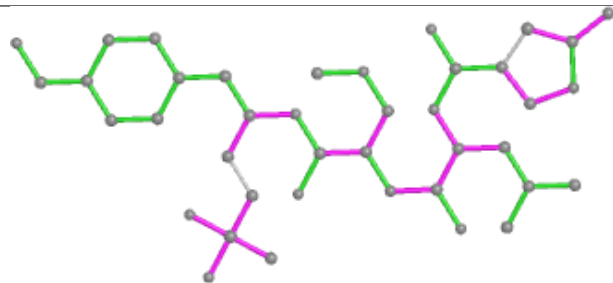
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	Y	301	GT5	1	0
17	K	301	GT5	1	0

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.

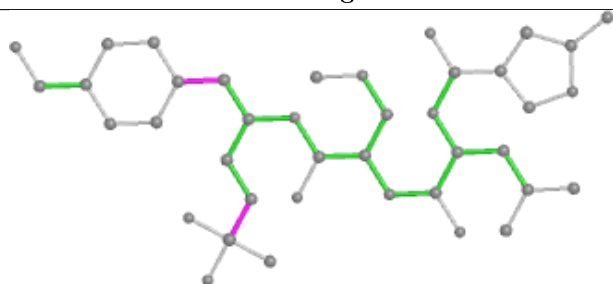
Ligand GT5 Y 301



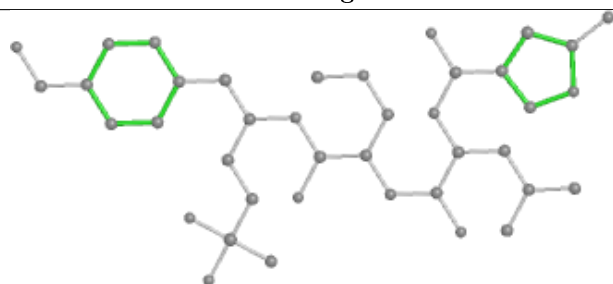
Bond lengths



Bond angles

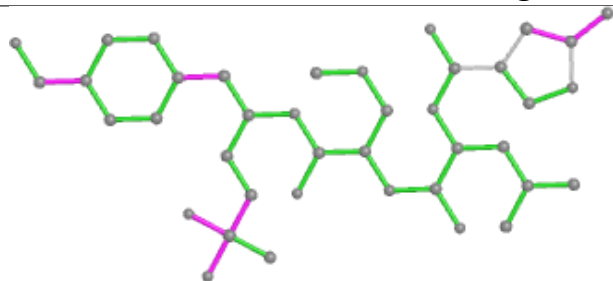


Torsions

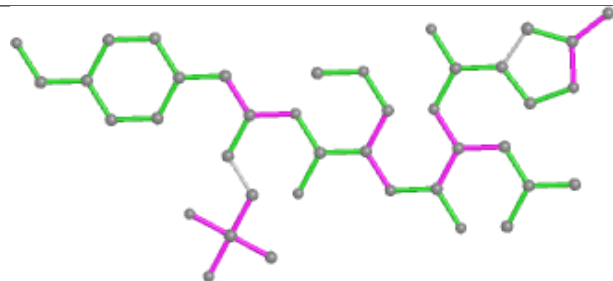


Rings

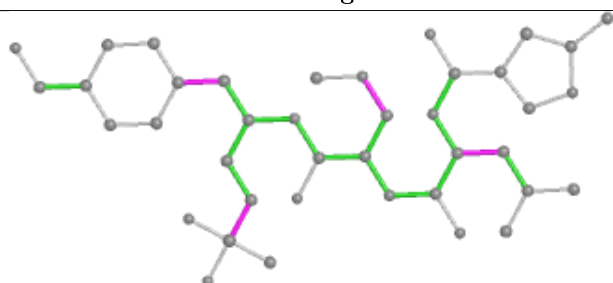
Ligand GT5 V 301



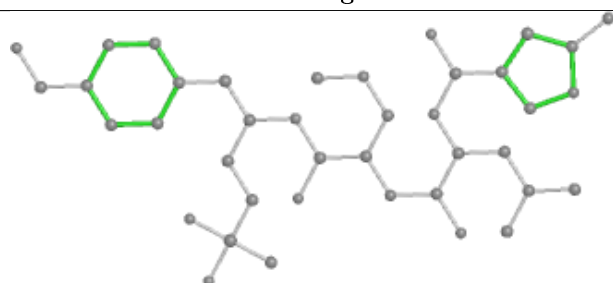
Bond lengths



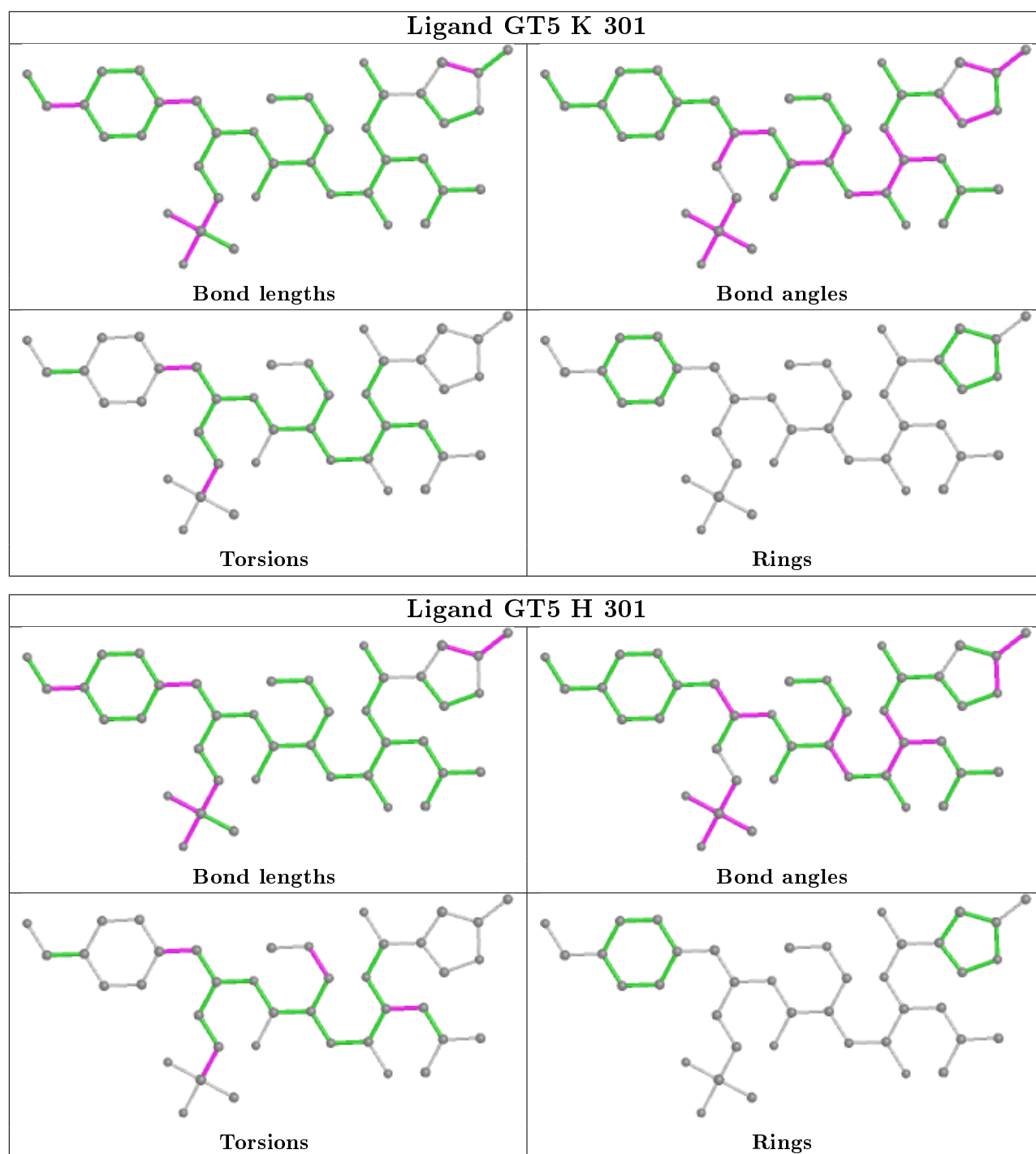
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/250 (100%)	-0.34	7 (2%) 53 49	42, 60, 98, 119	0
1	O	250/250 (100%)	-0.27	8 (3%) 47 43	48, 69, 108, 132	0
2	B	244/258 (94%)	-0.30	8 (3%) 46 41	43, 63, 104, 121	0
2	P	244/258 (94%)	-0.25	13 (5%) 26 22	49, 68, 105, 127	0
3	C	240/254 (94%)	-0.18	14 (5%) 23 19	42, 69, 122, 161	0
3	Q	240/254 (94%)	0.06	14 (5%) 23 19	52, 85, 152, 194	0
4	D	235/260 (90%)	-0.35	2 (0%) 84 84	51, 70, 99, 137	0
4	R	235/260 (90%)	-0.22	7 (2%) 50 45	58, 77, 107, 144	0
5	E	231/234 (98%)	-0.21	3 (1%) 77 77	53, 73, 110, 130	0
5	S	231/234 (98%)	-0.10	7 (3%) 50 45	59, 84, 128, 149	0
6	F	243/288 (84%)	-0.38	6 (2%) 57 55	44, 67, 109, 128	0
6	T	243/288 (84%)	-0.32	4 (1%) 72 71	50, 76, 123, 151	0
7	G	241/252 (95%)	-0.42	3 (1%) 79 79	43, 62, 97, 133	0
7	U	241/252 (95%)	-0.37	4 (1%) 70 69	47, 65, 97, 133	0
8	H	226/226 (100%)	-0.34	8 (3%) 44 38	45, 58, 91, 145	0
8	V	223/226 (98%)	-0.45	3 (1%) 77 77	43, 60, 86, 127	0
9	I	204/205 (99%)	-0.67	1 (0%) 91 91	40, 54, 78, 93	0
9	W	204/205 (99%)	-0.66	2 (0%) 82 82	40, 56, 80, 97	0
10	J	195/198 (98%)	-0.46	2 (1%) 82 82	43, 59, 83, 99	0
10	X	195/198 (98%)	-0.36	3 (1%) 73 73	45, 61, 85, 108	0
11	K	212/212 (100%)	-0.57	1 (0%) 91 91	42, 56, 83, 98	0
11	Y	212/212 (100%)	-0.58	2 (0%) 84 84	45, 59, 86, 101	0
12	L	222/222 (100%)	-0.54	0 100 100	43, 59, 88, 103	0
12	Z	222/222 (100%)	-0.53	1 (0%) 91 91	43, 59, 91, 106	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.52	3 (1%)	77 77	40, 57, 84, 99	0
13	a	233/246 (94%)	-0.52	2 (0%)	84 84	40, 58, 83, 97	0
14	N	196/196 (100%)	-0.57	1 (0%)	91 91	42, 54, 81, 94	0
14	b	196/196 (100%)	-0.55	1 (0%)	91 91	41, 56, 83, 97	0
All	All	6341/6602 (96%)	-0.38	130 (2%)	63 61	40, 64, 107, 194	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	H	224	GLN	10.3
2	P	220	ASN	7.1
3	Q	50	LEU	6.3
2	B	221	ASP	5.8
3	Q	49	THR	5.7
8	H	226	GLU	5.7
2	B	220	ASN	5.6
2	P	52	THR	5.1
8	H	225	GLU	5.1
2	P	221	ASP	4.9
10	X	1	MET	4.8
5	E	202	ASP	4.7
1	A	228	PRO	4.7
1	A	229	THR	4.6
3	Q	206	LYS	4.4
8	V	223	ILE	4.4
1	O	249	ALA	4.4
3	Q	240	GLU	4.4
1	O	229	THR	4.4
3	Q	202	GLN	4.4
10	J	1	MET	4.4
5	S	202	ASP	4.2
8	H	222	ASP	4.1
8	V	222	ASP	4.0
2	P	219	ALA	4.0
3	Q	236	GLN	3.9
5	S	54	GLU	3.9
1	O	231	LYS	3.9
8	V	221	CYS	3.9
1	O	228	PRO	3.9
3	C	202	GLN	3.8
3	Q	239	GLN	3.8

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Mol	Chain	Res	Type	RSRZ
3	C	238	LYS	3.6
6	F	205	GLU	3.6
5	S	225	ASP	3.5
7	U	242	GLN	3.5
10	X	194	ASP	3.5
11	K	212	GLY	3.4
3	C	49	THR	3.3
1	A	201	GLU	3.3
13	a	1	THR	3.3
1	A	249	ALA	3.3
3	Q	238	LYS	3.2
6	T	244	ASN	3.2
8	H	221	CYS	3.1
14	b	195	GLN	3.1
2	P	59	ASP	3.1
13	M	47	ASP	3.1
3	C	236	GLN	3.1
9	W	1	SER	3.1
1	O	201	GLU	3.0
7	G	240	ALA	3.0
13	M	1	THR	3.0
8	H	223	ILE	2.9
1	O	250	LEU	2.9
3	C	50	LEU	2.9
2	B	52	THR	2.8
5	E	201	ARG	2.8
10	X	193	ASP	2.8
6	F	202	ASP	2.7
4	R	241	ALA	2.7
4	D	242	GLU	2.7
7	G	242	GLN	2.7
5	E	233	ILE	2.6
14	N	105	LYS	2.6
3	C	216	ASP	2.6
1	A	1	MET	2.6
3	Q	48	SER	2.6
4	R	1	ASP	2.6
6	F	241	LYS	2.6
2	B	51	VAL	2.5
2	B	203	SER	2.5
6	F	181	GLU	2.5
4	D	1	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
6	T	2	THR	2.5
3	C	235	GLU	2.4
1	O	52	SER	2.4
13	M	216	ASN	2.4
5	S	173	ARG	2.4
7	U	181	LYS	2.4
1	A	231	LYS	2.4
2	P	230	LYS	2.3
1	O	1	MET	2.3
5	S	187	GLU	2.3
2	P	51	VAL	2.3
5	S	165	GLN	2.3
4	R	54	ASP	2.3
2	B	217	LYS	2.3
4	R	116	GLY	2.2
6	F	2	THR	2.2
5	S	180	LYS	2.2
3	C	239	GLN	2.2
6	F	244	ASN	2.2
7	G	222	ASP	2.2
3	C	59	PRO	2.2
4	R	242	GLU	2.2
10	J	194	ASP	2.2
6	T	201	GLU	2.2
8	H	198	GLU	2.2
2	P	225	TYR	2.2
13	a	216	ASN	2.2
4	R	125	LEU	2.2
9	I	1	SER	2.2
3	C	175	LYS	2.2
3	Q	181	GLU	2.2
3	Q	187	GLU	2.2
6	T	181	GLU	2.1
3	Q	223	SER	2.1
2	P	222	GLY	2.1
7	U	222	ASP	2.1
2	P	217	LYS	2.1
11	Y	106	ARG	2.1
3	C	27	ARG	2.1
9	W	160	GLU	2.1
12	Z	1	GLN	2.1
2	P	60	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	218	GLY	2.1
3	C	48	SER	2.1
8	H	10	ASP	2.1
4	R	141	ALA	2.1
1	A	248	GLU	2.1
11	Y	212	GLY	2.1
3	Q	235	GLU	2.0
3	C	1	GLY	2.0
3	C	204	GLY	2.0
7	U	230	GLU	2.0
2	P	61	SER	2.0
2	P	182	ASP	2.0
3	Q	237	GLU	2.0
2	B	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 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
17	GT5	H	301	40/40	0.88	0.23	48,71,76,79	0
15	MG	I	302	1/1	0.89	0.19	66,66,66,66	0
17	GT5	V	301	40/40	0.91	0.19	40,63,68,71	0
15	MG	K	302	1/1	0.93	0.08	60,60,60,60	0
15	MG	W	301	1/1	0.94	0.34	75,75,75,75	0
17	GT5	Y	301	40/40	0.94	0.17	39,50,60,67	0
15	MG	N	201	1/1	0.94	0.17	54,54,54,54	0
15	MG	Z	301	1/1	0.95	0.26	64,64,64,64	0
17	GT5	K	301	40/40	0.95	0.16	39,51,60,65	0

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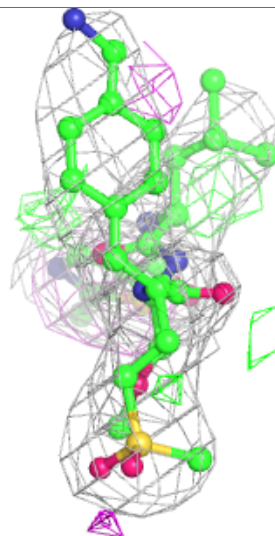
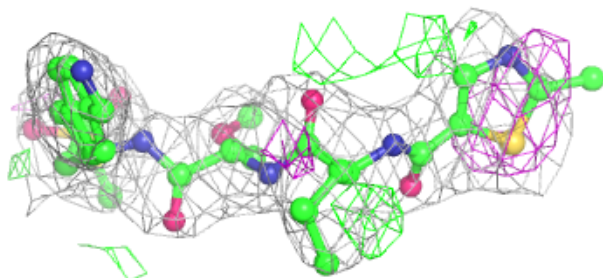
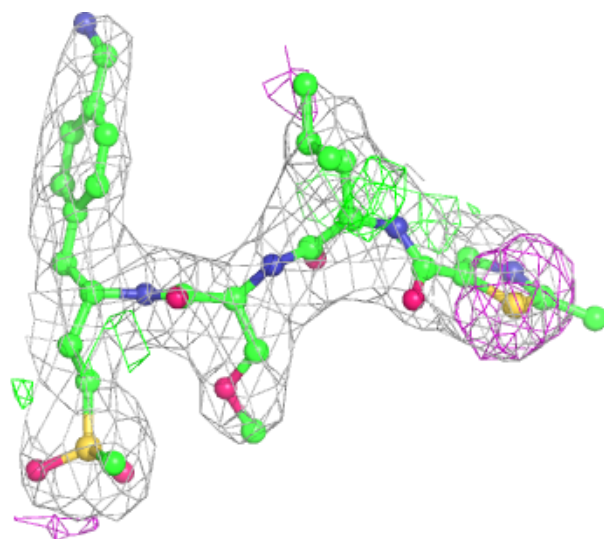
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
15	MG	L	301	1/1	0.96	0.11	65,65,65,65	0
15	MG	I	301	1/1	0.97	0.26	63,63,63,63	0
15	MG	G	301	1/1	0.97	0.06	56,56,56,56	0
16	CL	G	302	1/1	0.98	0.08	45,45,45,45	0
16	CL	U	301	1/1	0.99	0.17	52,52,52,52	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.

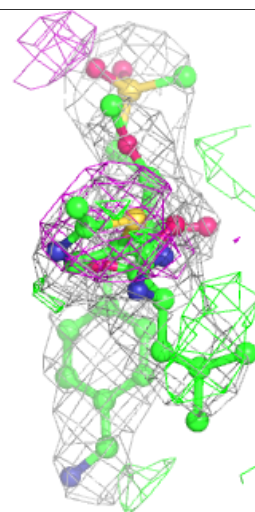
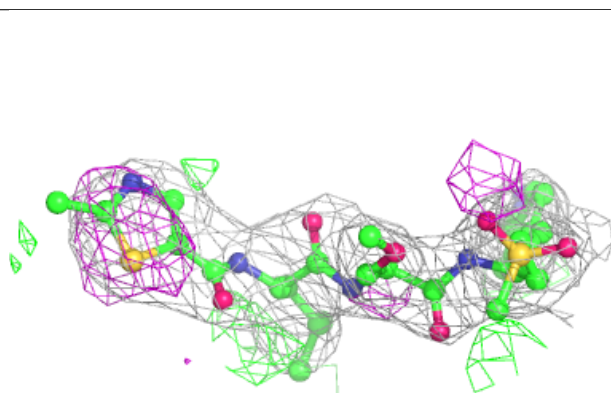
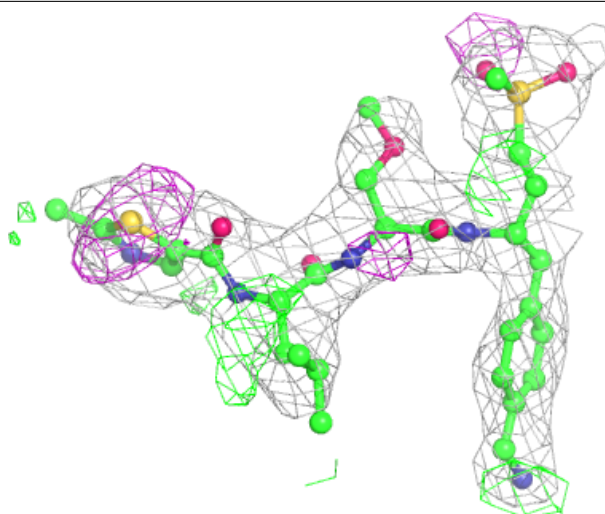
Electron density around GT5 H 301:

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



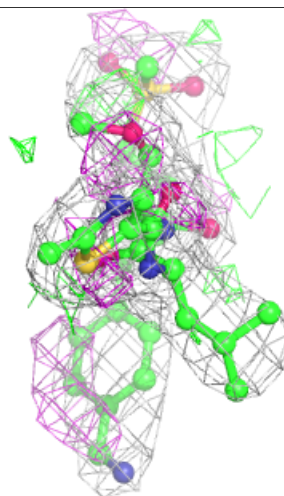
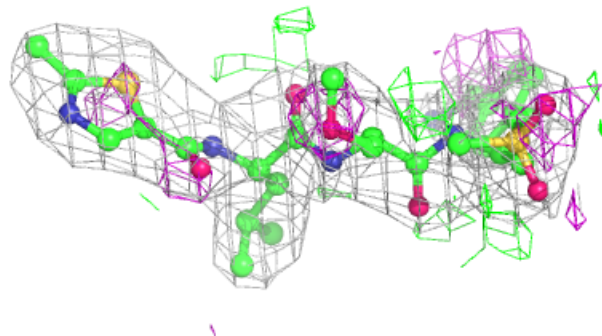
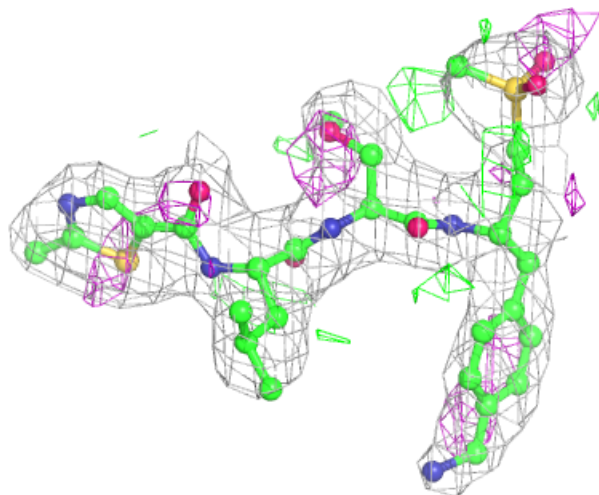
Electron density around GT5 V 301:

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



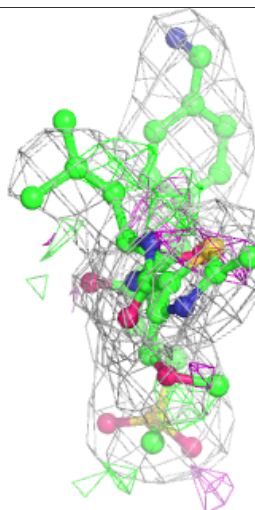
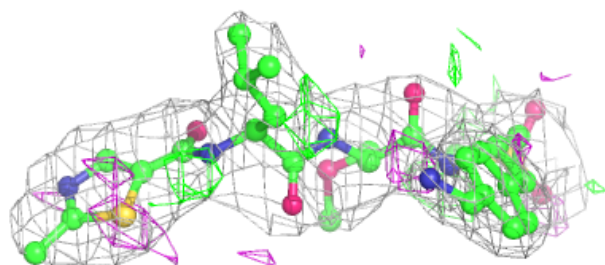
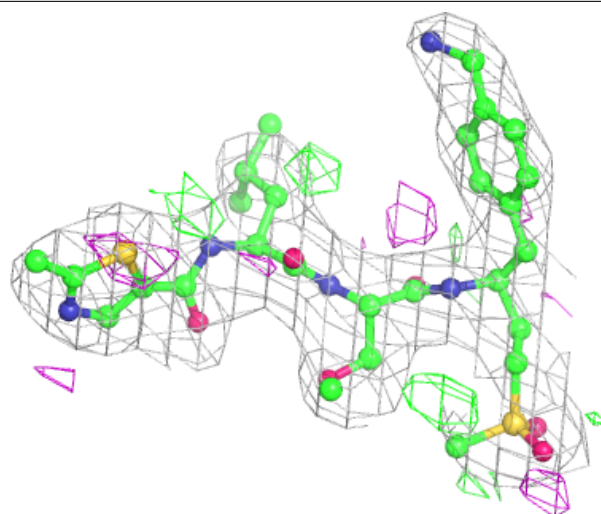
Electron density around GT5 Y 301:

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



Electron density around GT5 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.