



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 10:07 pm BST

PDB ID : 6HWE
Title : Yeast 20S proteasome beta2-G45A mutant in complex with carfilzomib
Authors : Huber, E.M.; Groll, M.
Deposited on : 2018-10-11
Resolution : 2.30 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

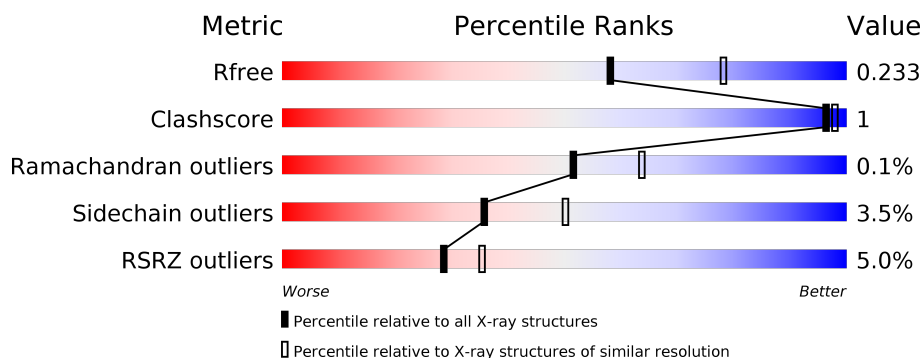
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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>4%</div> <div>98%</div> <div>•</div> </div>
1	O	250	<div> <div>5%</div> <div>98%</div> <div>•</div> </div>
2	B	258	<div> <div>7%</div> <div>88%</div> <div>6% 5%</div> </div>
2	P	258	<div> <div>8%</div> <div>89%</div> <div>5% 5%</div> </div>
3	C	254	<div> <div>9%</div> <div>88%</div> <div>6% 6%</div> </div>
3	Q	254	<div> <div>15%</div> <div>89%</div> <div>5% 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	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	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	MES	V	302	-	-	-	X

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 52005 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	226	Total	C	N	O	S	0	0	0
			1720	1083	298	332	7			
8	V	226	Total	C	N	O	S	0	0	0
			1720	1083	298	332	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	45	ALA	GLY	engineered mutation	UNP P25043
V	45	ALA	GLY	engineered mutation	UNP P25043

- 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			
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			

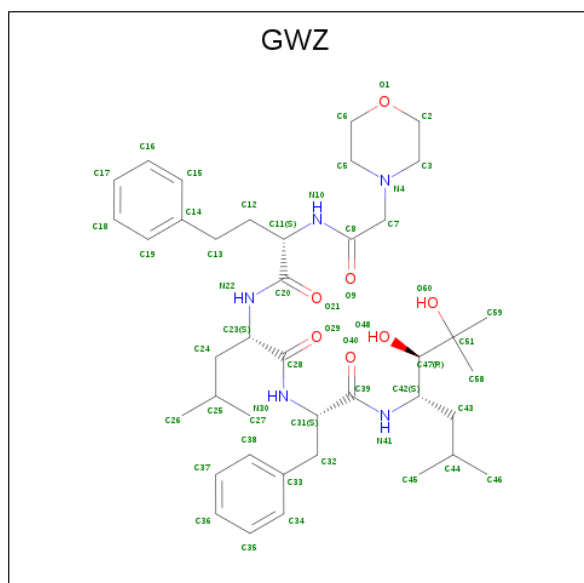
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

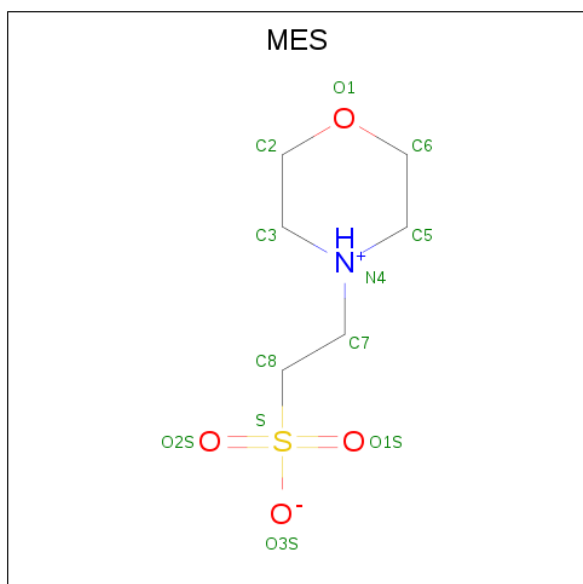
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total Cl 1 1	0	0
16	U	1	Total Cl 1 1	0	0

- Molecule 17 is (2 {S})- {N}-[(2 {S})-1-[(3 {R},4 {S})-2,6-dimethyl-2,3-bis(oxidanyl)heptan-4-yl]amino]-1-oxidanylidene-3-phenyl-propan-2-yl]-4-methyl-2-[(2 {S})-2-(2-morpholin-4-yl ethanoylamino)-4-phenyl-butanoyl]amino]pentanamide (three-letter code: GWZ) (formula: C₄₀H₆₁N₅O₇).



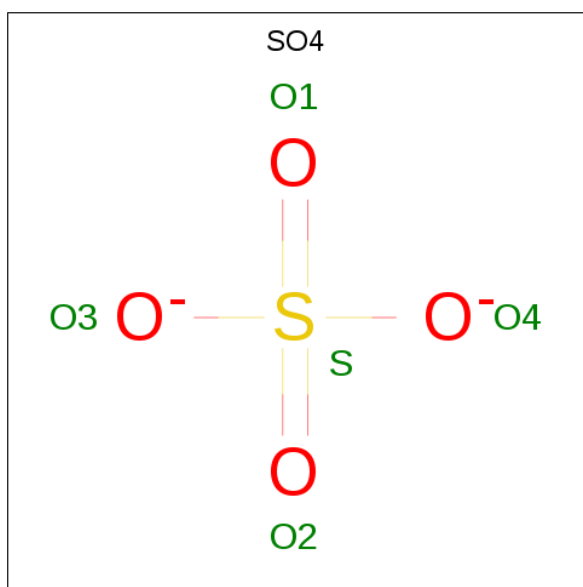
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	H	1	Total	C	N	O	0	0
			52	40	5	7		
17	K	1	Total	C	N	O	0	0
			52	40	5	7		
17	N	1	Total	C	N	O	0	0
			52	40	5	7		
17	V	1	Total	C	N	O	0	0
			52	40	5	7		
17	Y	1	Total	C	N	O	0	0
			52	40	5	7		
17	b	1	Total	C	N	O	0	0
			52	40	5	7		

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



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

- Molecule 19 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	123	Total	O	0	0
			123	123		
20	B	76	Total	O	0	0
			76	76		
20	C	61	Total	O	0	0
			61	61		
20	D	59	Total	O	0	0
			59	59		
20	E	34	Total	O	0	0
			34	34		
20	F	74	Total	O	0	0
			74	74		
20	G	98	Total	O	0	0
			98	98		
20	H	108	Total	O	0	0
			108	108		
20	I	84	Total	O	0	0
			84	84		
20	J	88	Total	O	0	0
			88	88		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	K	103	Total 103	O 103	0	0
20	L	104	Total 104	O 104	0	0
20	M	113	Total 113	O 113	0	0
20	N	94	Total 94	O 94	0	0
20	O	70	Total 70	O 70	0	0
20	P	55	Total 55	O 55	0	0
20	Q	43	Total 43	O 43	0	0
20	R	56	Total 56	O 56	0	0
20	S	39	Total 39	O 39	0	0
20	T	66	Total 66	O 66	0	0
20	U	104	Total 104	O 104	0	0
20	V	72	Total 72	O 72	0	0
20	W	66	Total 66	O 66	0	0
20	X	83	Total 83	O 83	0	0
20	Y	81	Total 81	O 81	0	0
20	Z	100	Total 100	O 100	0	0
20	a	114	Total 114	O 114	0	0
20	b	89	Total 89	O 89	0	0

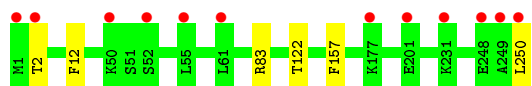
3 Residue-property plots [i](#)

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.

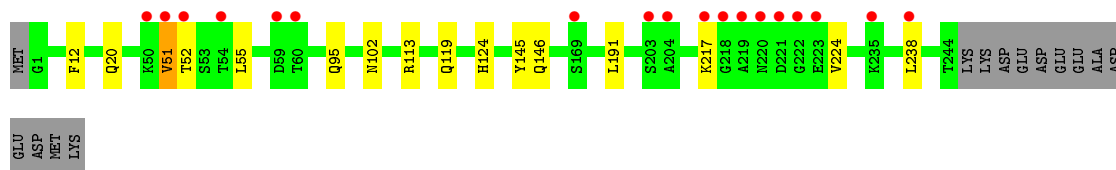
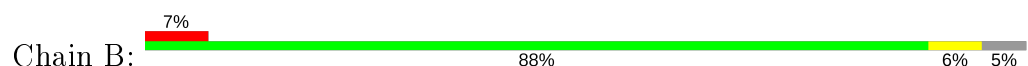
- Molecule 1: Proteasome subunit alpha type-2



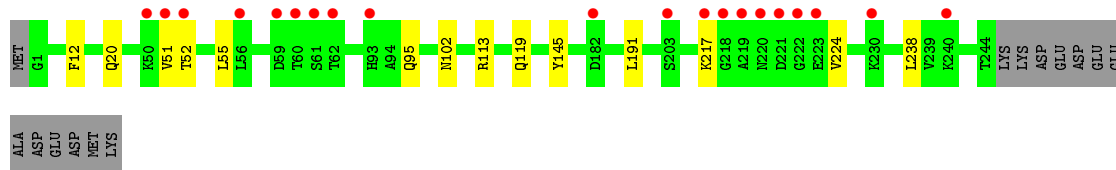
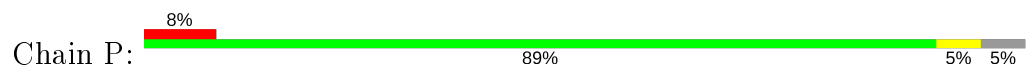
- Molecule 1: Proteasome subunit alpha type-2



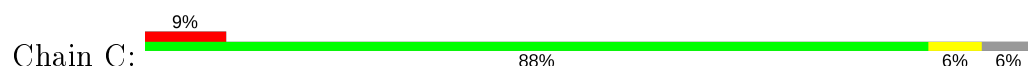
- Molecule 2: Proteasome subunit alpha type-3

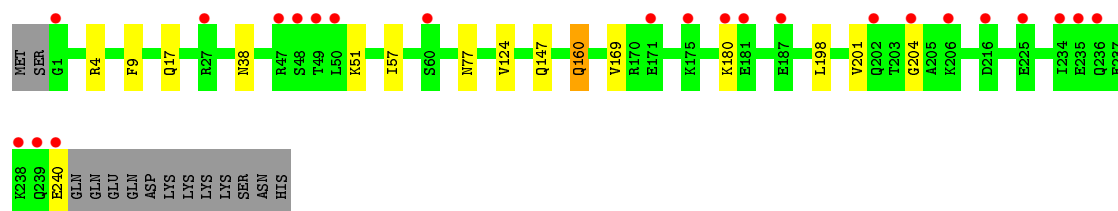


- Molecule 2: Proteasome subunit alpha type-3

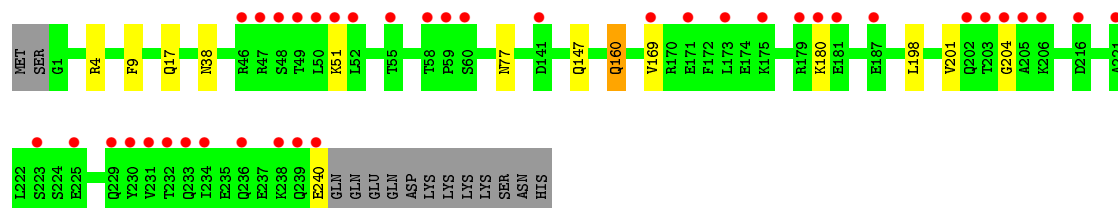
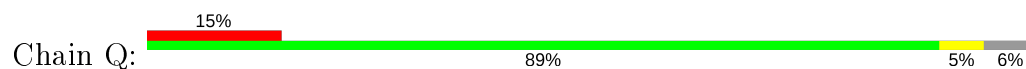


- Molecule 3: Proteasome subunit alpha type-4

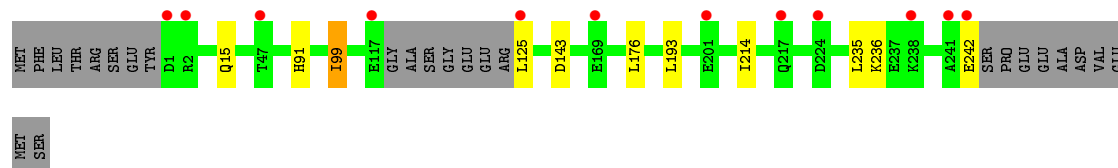
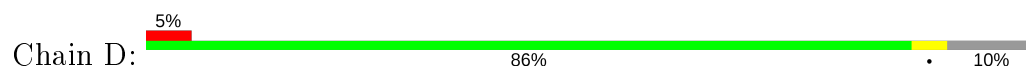




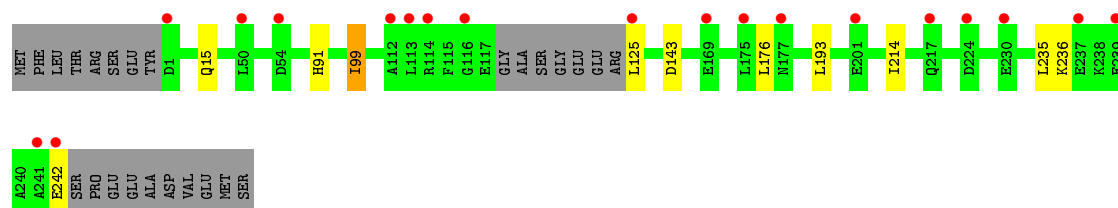
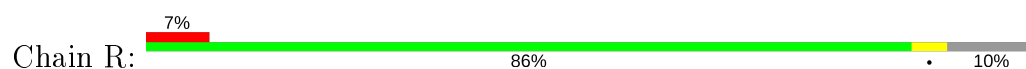
• Molecule 3: Proteasome subunit alpha type-4



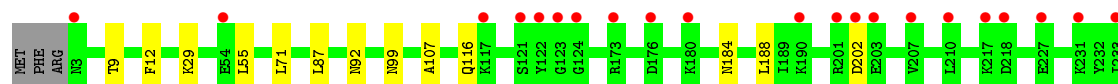
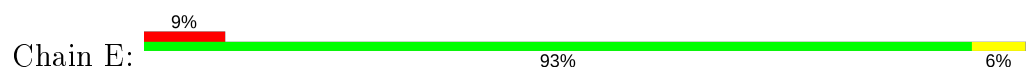
• Molecule 4: Proteasome subunit alpha type-5



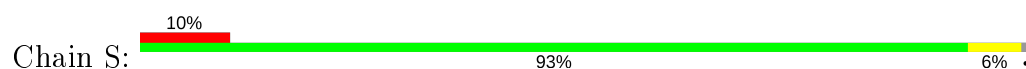
• Molecule 4: Proteasome subunit alpha type-5

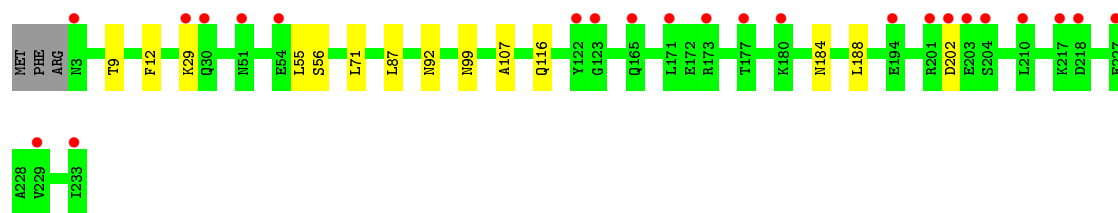


• Molecule 5: Proteasome subunit alpha type-6

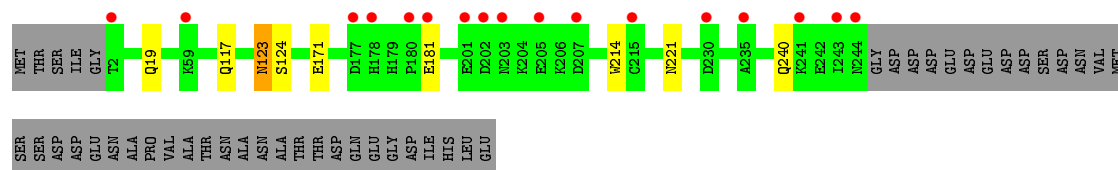
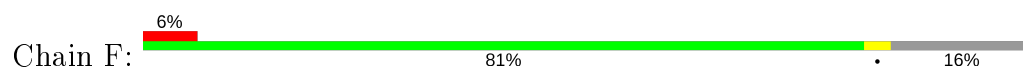


• Molecule 5: Proteasome subunit alpha type-6

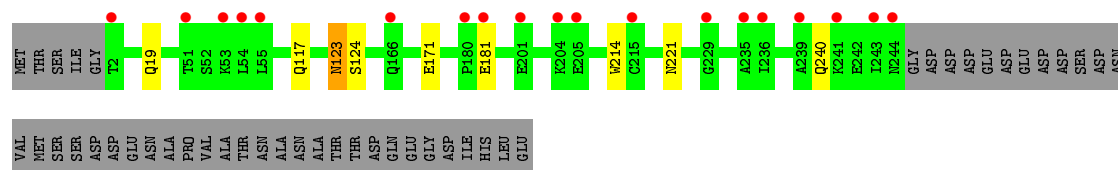
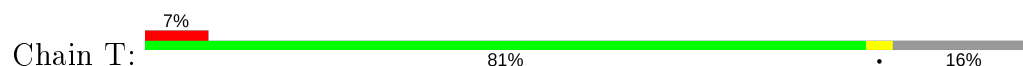




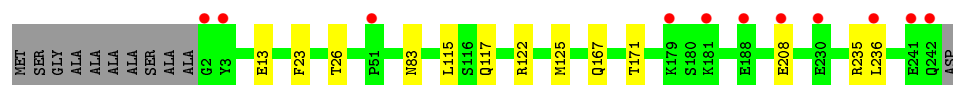
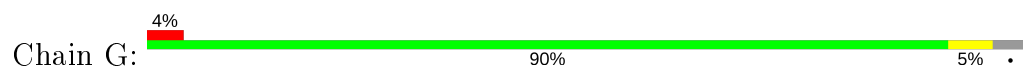
- Molecule 6: Probable proteasome subunit alpha type-7



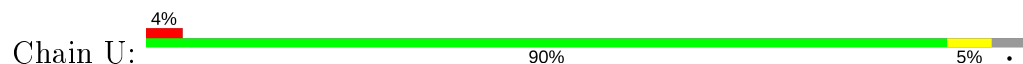
- Molecule 6: Probable proteasome subunit alpha type-7



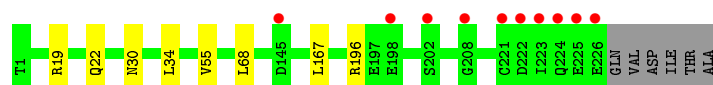
- Molecule 7: Proteasome subunit alpha type-1



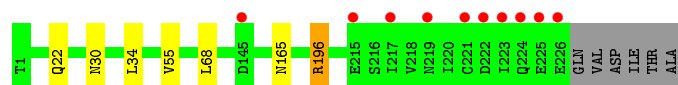
- Molecule 7: Proteasome subunit alpha type-1



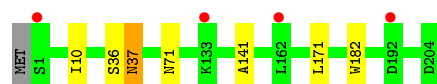
- Molecule 8: Proteasome subunit beta type-2



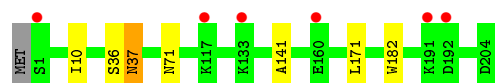
- Molecule 8: Proteasome subunit beta type-2



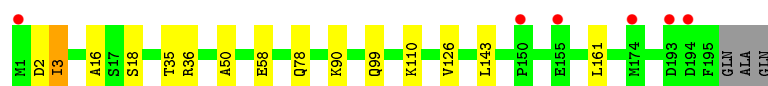
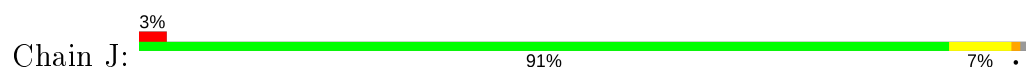
- Molecule 9: Proteasome subunit beta type-3



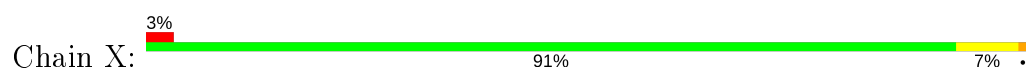
- Molecule 9: Proteasome subunit beta type-3



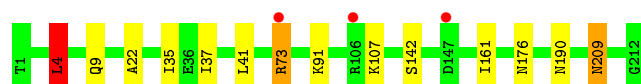
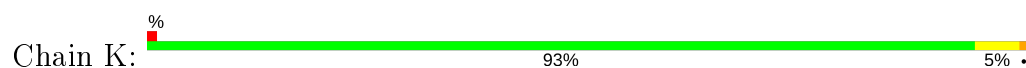
- Molecule 10: Proteasome subunit beta type-4



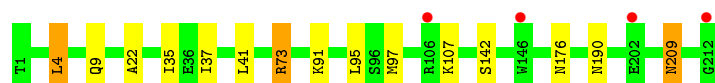
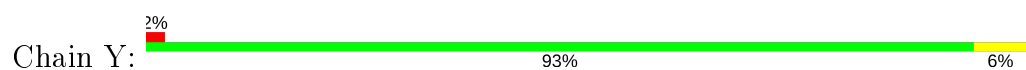
- Molecule 10: Proteasome subunit beta type-4



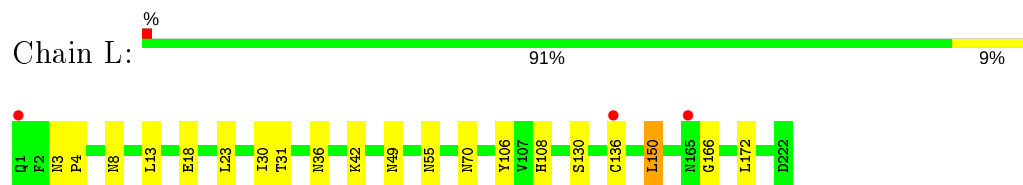
- Molecule 11: Proteasome subunit beta type-5



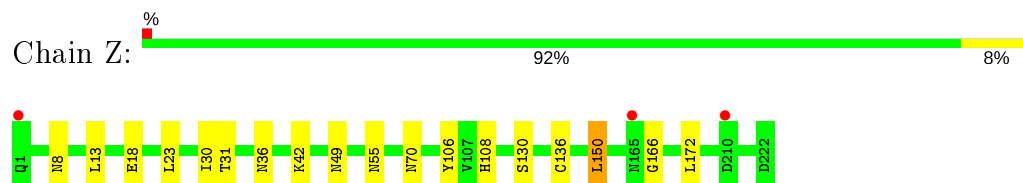
- Molecule 11: Proteasome subunit beta type-5



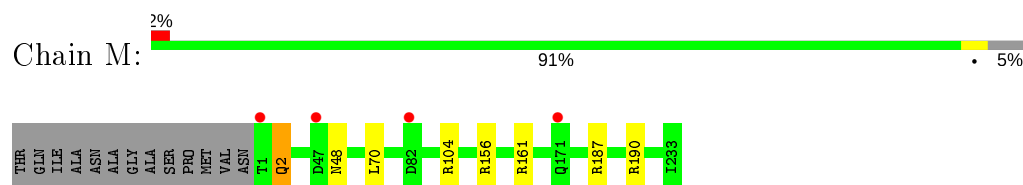
- Molecule 12: Proteasome subunit beta type-6



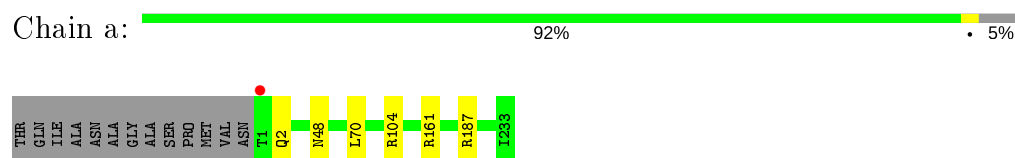
- Molecule 12: Proteasome subunit beta type-6



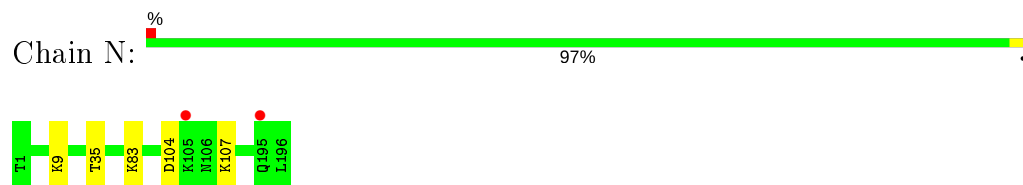
- Molecule 13: Proteasome subunit beta type-7



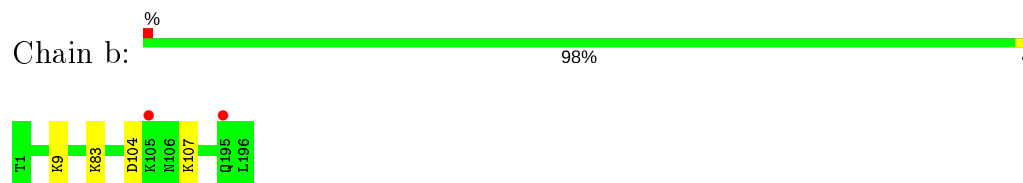
- Molecule 13: Proteasome subunit beta type-7



- 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	136.78Å 300.17Å 145.49Å 90.00° 113.29° 90.00°	Depositor
Resolution (Å)	15.00 – 2.30 15.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.1 (15.00-2.30) 98.5 (15.00-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.204 , 0.231 0.208 , 0.233	Depositor DCC
R_{free} test set	23307 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	42.0	Xtriage
Anisotropy	0.671	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.5	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	0.96	EDS
Total number of atoms	52005	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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, GWZ, SO4, MES, 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	0.38	0/1952	0.58	0/2642
1	O	0.38	0/1952	0.57	0/2642
2	B	0.39	0/1934	0.65	2/2618 (0.1%)
2	P	0.39	0/1934	0.65	2/2618 (0.1%)
3	C	0.39	0/1910	0.63	0/2586
3	Q	0.39	0/1910	0.63	0/2586
4	D	0.38	0/1837	0.59	0/2475
4	R	0.37	0/1837	0.59	0/2475
5	E	0.38	0/1800	0.57	0/2433
5	S	0.38	0/1800	0.58	0/2433
6	F	0.39	0/1932	0.56	0/2609
6	T	0.38	0/1932	0.56	0/2609
7	G	0.38	0/1945	0.58	0/2634
7	U	0.38	0/1945	0.57	0/2634
8	H	0.35	0/1751	0.60	0/2375
8	V	0.36	0/1751	0.60	1/2375 (0.0%)
9	I	0.37	0/1611	0.59	0/2174
9	W	0.37	0/1611	0.59	0/2174
10	J	0.37	0/1589	0.63	0/2142
10	X	0.38	0/1589	0.63	0/2142
11	K	0.37	0/1681	0.87	4/2274 (0.2%)
11	Y	0.36	0/1681	0.85	5/2274 (0.2%)
12	L	0.38	0/1795	0.62	0/2420
12	Z	0.38	0/1795	0.62	0/2420
13	M	0.38	0/1855	0.64	0/2514
13	a	0.38	0/1855	0.65	0/2514
14	N	0.36	0/1541	0.59	0/2087
14	b	0.36	0/1541	0.60	0/2087
All	All	0.38	0/50266	0.62	14/67966 (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
11	K	0	1
11	Y	0	1
All	All	0	2

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	73	ARG	NE-CZ-NH2	-21.13	109.73	120.30
11	Y	73	ARG	NE-CZ-NH1	-18.78	110.91	120.30
11	Y	73	ARG	NE-CZ-NH2	16.48	128.54	120.30
11	K	73	ARG	NE-CZ-NH1	15.31	127.95	120.30
11	K	73	ARG	CD-NE-CZ	10.50	138.30	123.60
11	Y	73	ARG	CD-NE-CZ	8.75	135.85	123.60
2	B	51	VAL	CG1-CB-CG2	5.75	120.10	110.90
2	P	224	VAL	CG1-CB-CG2	5.68	119.99	110.90
11	Y	4	LEU	CA-CB-CG	5.38	127.67	115.30
2	B	224	VAL	CG1-CB-CG2	5.28	119.35	110.90
11	K	4	LEU	CB-CG-CD2	5.27	119.96	111.00
11	Y	4	LEU	CB-CG-CD1	5.20	119.84	111.00
2	P	51	VAL	CG1-CB-CG2	5.13	119.11	110.90
8	V	196	ARG	NE-CZ-NH1	5.03	122.81	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	K	73	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	2	0
2	B	1904	0	1904	7	0
2	P	1904	0	1904	5	0
3	C	1881	0	1895	6	0
3	Q	1881	0	1895	4	0
4	D	1813	0	1797	3	0
4	R	1813	0	1797	2	0
5	E	1773	0	1775	5	0
5	S	1773	0	1775	5	0
6	F	1892	0	1883	3	0
6	T	1892	0	1883	3	0
7	G	1907	0	1901	2	0
7	U	1907	0	1901	3	0
8	H	1720	0	1718	2	0
8	V	1720	0	1718	2	0
9	I	1581	0	1574	5	0
9	W	1581	0	1574	5	0
10	J	1561	0	1569	6	0
10	X	1561	0	1569	6	0
11	K	1644	0	1592	9	0
11	Y	1644	0	1592	8	0
12	L	1757	0	1711	10	0
12	Z	1757	0	1711	9	0
13	M	1824	0	1832	3	0
13	a	1824	0	1832	0	0
14	N	1512	0	1478	1	0
14	b	1512	0	1478	0	0
15	G	1	0	0	0	0
15	I	2	0	0	0	0
15	K	1	0	0	0	0
15	L	1	0	0	0	0
15	N	1	0	0	0	0
15	W	1	0	0	0	0
15	Z	1	0	0	0	0
16	G	1	0	0	0	0
16	U	1	0	0	0	0
17	H	52	0	0	1	0
17	K	52	0	0	2	0
17	N	52	0	0	0	0
17	V	52	0	0	1	0
17	Y	52	0	0	2	0
17	b	52	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	H	12	0	13	0	0
18	K	12	0	13	0	0
18	V	12	0	13	0	0
18	Y	12	0	13	0	0
19	N	5	0	0	0	0
19	b	5	0	0	0	0
20	A	123	0	0	0	0
20	B	76	0	0	0	0
20	C	61	0	0	0	0
20	D	59	0	0	0	0
20	E	34	0	0	0	0
20	F	74	0	0	0	0
20	G	98	0	0	0	0
20	H	108	0	0	0	0
20	I	84	0	0	0	0
20	J	88	0	0	0	0
20	K	103	0	0	0	0
20	L	104	0	0	0	0
20	M	113	0	0	2	0
20	N	94	0	0	1	0
20	O	70	0	0	0	0
20	P	55	0	0	0	0
20	Q	43	0	0	0	0
20	R	56	0	0	0	0
20	S	39	0	0	0	0
20	T	66	0	0	0	0
20	U	104	0	0	0	0
20	V	72	0	0	0	0
20	W	66	0	0	0	0
20	X	83	0	0	0	0
20	Y	81	0	0	0	0
20	Z	100	0	0	0	0
20	a	114	0	0	0	0
20	b	89	0	0	0	0
All	All	52005	0	49168	87	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 (87) 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)
5:S:92:ASN:HD21	12:Z:70:ASN:HD21	1.29	0.80
5:E:92:ASN:HD21	12:L:70:ASN:HD21	1.30	0.78
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.50	0.76
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.53	0.73
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.36	0.71
2:P:95:GLN:HE22	9:W:71:ASN:HD22	1.40	0.69
5:S:92:ASN:HD21	12:Z:70:ASN:ND2	1.91	0.69
5:S:12:PHE:H	6:T:19:GLN:HE22	1.40	0.68
5:E:12:PHE:H	6:F:19:GLN:HE22	1.42	0.68
5:E:92:ASN:HD21	12:L:70:ASN:ND2	1.93	0.66
2:B:12:PHE:H	3:C:17:GLN:HE22	1.42	0.66
1:O:12:PHE:H	2:P:20:GLN:HE22	1.44	0.66
5:S:92:ASN:ND2	12:Z:70:ASN:HD21	1.94	0.66
5:E:92:ASN:ND2	12:L:70:ASN:HD21	1.96	0.64
3:C:160:GLN:HA	3:C:160:GLN:HE21	1.62	0.63
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.64	0.62
11:K:209:ASN:O	9:W:37:ASN:ND2	2.33	0.62
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.47	0.62
1:A:12:PHE:H	2:B:20:GLN:HE22	1.49	0.61
2:B:145:TYR:OH	2:B:217:LYS:N	2.35	0.60
9:I:37:ASN:ND2	11:Y:209:ASN:O	2.34	0.60
2:P:145:TYR:OH	2:P:217:LYS:N	2.35	0.59
6:F:123:ASN:HD22	6:F:124:SER:N	2.00	0.59
12:Z:42:LYS:HD2	12:Z:55:ASN:HD22	1.68	0.58
12:L:42:LYS:HD2	12:L:55:ASN:HD22	1.69	0.58
6:T:123:ASN:HD22	6:T:124:SER:N	2.00	0.58
8:H:22:GLN:HE21	17:H:301:GWZ:C5	2.18	0.56
11:K:4:LEU:HD23	11:K:161:ILE:HD11	1.86	0.56
7:U:23:PHE:O	7:U:26:THR:HB	2.05	0.55
3:C:9:PHE:H	4:D:15:GLN:HE22	1.53	0.55
2:P:95:GLN:NE2	9:W:71:ASN:HD22	2.04	0.55
2:B:95:GLN:NE2	9:I:71:ASN:HD22	2.05	0.54
10:J:50:ALA:O	11:K:91:LYS:NZ	2.40	0.54
8:V:22:GLN:HE21	17:V:301:GWZ:C5	2.20	0.54
13:M:2:GLN:NE2	20:M:301:HOH:O	2.40	0.54
11:K:142:SER:OG	10:X:143:LEU:HD21	2.07	0.54
10:X:50:ALA:O	11:Y:91:LYS:NZ	2.39	0.54
7:G:23:PHE:O	7:G:26:THR:HB	2.08	0.54
11:K:176:ASN:ND2	11:K:190:ASN:HD22	2.06	0.53
17:K:301:GWZ:C3	12:L:108:HIS:HE1	2.22	0.53
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.91	0.53
11:Y:176:ASN:ND2	11:Y:190:ASN:HD22	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.91	0.50
10:J:143:LEU:HD21	11:Y:142:SER:OG	2.13	0.48
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.62	0.48
6:T:123:ASN:C	6:T:123:ASN:HD22	2.18	0.47
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.95	0.47
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.96	0.47
10:X:3:ILE:HG23	10:X:18:SER:HB3	1.97	0.46
11:Y:176:ASN:HD21	11:Y:190:ASN:HD22	1.64	0.46
14:N:35:THR:HG22	20:N:322:HOH:O	2.15	0.46
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.97	0.46
13:M:156:ARG:HH11	8:V:165:ASN:HD22	1.64	0.46
11:K:176:ASN:HD21	11:K:190:ASN:HD22	1.64	0.45
10:J:3:ILE:HG23	10:J:18:SER:HB3	1.97	0.45
9:W:36:SER:HB2	10:X:126:VAL:HG11	1.99	0.45
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.97	0.45
6:F:123:ASN:C	6:F:123:ASN:HD22	2.19	0.45
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.97	0.45
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.47	0.45
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.46	0.45
13:M:190:ARG:NH2	20:M:303:HOH:O	2.49	0.45
11:K:4:LEU:HD23	11:K:161:ILE:CD1	2.47	0.44
17:Y:301:GWZ:C3	12:Z:108:HIS:HE1	2.31	0.44
2:B:146:GLN:HG2	3:C:57:ILE:HG21	2.00	0.43
10:J:36:ARG:NH1	10:J:58:GLU:OE2	2.50	0.43
7:G:167:GLN:HE21	7:G:171:THR:HG23	1.83	0.43
10:X:36:ARG:NH1	10:X:58:GLU:OE2	2.51	0.43
9:I:10:ILE:HG21	9:I:141:ALA:HB3	2.01	0.43
3:Q:198:LEU:HA	3:Q:201:VAL:HG12	2.01	0.43
3:C:198:LEU:HA	3:C:201:VAL:HG12	2.00	0.43
12:L:8:ASN:HA	12:L:30:ILE:O	2.19	0.43
7:U:61:SER:OG	7:U:215:GLU:OE2	2.25	0.42
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.49	0.42
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.50	0.42
11:Y:37:ILE:HB	11:Y:41:LEU:HB3	2.01	0.42
2:B:124:HIS:HB3	3:C:124:VAL:HG12	2.02	0.42
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.19	0.42
11:K:37:ILE:HB	11:K:41:LEU:HB3	2.02	0.42
12:L:3:ASN:HD22	12:L:4:PRO:HD2	1.84	0.42
8:H:19:ARG:NH1	8:H:167:LEU:O	2.52	0.41
11:Y:95:LEU:HD13	11:Y:97:MET:HE1	2.01	0.41
1:O:83:ARG:HE	7:U:114:ASN:ND2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:10:ILE:HG21	9:W:141:ALA:HB3	2.02	0.40
4:D:91:HIS:HB3	4:D:99:ILE:HG21	2.03	0.40
11:Y:22:ALA:HB1	17:Y:301:GWZ:C5	2.51	0.40
11:K:22:ALA:HB1	17:K:301:GWZ:C5	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	242 (98%)	6 (2%)	0	100	100
1	O	248/250 (99%)	241 (97%)	7 (3%)	0	100	100
2	B	242/258 (94%)	235 (97%)	7 (3%)	0	100	100
2	P	242/258 (94%)	234 (97%)	8 (3%)	0	100	100
3	C	238/254 (94%)	235 (99%)	2 (1%)	1 (0%)	34	42
3	Q	238/254 (94%)	235 (99%)	2 (1%)	1 (0%)	34	42
4	D	231/260 (89%)	228 (99%)	3 (1%)	0	100	100
4	R	231/260 (89%)	227 (98%)	4 (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%)	237 (98%)	4 (2%)	0	100	100
6	T	241/288 (84%)	238 (99%)	3 (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	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
8	V	224/232 (97%)	218 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	189 (98%)	4 (2%)	0	100	100
10	X	193/198 (98%)	189 (98%)	4 (2%)	0	100	100
11	K	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
11	Y	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
12	L	220/222 (99%)	214 (97%)	5 (2%)	1 (0%)	29	35
12	Z	220/222 (99%)	214 (97%)	5 (2%)	1 (0%)	29	35
13	M	231/246 (94%)	223 (96%)	8 (4%)	0	100	100
13	a	231/246 (94%)	223 (96%)	8 (4%)	0	100	100
14	N	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
14	b	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
All	All	6284/6614 (95%)	6136 (98%)	144 (2%)	4 (0%)	51	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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	73
1	O	209/209 (100%)	205 (98%)	4 (2%)	57	73
2	B	203/216 (94%)	195 (96%)	8 (4%)	32	46
2	P	203/216 (94%)	196 (97%)	7 (3%)	37	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	212/226 (94%)	203 (96%)	9 (4%)	30	42
3	Q	212/226 (94%)	203 (96%)	9 (4%)	30	42
4	D	194/215 (90%)	185 (95%)	9 (5%)	27	38
4	R	194/215 (90%)	185 (95%)	9 (5%)	27	38
5	E	190/193 (98%)	181 (95%)	9 (5%)	26	37
5	S	190/193 (98%)	180 (95%)	10 (5%)	22	31
6	F	201/239 (84%)	194 (96%)	7 (4%)	36	50
6	T	201/239 (84%)	194 (96%)	7 (4%)	36	50
7	G	206/210 (98%)	197 (96%)	9 (4%)	28	39
7	U	206/210 (98%)	198 (96%)	8 (4%)	32	46
8	H	185/190 (97%)	180 (97%)	5 (3%)	44	61
8	V	185/190 (97%)	180 (97%)	5 (3%)	44	61
9	I	172/173 (99%)	169 (98%)	3 (2%)	60	76
9	W	172/173 (99%)	169 (98%)	3 (2%)	60	76
10	J	173/175 (99%)	166 (96%)	7 (4%)	31	44
10	X	173/175 (99%)	166 (96%)	7 (4%)	31	44
11	K	169/169 (100%)	164 (97%)	5 (3%)	41	57
11	Y	169/169 (100%)	164 (97%)	5 (3%)	41	57
12	L	185/185 (100%)	177 (96%)	8 (4%)	29	40
12	Z	185/185 (100%)	177 (96%)	8 (4%)	29	40
13	M	199/208 (96%)	193 (97%)	6 (3%)	41	57
13	a	199/208 (96%)	193 (97%)	6 (3%)	41	57
14	N	162/162 (100%)	158 (98%)	4 (2%)	47	65
14	b	162/162 (100%)	158 (98%)	4 (2%)	47	65
All	All	5320/5540 (96%)	5135 (96%)	185 (4%)	36	50

All (185) 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	51	VAL

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Mol	Chain	Res	Type
2	B	52	THR
2	B	55	LEU
2	B	102	ASN
2	B	113	ARG
2	B	119	GLN
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
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	9	THR
5	E	29	LYS
5	E	55	LEU
5	E	71	LEU
5	E	99	ASN
5	E	116	GLN
5	E	184	ASN
5	E	188	LEU
5	E	202	ASP
6	F	117	GLN
6	F	123	ASN
6	F	171	GLU
6	F	181	GLU
6	F	214	TRP
6	F	221	ASN
6	F	240	GLN
7	G	13	GLU

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Mol	Chain	Res	Type
7	G	83	ASN
7	G	115	LEU
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	30	ASN
8	H	34	LEU
8	H	55	VAL
8	H	68	LEU
8	H	196	ARG
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
10	J	110	LYS
11	K	4	LEU
11	K	9	GLN
11	K	35	ILE
11	K	107	LYS
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	136	CYS
12	L	150	LEU
12	L	172	LEU
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG

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Mol	Chain	Res	Type
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	52	THR
2	P	55	LEU
2	P	102	ASN
2	P	113	ARG
2	P	119	GLN
2	P	191	LEU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
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
4	R	125	LEU
4	R	143	ASP
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	55	LEU
5	S	56	SER
5	S	71	LEU
5	S	99	ASN
5	S	116	GLN
5	S	184	ASN
5	S	188	LEU

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Mol	Chain	Res	Type
5	S	202	ASP
6	T	117	GLN
6	T	123	ASN
6	T	171	GLU
6	T	181	GLU
6	T	214	TRP
6	T	221	ASN
6	T	240	GLN
7	U	13	GLU
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
8	V	30	ASN
8	V	34	LEU
8	V	55	VAL
8	V	68	LEU
8	V	196	ARG
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
10	X	110	LYS
11	Y	4	LEU
11	Y	9	GLN
11	Y	35	ILE
11	Y	107	LYS
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	136	CYS

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Mol	Chain	Res	Type
12	Z	150	LEU
12	Z	172	LEU
13	a	2	GLN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
14	b	9	LYS
14	b	83	LYS
14	b	104	ASP
14	b	107	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (134) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	20	GLN
2	B	58	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
3	C	17	GLN
3	C	38	ASN
3	C	77	ASN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	91	HIS
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	184	ASN
6	F	19	GLN

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Mol	Chain	Res	Type
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
7	G	166	GLN
7	G	167	GLN
7	G	175	ASN
8	H	22	GLN
8	H	30	ASN
8	H	66	HIS
8	H	165	ASN
8	H	172	ASN
8	H	189	ASN
10	J	55	GLN
10	J	118	GLN
11	K	9	GLN
11	K	85	ASN
11	K	176	ASN
11	K	209	ASN
12	L	3	ASN
12	L	36	ASN
12	L	49	ASN
12	L	55	ASN
12	L	70	ASN
12	L	79	HIS
12	L	108	HIS
12	L	158	ASN
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	108	ASN
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
14	N	69	GLN
14	N	161	GLN
1	O	94	HIS

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Mol	Chain	Res	Type
2	P	20	GLN
2	P	58	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	176	GLN
3	Q	17	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	91	HIS
4	R	225	ASN
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	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	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	167	GLN
7	U	175	ASN
8	V	22	GLN
8	V	30	ASN
8	V	35	HIS
8	V	165	ASN
8	V	172	ASN
8	V	189	ASN
10	X	55	GLN

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Mol	Chain	Res	Type
10	X	78	GLN
10	X	86	GLN
10	X	118	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	176	ASN
11	Y	209	ASN
12	Z	3	ASN
12	Z	36	ASN
12	Z	49	ASN
12	Z	55	ASN
12	Z	70	ASN
12	Z	79	HIS
12	Z	108	HIS
12	Z	158	ASN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN
13	a	179	ASN
13	a	194	ASN
13	a	213	GLN
14	b	69	GLN
14	b	161	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 22 ligands modelled in this entry, 10 are monoatomic - leaving 12 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	GWZ	N	201	14	54,54,54	1.16	3 (5%)	71,73,73	0.96	1 (1%)
18	MES	K	303	-	12,12,12	2.31	1 (8%)	14,16,16	1.49	2 (14%)
17	GWZ	K	301	11	54,54,54	1.24	4 (7%)	71,73,73	1.12	4 (5%)
17	GWZ	V	301	8	54,54,54	1.26	5 (9%)	71,73,73	1.29	4 (5%)
19	SO4	N	203	-	4,4,4	0.28	0	6,6,6	0.07	0
18	MES	Y	302	-	12,12,12	2.26	1 (8%)	14,16,16	1.42	1 (7%)
17	GWZ	H	301	8	54,54,54	1.28	5 (9%)	71,73,73	1.27	3 (4%)
17	GWZ	Y	301	11	54,54,54	1.26	3 (5%)	71,73,73	1.13	4 (5%)
19	SO4	b	202	-	4,4,4	0.27	0	6,6,6	0.15	0
17	GWZ	b	201	14	54,54,54	1.24	3 (5%)	71,73,73	1.01	1 (1%)
18	MES	H	302	-	12,12,12	2.28	1 (8%)	14,16,16	1.60	2 (14%)
18	MES	V	302	-	12,12,12	2.24	1 (8%)	14,16,16	1.44	2 (14%)

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	GWZ	N	201	14	-	2/59/67/67	0/3/3/3
18	MES	K	303	-	-	2/6/14/14	0/1/1/1
17	GWZ	K	301	11	-	2/59/67/67	0/3/3/3
17	GWZ	V	301	8	-	7/59/67/67	0/3/3/3
18	MES	Y	302	-	-	4/6/14/14	0/1/1/1
17	GWZ	H	301	8	-	6/59/67/67	0/3/3/3
17	GWZ	Y	301	11	-	2/59/67/67	0/3/3/3
17	GWZ	b	201	14	-	2/59/67/67	0/3/3/3
18	MES	H	302	-	-	2/6/14/14	0/1/1/1
18	MES	V	302	-	-	5/6/14/14	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	K	303	MES	C8-S	-7.83	1.66	1.77
18	Y	302	MES	C8-S	-7.62	1.66	1.77
18	H	302	MES	C8-S	-7.60	1.66	1.77
18	V	302	MES	C8-S	-7.52	1.66	1.77
17	b	201	GWZ	C32-C33	-5.04	1.39	1.51
17	K	301	GWZ	C32-C33	-5.03	1.39	1.51
17	N	201	GWZ	C32-C33	-4.91	1.39	1.51
17	Y	301	GWZ	C32-C33	-4.89	1.39	1.51
17	H	301	GWZ	C32-C33	-4.83	1.39	1.51
17	V	301	GWZ	C32-C33	-4.69	1.40	1.51
17	K	301	GWZ	C13-C14	-4.53	1.38	1.51
17	Y	301	GWZ	C13-C14	-4.49	1.38	1.51
17	b	201	GWZ	C58-C51	4.41	1.59	1.52
17	H	301	GWZ	C58-C51	4.20	1.59	1.52
17	V	301	GWZ	C58-C51	4.19	1.59	1.52
17	Y	301	GWZ	C58-C51	4.13	1.59	1.52
17	b	201	GWZ	C13-C14	-3.97	1.40	1.51
17	H	301	GWZ	C13-C14	-3.89	1.40	1.51
17	N	201	GWZ	C13-C14	-3.89	1.40	1.51
17	V	301	GWZ	C13-C14	-3.81	1.40	1.51
17	K	301	GWZ	C58-C51	3.44	1.58	1.52
17	H	301	GWZ	C51-C47	3.30	1.61	1.54
17	N	201	GWZ	C58-C51	3.08	1.57	1.52
17	V	301	GWZ	C51-C47	3.04	1.60	1.54
17	H	301	GWZ	C59-C51	2.36	1.56	1.52
17	K	301	GWZ	C43-C42	2.22	1.56	1.52
17	V	301	GWZ	C59-C51	2.22	1.56	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	H	301	GWZ	C59-C51-C58	-6.65	101.06	110.56
17	V	301	GWZ	C59-C51-C58	-6.63	101.08	110.56
18	Y	302	MES	O3S-S-C8	3.96	112.17	105.77
17	Y	301	GWZ	C58-C51-C47	3.71	118.23	111.28
18	V	302	MES	O3S-S-C8	3.67	111.71	105.77
17	K	301	GWZ	C58-C51-C47	3.52	117.88	111.28
18	K	303	MES	O1S-S-C8	3.29	110.87	106.92
18	H	302	MES	O1S-S-C8	3.11	110.66	106.92
17	V	301	GWZ	C58-C51-C47	3.01	116.91	111.28
18	K	303	MES	O3S-S-C8	2.93	110.51	105.77
17	H	301	GWZ	C58-C51-C47	2.91	116.73	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	201	GWZ	C20-C11-N10	-2.90	103.28	111.16
17	N	201	GWZ	C20-C11-N10	-2.78	103.58	111.16
18	H	302	MES	O2S-S-C8	2.78	110.26	106.92
17	K	301	GWZ	C7-N4-C5	2.69	115.27	111.09
17	Y	301	GWZ	C7-N4-C5	2.44	114.87	111.09
18	V	302	MES	O1S-S-C8	2.40	109.81	106.92
17	Y	301	GWZ	C23-C28-N30	-2.29	111.69	116.70
17	V	301	GWZ	O60-C51-C58	2.27	112.78	107.90
17	V	301	GWZ	C59-C51-C47	2.26	115.51	111.28
17	H	301	GWZ	C59-C51-C47	2.23	115.46	111.28
17	K	301	GWZ	C23-C28-N30	-2.16	111.96	116.70
17	K	301	GWZ	C33-C32-C31	-2.14	107.47	113.39
17	Y	301	GWZ	C33-C32-C31	-2.00	107.85	113.39

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	K	301	GWZ	C8-C7-N4-C5
17	V	301	GWZ	C42-C47-C51-C58
17	V	301	GWZ	C42-C47-C51-C59
17	V	301	GWZ	O48-C47-C51-C58
17	V	301	GWZ	O48-C47-C51-C59
17	V	301	GWZ	O48-C47-C51-O60
18	H	302	MES	N4-C7-C8-S
17	H	301	GWZ	C42-C47-C51-C58
17	H	301	GWZ	C42-C47-C51-C59
17	H	301	GWZ	C42-C47-C51-O60
17	H	301	GWZ	O48-C47-C51-C58
17	H	301	GWZ	O48-C47-C51-C59
17	H	301	GWZ	O48-C47-C51-O60
17	Y	301	GWZ	C8-C7-N4-C5
18	V	302	MES	C7-C8-S-O1S
18	V	302	MES	C7-C8-S-O3S
18	K	303	MES	C8-C7-N4-C3
18	K	303	MES	C8-C7-N4-C5
18	V	302	MES	C8-C7-N4-C3
18	V	302	MES	C8-C7-N4-C5
17	b	201	GWZ	N10-C11-C20-N22
17	b	201	GWZ	N10-C11-C20-O21
17	N	201	GWZ	N10-C11-C20-N22
17	V	301	GWZ	C42-C47-C51-O60

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Mol	Chain	Res	Type	Atoms
17	N	201	GWZ	N10-C11-C20-O21
18	V	302	MES	C7-C8-S-O2S
18	H	302	MES	C8-C7-N4-C5
18	Y	302	MES	C8-C7-N4-C3
18	Y	302	MES	C7-C8-S-O3S
17	K	301	GWZ	N10-C11-C20-O21
17	Y	301	GWZ	N10-C11-C20-O21
18	Y	302	MES	C7-C8-S-O1S
18	Y	302	MES	C8-C7-N4-C5
17	V	301	GWZ	N30-C31-C39-O40

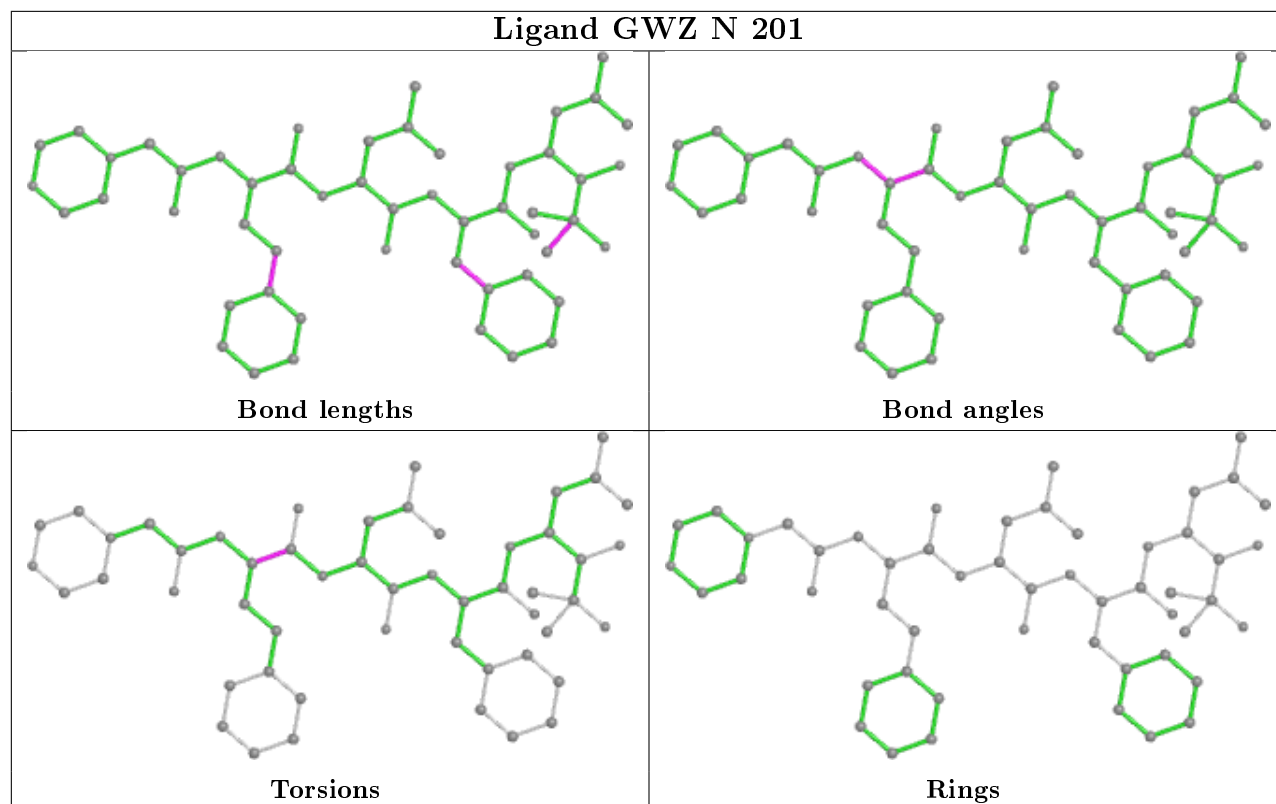
There are no ring outliers.

4 monomers are involved in 6 short contacts:

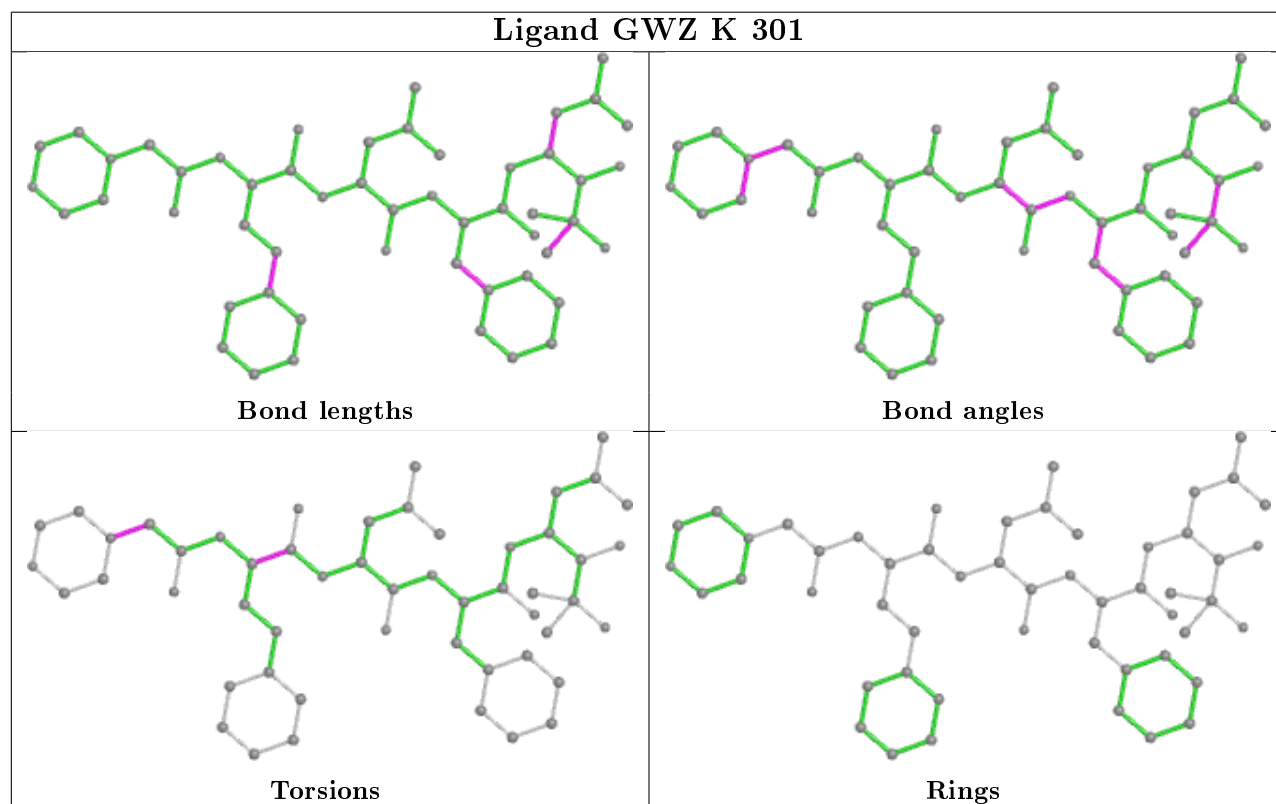
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	K	301	GWZ	2	0
17	V	301	GWZ	1	0
17	H	301	GWZ	1	0
17	Y	301	GWZ	2	0

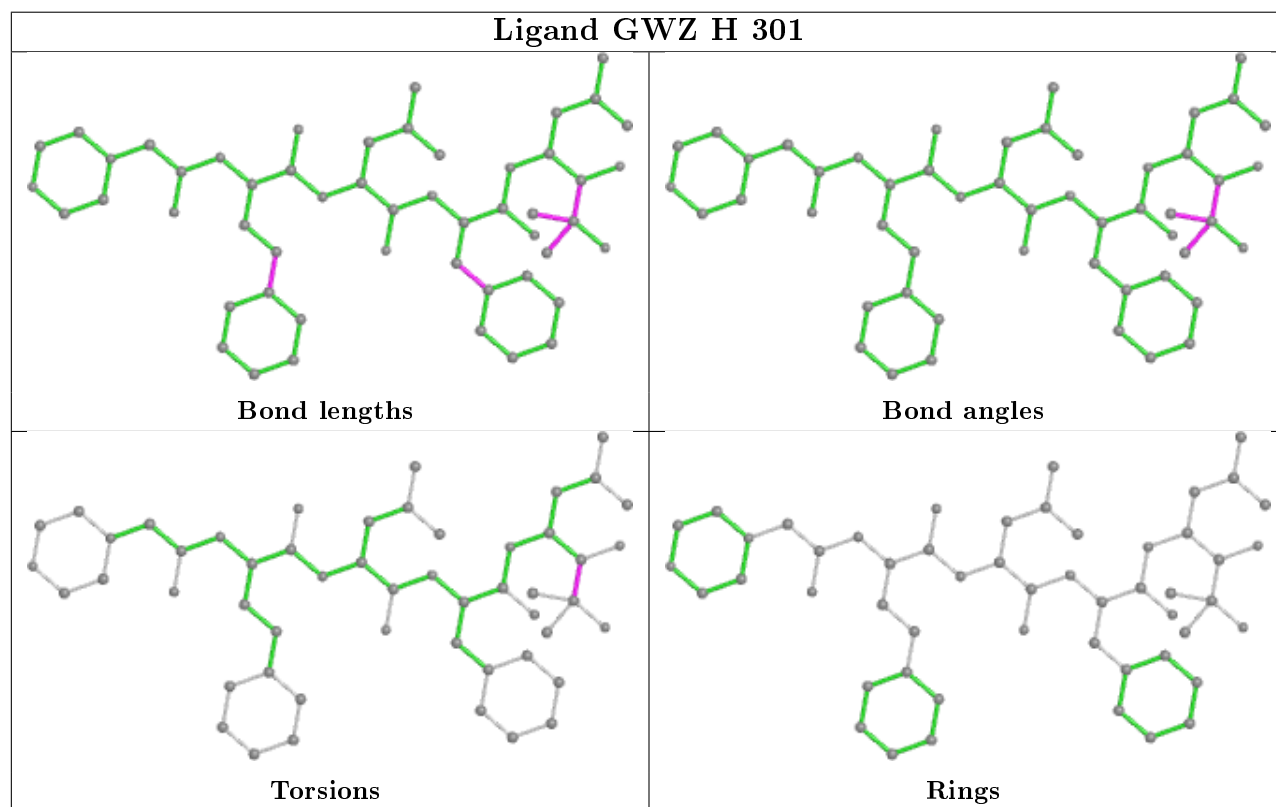
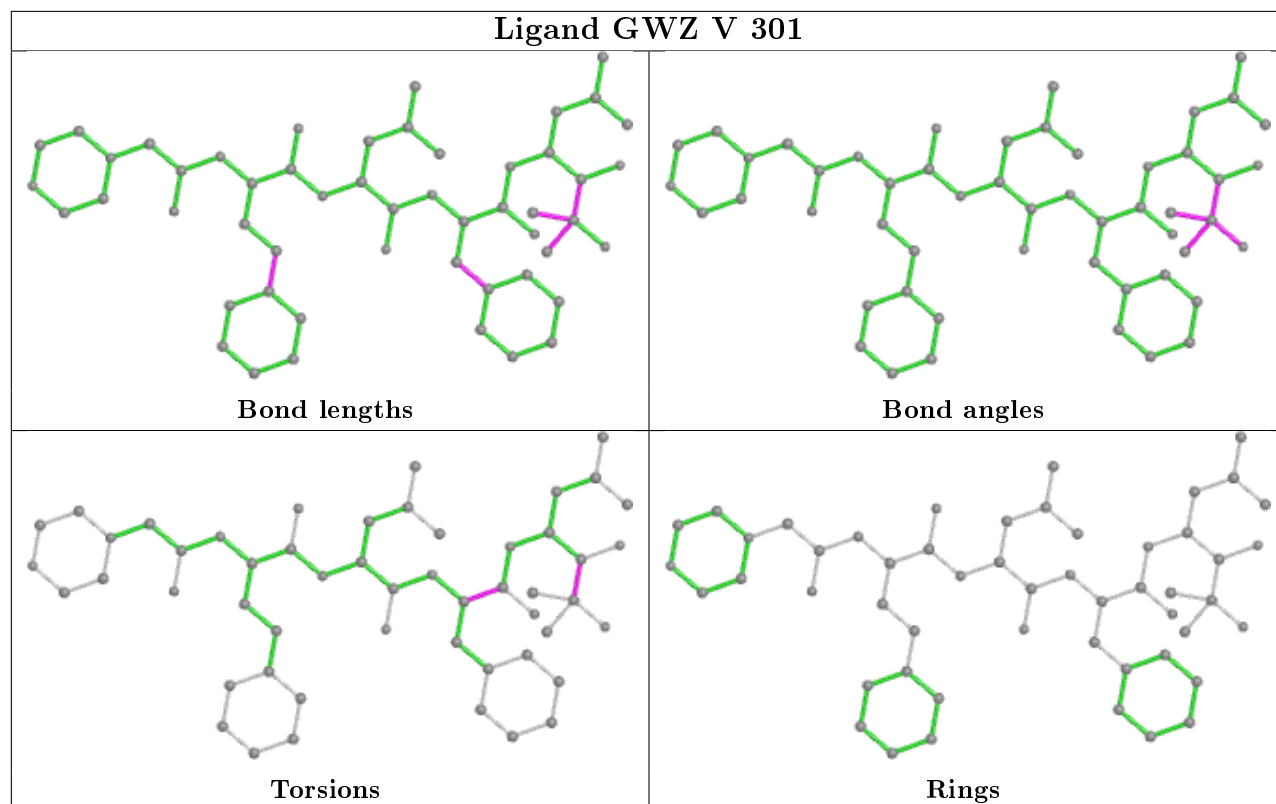
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

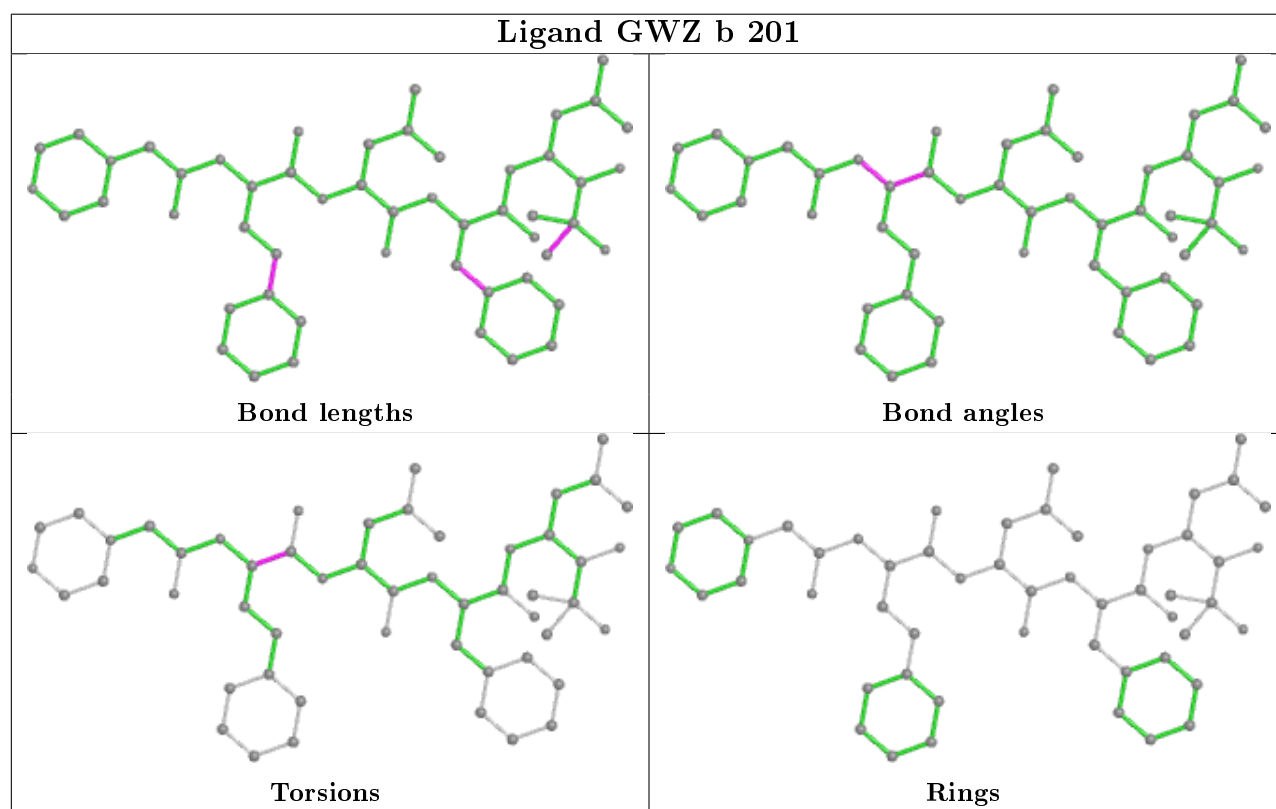
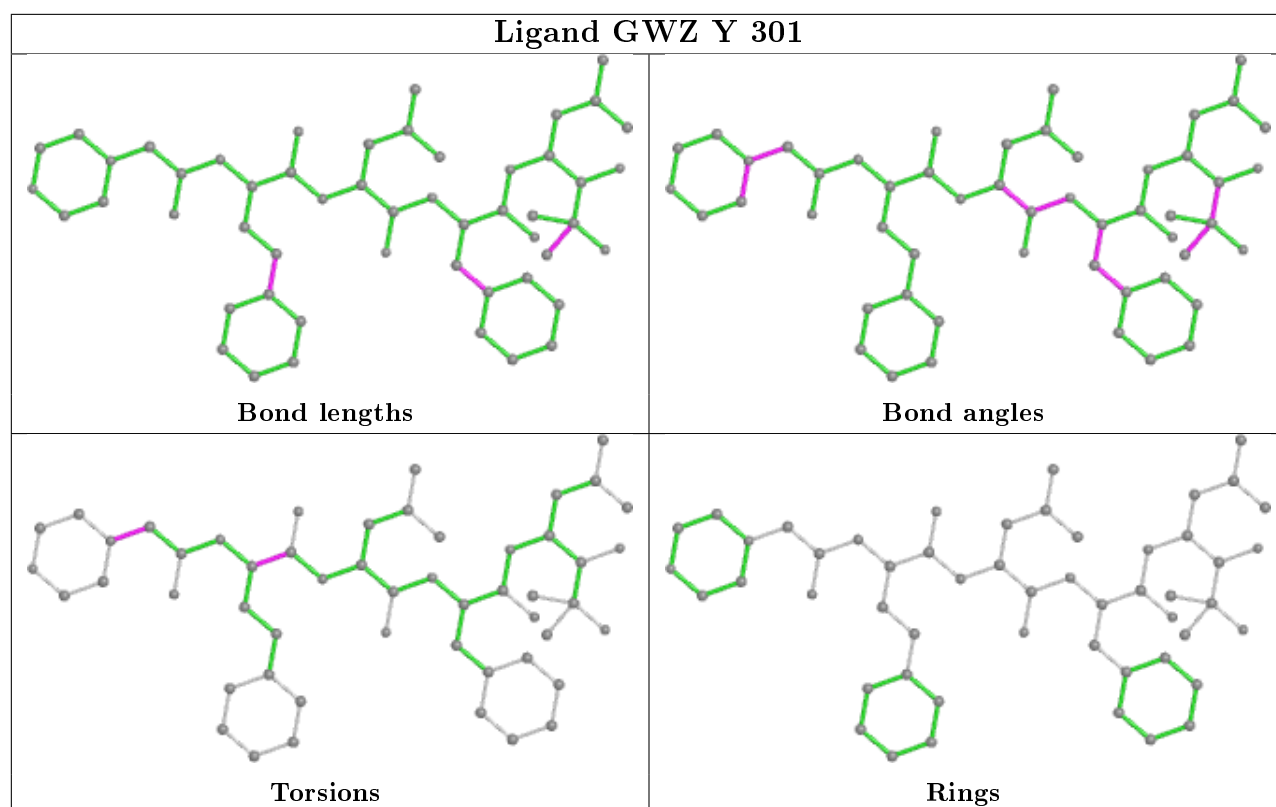
Ligand GWZ N 201



Ligand GWZ K 301







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 ⓘ

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%)	0.03	11 (4%) 34 41	35, 50, 88, 115	0
1	O	250/250 (100%)	0.16	12 (4%) 30 37	39, 59, 100, 130	0
2	B	244/258 (94%)	0.26	18 (7%) 14 19	35, 54, 96, 120	0
2	P	244/258 (94%)	0.30	20 (8%) 11 15	37, 58, 97, 128	0
3	C	240/254 (94%)	0.31	23 (9%) 8 10	33, 57, 112, 152	0
3	Q	240/254 (94%)	0.73	39 (16%) 1 2	40, 70, 148, 196	0
4	D	235/260 (90%)	-0.00	12 (5%) 28 35	38, 58, 87, 132	0
4	R	235/260 (90%)	0.24	19 (8%) 12 16	44, 63, 99, 138	0
5	E	231/234 (98%)	0.27	21 (9%) 9 12	43, 62, 98, 119	0
5	S	231/234 (98%)	0.39	23 (9%) 7 10	43, 65, 110, 131	0
6	F	243/288 (84%)	0.06	17 (6%) 16 21	32, 55, 97, 119	0
6	T	243/288 (84%)	0.18	19 (7%) 13 17	33, 60, 108, 139	0
7	G	241/252 (95%)	-0.03	11 (4%) 32 39	33, 50, 84, 133	0
7	U	241/252 (95%)	-0.04	10 (4%) 37 44	36, 51, 83, 120	0
8	H	226/232 (97%)	0.00	10 (4%) 34 41	38, 43, 71, 140	0
8	V	226/232 (97%)	-0.01	10 (4%) 34 41	38, 44, 76, 152	0
9	I	204/205 (99%)	-0.28	4 (1%) 65 71	29, 44, 71, 90	0
9	W	204/205 (99%)	-0.27	6 (2%) 51 58	30, 48, 72, 91	0
10	J	195/198 (98%)	-0.09	6 (3%) 49 56	31, 48, 72, 96	0
10	X	195/198 (98%)	-0.08	5 (2%) 56 63	34, 50, 74, 104	0
11	K	212/212 (100%)	-0.25	3 (1%) 75 80	30, 46, 71, 87	0
11	Y	212/212 (100%)	-0.23	4 (1%) 66 73	26, 47, 72, 88	0
12	L	222/222 (100%)	-0.25	3 (1%) 75 80	33, 48, 77, 97	0
12	Z	222/222 (100%)	-0.29	3 (1%) 75 80	34, 45, 76, 96	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.27	4 (1%)	70 76	30, 47, 70, 82	0
13	a	233/246 (94%)	-0.26	1 (0%)	92 95	28, 44, 65, 79	0
14	N	196/196 (100%)	-0.27	2 (1%)	82 86	26, 43, 70, 87	0
14	b	196/196 (100%)	-0.25	2 (1%)	82 86	26, 45, 71, 88	0
All	All	6344/6614 (95%)	0.01	318 (5%)	28 35	26, 51, 95, 196	0

All (318) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	50	LEU	10.9
2	P	218	GLY	8.7
2	B	218	GLY	8.5
2	B	219	ALA	8.5
1	O	249	ALA	8.4
3	Q	49	THR	8.3
3	Q	202	GLN	8.1
2	B	220	ASN	7.6
2	P	219	ALA	7.6
3	Q	206	LYS	7.6
3	Q	204	GLY	7.5
2	B	221	ASP	7.4
3	C	238	LYS	7.4
3	Q	48	SER	7.3
10	X	1	MET	6.9
3	C	49	THR	6.8
8	V	224	GLN	6.8
2	P	220	ASN	6.5
2	P	52	THR	6.5
5	S	202	ASP	6.4
8	V	221	CYS	6.4
8	H	224	GLN	6.3
2	P	51	VAL	6.2
2	B	217	LYS	5.8
2	B	52	THR	5.8
8	V	222	ASP	5.8
3	C	202	GLN	5.8
2	B	51	VAL	5.7
1	A	249	ALA	5.6
10	J	1	MET	5.6
10	X	194	ASP	5.5
2	P	221	ASP	5.4

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Mol	Chain	Res	Type	RSRZ
4	R	113	LEU	5.4
3	Q	240	GLU	5.4
8	V	226	GLU	5.3
6	T	241	LYS	5.2
3	C	50	LEU	5.2
3	C	236	GLN	5.2
2	P	59	ASP	5.2
7	U	242	GLN	5.1
10	J	194	ASP	5.1
3	C	206	LYS	5.1
6	T	243	ILE	5.1
3	Q	239	GLN	5.1
14	N	195	GLN	5.1
4	D	242	GLU	5.0
1	O	52	SER	4.9
1	A	1	MET	4.9
13	a	1	THR	4.9
1	A	250	LEU	4.8
5	S	210	LEU	4.8
7	G	2	GLY	4.8
5	E	202	ASP	4.8
3	Q	205	ALA	4.8
3	Q	221	ALA	4.8
14	b	195	GLN	4.8
6	F	205	GLU	4.7
6	T	244	ASN	4.7
7	G	242	GLN	4.6
5	S	173	ARG	4.5
3	Q	51	LYS	4.5
3	Q	236	GLN	4.5
3	Q	238	LYS	4.4
8	H	226	GLU	4.4
9	W	1	SER	4.3
1	O	1	MET	4.2
3	C	225	GLU	4.2
3	C	204	GLY	4.2
3	C	180	LYS	4.2
7	G	3	TYR	4.2
3	Q	223	SER	4.1
6	F	2	THR	4.1
7	U	2	GLY	4.1
3	Q	52	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
12	L	165	ASN	4.1
8	H	221	CYS	4.1
6	T	181	GLU	4.0
3	C	240	GLU	4.0
6	F	243	ILE	4.0
2	P	222	GLY	3.9
11	Y	106	ARG	3.9
1	O	231	LYS	3.9
6	T	180	PRO	3.9
3	Q	225	GLU	3.9
4	R	242	GLU	3.9
3	Q	232	THR	3.8
5	S	180	LYS	3.8
1	O	55	LEU	3.8
1	O	250	LEU	3.8
5	E	123	GLY	3.7
9	I	1	SER	3.7
5	E	173	ARG	3.7
2	B	50	LYS	3.6
5	S	203	GLU	3.6
9	W	191	LYS	3.6
1	A	55	LEU	3.6
10	X	193	ASP	3.6
5	E	201	ARG	3.5
1	O	201	GLU	3.5
3	C	48	SER	3.5
1	O	2	THR	3.5
2	P	240	LYS	3.5
10	J	193	ASP	3.5
6	T	235	ALA	3.5
3	C	216	ASP	3.5
7	G	241	GLU	3.5
3	C	239	GLN	3.4
6	T	205	GLU	3.4
5	E	117	LYS	3.4
3	Q	55	THR	3.4
5	E	233	ILE	3.4
6	T	53	LYS	3.4
4	R	217	GLN	3.3
3	Q	60	SER	3.3
4	R	125	LEU	3.3
2	B	203	SER	3.3

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Mol	Chain	Res	Type	RSRZ
3	Q	58	THR	3.3
5	S	233	ILE	3.3
7	U	51	PRO	3.3
3	Q	181	GLU	3.3
6	F	178	HIS	3.2
2	P	50	LYS	3.2
6	F	201	GLU	3.2
5	S	3	ASN	3.2
2	P	61	SER	3.2
3	Q	180	LYS	3.2
3	Q	47	ARG	3.2
14	b	105	LYS	3.1
2	P	223	GLU	3.1
5	S	204	SER	3.1
4	D	1	ASP	3.1
3	C	187	GLU	3.1
5	S	171	LEU	3.1
2	B	60	THR	3.1
3	Q	59	PRO	3.1
6	F	244	ASN	3.1
7	G	181	LYS	3.1
5	S	54	GLU	3.1
1	A	229	THR	3.1
2	P	203	SER	3.1
7	U	3	TYR	3.0
4	R	201	GLU	3.0
8	H	222	ASP	3.0
6	F	241	LYS	3.0
5	S	29	LYS	3.0
2	P	230	LYS	3.0
3	Q	175	LYS	3.0
5	E	121	SER	3.0
14	N	105	LYS	3.0
6	T	2	THR	3.0
4	R	116	GLY	3.0
1	A	2	THR	3.0
2	P	62	THR	3.0
13	M	1	THR	3.0
6	F	181	GLU	2.9
5	E	3	ASN	2.9
4	R	1	ASP	2.9
8	H	223	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
7	G	188	GLU	2.9
3	Q	171	GLU	2.9
4	D	241	ALA	2.9
2	B	59	ASP	2.9
7	U	183	ASP	2.9
4	R	241	ALA	2.9
2	P	217	LYS	2.9
12	Z	165	ASN	2.8
9	W	192	ASP	2.8
3	Q	187	GLU	2.8
7	G	230	GLU	2.8
5	S	201	ARG	2.8
5	E	122	TYR	2.8
13	M	47	ASP	2.8
1	A	248	GLU	2.8
3	Q	141	ASP	2.8
3	C	60	SER	2.8
5	S	218	ASP	2.7
2	B	169	SER	2.7
6	F	235	ALA	2.7
3	Q	229	GLN	2.7
6	T	204	LYS	2.7
5	E	217	LYS	2.7
6	T	201	GLU	2.7
4	D	224	ASP	2.7
7	U	222	ASP	2.7
8	V	223	ILE	2.7
12	Z	1	GLN	2.7
4	D	238	LYS	2.7
3	Q	231	VAL	2.7
2	P	182	ASP	2.7
10	J	174	MET	2.7
4	D	47	THR	2.7
8	V	217	ILE	2.6
4	D	2	ARG	2.6
5	E	218	ASP	2.6
5	E	124	GLY	2.6
2	B	238	LEU	2.6
6	T	215	CYS	2.6
7	G	179	LYS	2.6
1	A	201	GLU	2.6
10	J	155	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
3	Q	234	ILE	2.6
2	P	60	THR	2.6
4	D	169	GLU	2.6
5	S	123	GLY	2.6
3	Q	179	ARG	2.6
1	O	61	LEU	2.6
5	E	207	VAL	2.6
3	Q	216	ASP	2.6
6	F	230	ASP	2.6
6	F	180	PRO	2.5
5	E	54	GLU	2.5
8	V	225	GLU	2.5
7	U	181	LYS	2.5
4	R	177	ASN	2.5
5	E	227	GLU	2.5
5	S	194	GLU	2.5
5	E	180	LYS	2.5
6	F	215	CYS	2.5
12	L	1	GLN	2.5
4	D	125	LEU	2.5
5	E	231	LYS	2.4
11	Y	212	GLY	2.4
1	A	59	GLU	2.4
1	A	54	PRO	2.4
4	R	169	GLU	2.4
5	S	122	TYR	2.4
9	W	133	LYS	2.4
4	R	230	GLU	2.4
6	T	229	GLY	2.4
7	G	208	GLU	2.4
5	S	177	THR	2.4
12	Z	210	ASP	2.4
9	I	133	LYS	2.4
6	F	59	LYS	2.4
8	H	202	SER	2.4
2	B	235	LYS	2.4
6	F	202	ASP	2.4
4	R	50	LEU	2.4
4	D	117	GLU	2.4
8	V	145	ASP	2.3
5	E	210	LEU	2.3
9	W	160	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
11	Y	202	GLU	2.3
5	S	30	GLN	2.3
6	T	166	GLN	2.3
3	Q	46	ARG	2.3
11	K	106	ARG	2.3
6	T	236	ILE	2.3
7	G	51	PRO	2.3
2	P	56	LEU	2.3
3	Q	173	LEU	2.3
9	I	192	ASP	2.3
5	E	190	LYS	2.3
3	C	47	ARG	2.3
4	R	239	GLU	2.3
5	S	227	GLU	2.3
7	U	230	GLU	2.3
11	K	147	ASP	2.3
9	I	162	LEU	2.3
3	C	1	GLY	2.3
1	O	50	LYS	2.3
3	C	175	LYS	2.3
12	L	136	CYS	2.2
6	F	203	ASN	2.2
4	D	217	GLN	2.2
1	O	248	GLU	2.2
4	R	114	ARG	2.2
5	E	203	GLU	2.2
7	U	241	GLU	2.2
8	H	198	GLU	2.2
2	B	54	THR	2.2
13	M	82	ASP	2.2
2	P	93	HIS	2.2
10	X	174	MET	2.2
3	C	171	GLU	2.2
8	H	225	GLU	2.2
2	B	223	GLU	2.2
2	B	222	GLY	2.2
4	D	201	GLU	2.2
4	R	237	GLU	2.2
3	Q	233	GLN	2.2
3	C	181	GLU	2.1
3	C	234	ILE	2.1
1	A	220	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
4	R	54	ASP	2.1
1	O	177	LYS	2.1
3	C	235	GLU	2.1
6	F	207	ASP	2.1
5	S	165	GLN	2.1
8	H	208	GLY	2.1
3	Q	169	VAL	2.1
4	R	112	ALA	2.1
6	T	51	THR	2.1
4	R	224	ASP	2.1
8	H	145	ASP	2.1
13	M	171	GLN	2.1
10	J	150	PRO	2.1
6	F	177	ASP	2.1
3	Q	203	THR	2.1
6	T	239	ALA	2.1
11	Y	146	TRP	2.1
5	S	51	ASN	2.1
9	W	117	LYS	2.1
6	T	54	LEU	2.1
3	Q	230	TYR	2.1
7	U	178	LYS	2.0
8	V	219	ASN	2.0
4	R	175	LEU	2.0
6	T	55	LEU	2.0
8	V	215	GLU	2.0
11	K	73	ARG	2.0
5	S	217	LYS	2.0
5	S	229	VAL	2.0
7	G	236	LEU	2.0
3	C	27	ARG	2.0
5	E	176	ASP	2.0
10	X	149	ARG	2.0
2	B	204	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

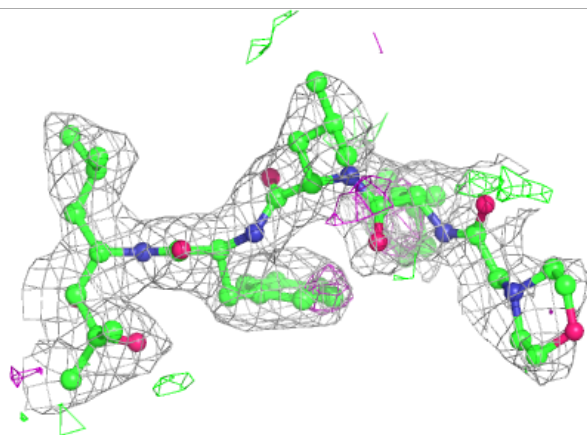
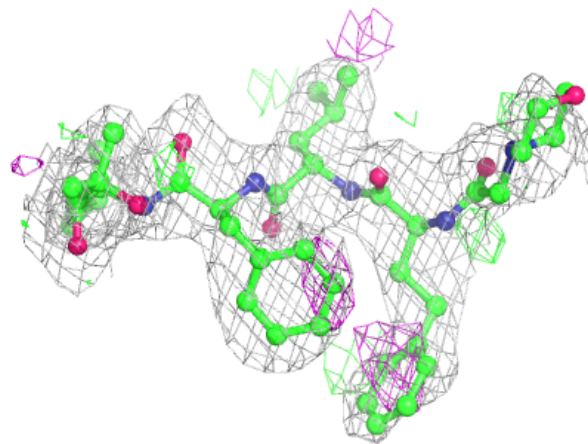
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	MG	K	302	1/1	0.77	0.33	90,90,90,90	0
18	MES	V	302	12/12	0.79	0.44	94,145,153,154	12
15	MG	I	302	1/1	0.89	0.26	76,76,76,76	0
18	MES	H	302	12/12	0.89	0.31	85,141,150,151	12
17	GWZ	b	201	52/52	0.90	0.16	24,35,113,117	0
18	MES	Y	302	12/12	0.90	0.34	55,101,104,104	12
15	MG	G	301	1/1	0.90	0.14	72,72,72,72	0
17	GWZ	N	201	52/52	0.90	0.17	24,32,113,116	0
17	GWZ	V	301	52/52	0.90	0.16	41,51,98,101	0
17	GWZ	H	301	52/52	0.91	0.16	41,52,104,106	0
15	MG	I	301	1/1	0.91	0.15	81,81,81,81	0
17	GWZ	Y	301	52/52	0.92	0.14	25,33,83,87	0
18	MES	K	303	12/12	0.93	0.34	58,101,104,105	12
17	GWZ	K	301	52/52	0.93	0.14	26,34,86,93	0
15	MG	Z	301	1/1	0.94	0.38	82,82,82,82	0
19	SO4	N	203	5/5	0.94	0.18	53,77,97,101	5
19	SO4	b	202	5/5	0.95	0.18	55,84,93,99	5
15	MG	W	301	1/1	0.95	0.30	71,71,71,71	0
15	MG	L	301	1/1	0.98	0.08	60,60,60,60	0
16	CL	U	301	1/1	0.98	0.07	56,56,56,56	0
15	MG	N	202	1/1	0.98	0.13	58,58,58,58	0
16	CL	G	302	1/1	0.99	0.07	48,48,48,48	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.

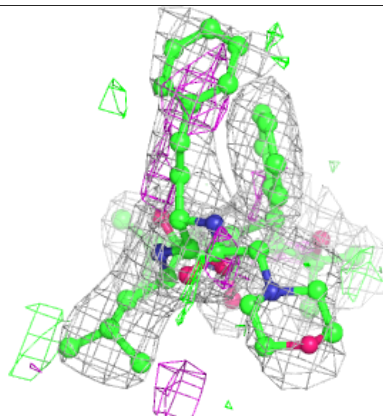
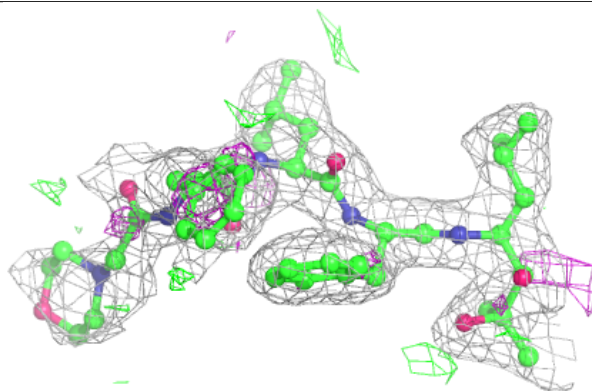
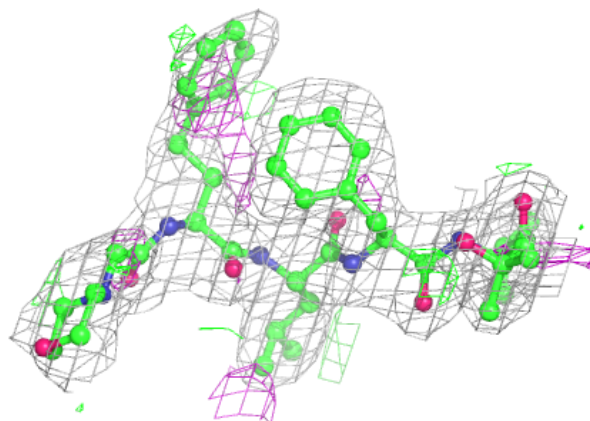
Electron density around GWZ b 201:

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

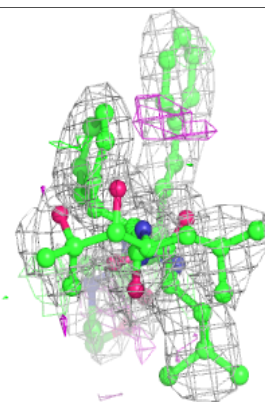
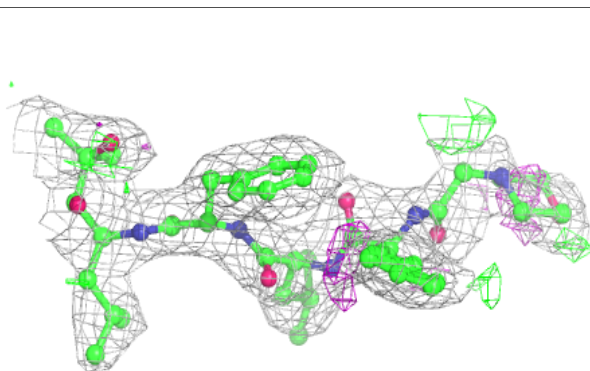
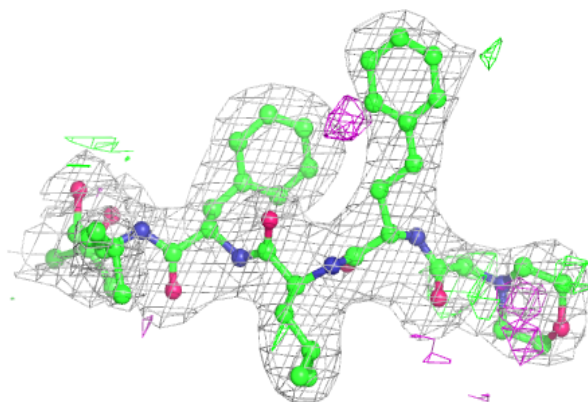


Electron density around GWZ N 201:

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

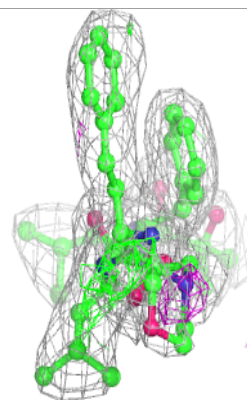
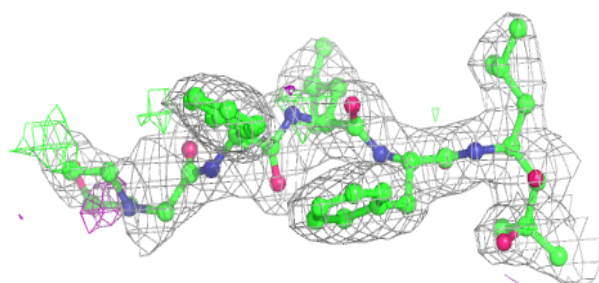
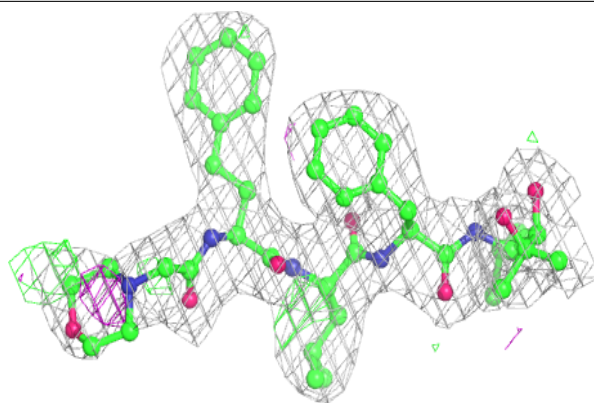
**Electron density around GWZ V 301:**

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

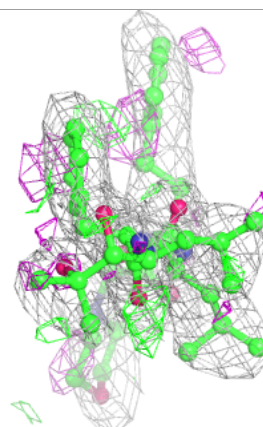
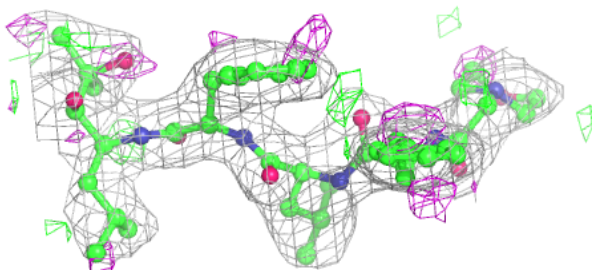
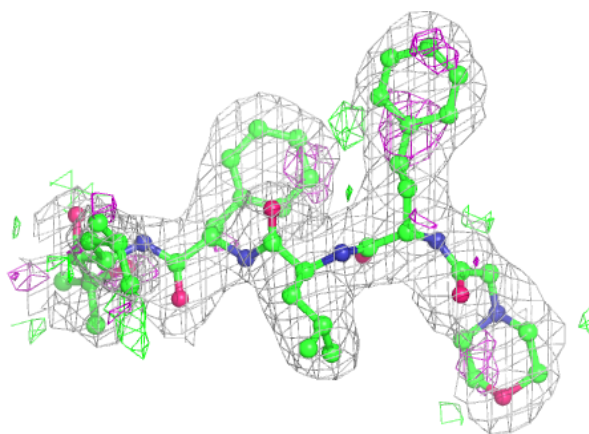


Electron density around GWZ H 301:

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

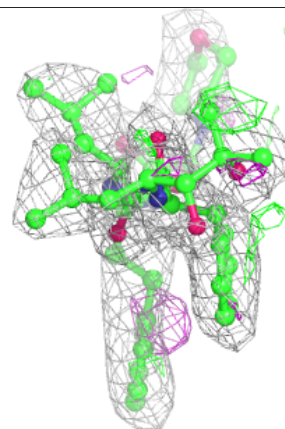
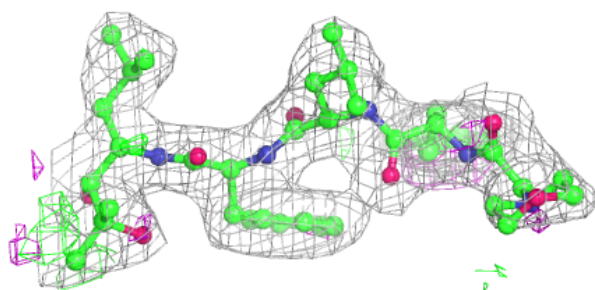
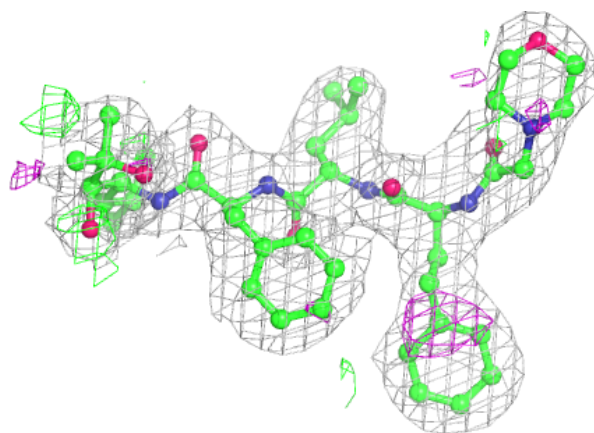
**Electron density around GWZ Y 301:**

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



Electron density around GWZ 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.