



# Full wwPDB X-ray Structure Validation Report ⓘ

May 10, 2021 – 02:25 pm BST

PDB ID : 6ZP8  
Title : Yeast 20S proteasome in complex with glidobactin-like natural product HB335  
Authors : Zhao, L.; Le Chapelain, C.; Brachmann, A.O.; Kaiser, M.; Groll, M.; Bode, H.B.  
Deposited on : 2020-07-08  
Resolution : 3.00 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](mailto: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.

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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 : 2.18  
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) : 2.18

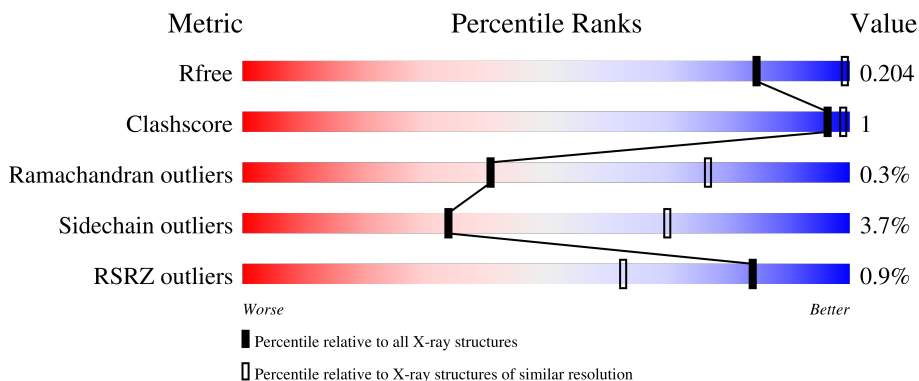
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	98%
1	O	250	98%
2	B	258	2% 88% 6% 5%
2	P	258	2% 88% 6% 5%
3	C	254	2% 86% 7% 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	3% 87% 7% • 6%
4	D	260	86% • • 10%
4	R	260	84% 6% 10%
5	E	234	% 93% 5% •
5	S	234	93% 6% •
6	F	288	80% • 16%
6	T	288	80% • 16%
7	G	252	90% 6% •
7	U	252	% 90% 6% •
8	H	232	3% 93% • • •
8	V	232	3% 92% • • •
9	I	205	94% 5%
9	W	205	95% 5%
10	J	198	% 93% 5% • •
10	X	198	% 93% 5% • •
11	K	212	92% 7% •
11	Y	212	93% 6%
12	L	222	96% •
12	Z	222	95% 5%
13	M	246	90% • 7%
13	a	246	91% • 6%
14	N	196	95% • •
14	b	196	% 97% •

## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 49792 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	212	1644	1045	280	312	7	0	0	0
11	Y	212	1644	1045	280	312	7	0	0	0

- Molecule 12 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	222	1757	1115	303	335	4	0	0	0
12	Z	222	1757	1115	303	335	4	0	0	0

- Molecule 13 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	M	229	1790	1133	306	344	7	0	0	0
13	a	232	1815	1148	311	349	7	0	0	0

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

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

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

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

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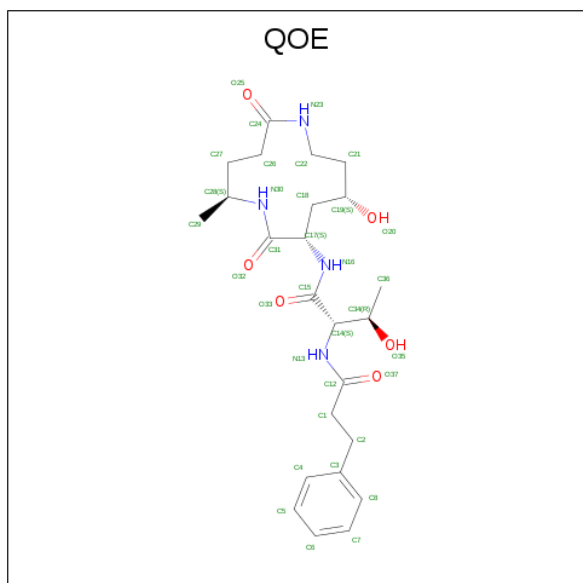
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	K	1	Total Mg 1 1	0	0
15	N	1	Total Mg 1 1	0	0
15	V	1	Total Mg 1 1	0	0
15	W	1	Total Mg 1 1	0	0
15	Y	1	Total Mg 1 1	0	0
15	Z	1	Total Mg 1 1	0	0

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

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

- Molecule 17 is (2 {S},3 {R})- {N}-[(5 {S},8 {S},10 {S})-5-methyl-10-oxidanyl-2,7-bis(oxidanylidene)-1,6-diazacyclododec-8-yl]-3-oxidanyl-2-(3-phenylpropanoylamino)butanamide (three-letter code: QOE) (formula: C<sub>24</sub>H<sub>36</sub>N<sub>4</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	H	1	Total	C	N	O	0	0
			34	24	4	6		
17	K	1	Total	C	N	O	0	0
			34	24	4	6		
17	V	1	Total	C	N	O	0	0
			34	24	4	6		
17	Y	1	Total	C	N	O	0	0
			34	24	4	6		

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	10	Total	O	0	0
			10	10		
18	B	17	Total	O	0	0
			17	17		
18	C	12	Total	O	0	0
			12	12		
18	D	5	Total	O	0	0
			5	5		
18	E	9	Total	O	0	0
			9	9		
18	F	14	Total	O	0	0
			14	14		
18	G	7	Total	O	0	0
			7	7		
18	H	13	Total	O	0	0
			13	13		
18	I	5	Total	O	0	0
			5	5		
18	J	13	Total	O	0	0
			13	13		
18	K	6	Total	O	0	0
			6	6		
18	L	21	Total	O	0	0
			21	21		
18	M	18	Total	O	0	0
			18	18		
18	N	11	Total	O	0	0
			11	11		
18	O	5	Total	O	0	0
			5	5		
18	P	14	Total	O	0	0
			14	14		

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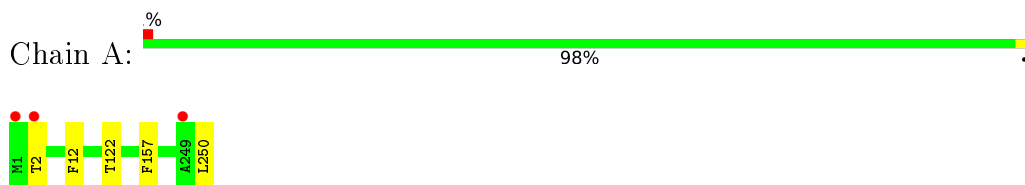
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
18	Q	11	Total 11	O 11	0	0
18	R	10	Total 10	O 10	0	0
18	S	7	Total 7	O 7	0	0
18	T	11	Total 11	O 11	0	0
18	U	15	Total 15	O 15	0	0
18	V	16	Total 16	O 16	0	0
18	W	7	Total 7	O 7	0	0
18	X	12	Total 12	O 12	0	0
18	Y	9	Total 9	O 9	0	0
18	Z	18	Total 18	O 18	0	0
18	a	14	Total 14	O 14	0	0
18	b	13	Total 13	O 13	0	0

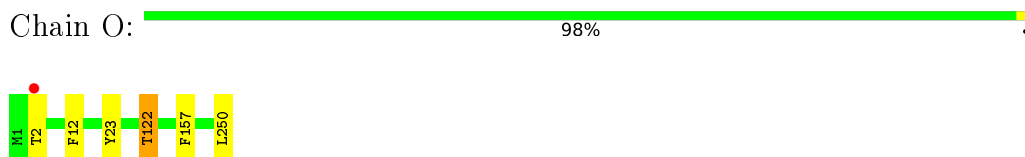
### 3 Residue-property plots [i](#)

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

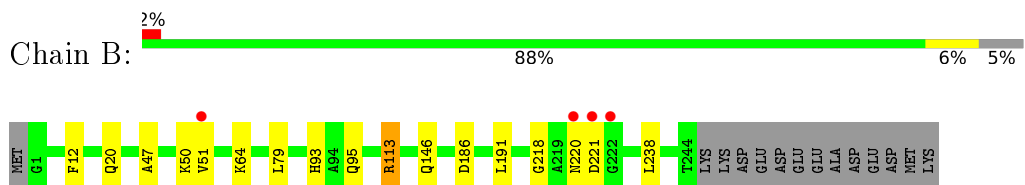
- Molecule 1: Proteasome subunit alpha type-2



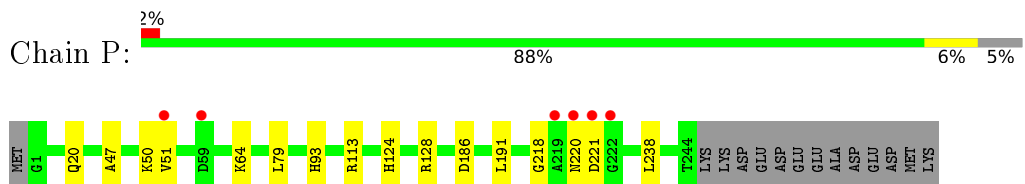
- Molecule 1: Proteasome subunit alpha type-2



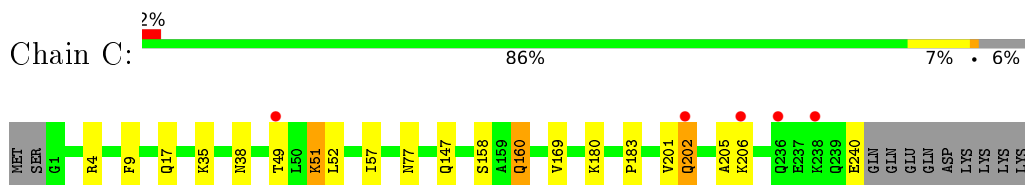
- Molecule 2: Proteasome subunit alpha type-3



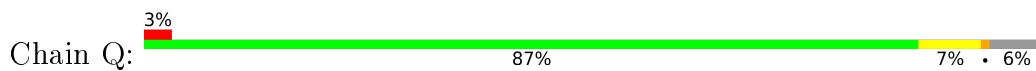
- Molecule 2: Proteasome subunit alpha type-3



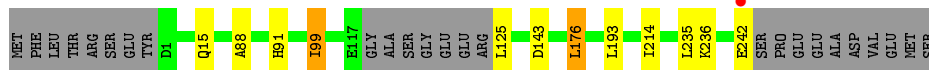
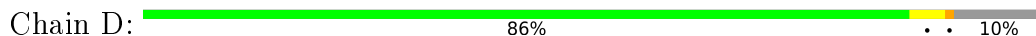
- Molecule 3: Proteasome subunit alpha type-4



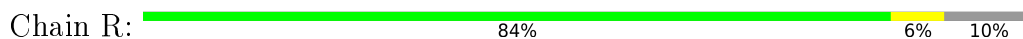
- Molecule 3: Proteasome subunit alpha type-4



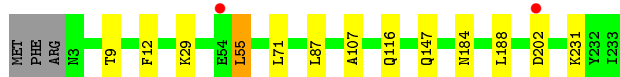
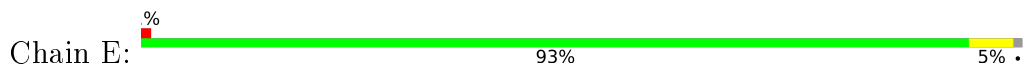
- Molecule 4: Proteasome subunit alpha type-5



- Molecule 4: Proteasome subunit alpha type-5



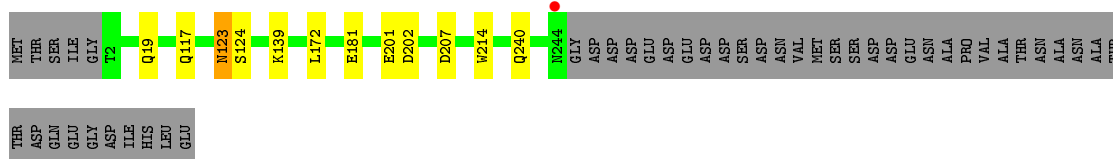
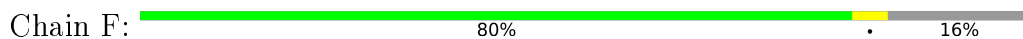
- Molecule 5: Proteasome subunit alpha type-6



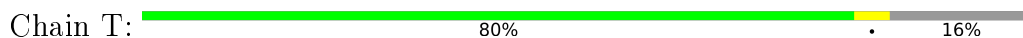
- Molecule 5: Proteasome subunit alpha type-6

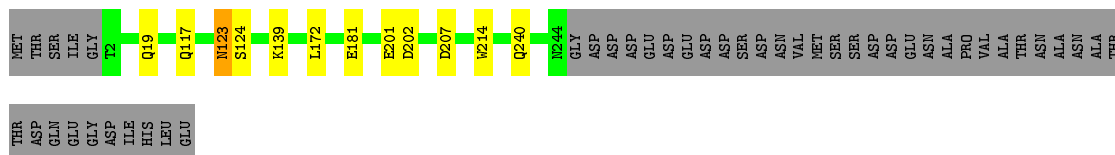


- Molecule 6: Probable proteasome subunit alpha type-7



- Molecule 6: Probable proteasome subunit alpha type-7





- Molecule 7: Proteasome subunit alpha type-1

Chain G: 90% 6%



- Molecule 7: Proteasome subunit alpha type-1

Chain U: 90% 6%



- Molecule 8: Proteasome subunit beta type-2

Chain H: 93% 3%



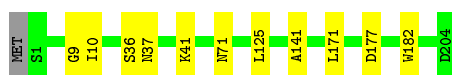
- Molecule 8: Proteasome subunit beta type-2

Chain V: 92% 3%



- Molecule 9: Proteasome subunit beta type-3

Chain I: 94% 5%

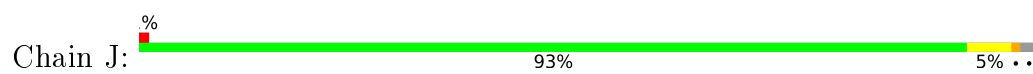


- Molecule 9: Proteasome subunit beta type-3

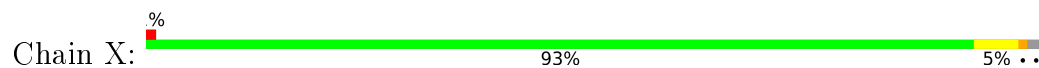
Chain W: 95% 5%



- 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



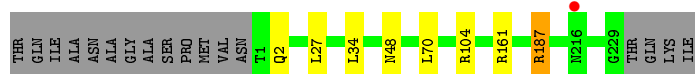
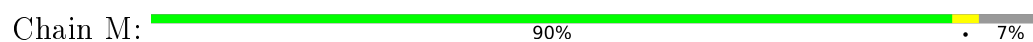
- Molecule 12: Proteasome subunit beta type-6




- Molecule 12: Proteasome subunit beta type-6

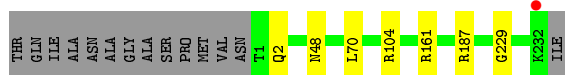


- Molecule 13: Proteasome subunit beta type-7



- Molecule 13: Proteasome subunit beta type-7

Chain a:  91%  6%



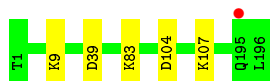
- Molecule 14: Proteasome subunit beta type-1

Chain N:  95% 



- Molecule 14: Proteasome subunit beta type-1

Chain b:  97% 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.16Å 300.12Å 144.83Å 90.00° 113.11° 90.00°	Depositor
Resolution (Å)	15.00 – 3.00 15.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.4 (15.00-3.00) 99.2 (15.00-3.00)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.50 (at 3.01Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.167 , 0.200 0.173 , 0.204	Depositor DCC
$R_{free}$ test set	10458 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.6	Xtrriage
Anisotropy	0.274	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 39.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	49792	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, QOE, 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	0.36	0/1952	0.57	0/2642
1	O	0.36	0/1952	0.58	0/2642
2	B	0.37	0/1934	0.62	0/2618
2	P	0.36	0/1934	0.62	0/2618
3	C	0.36	0/1910	0.64	0/2586
3	Q	0.36	0/1910	0.63	0/2586
4	D	0.35	0/1837	0.59	0/2475
4	R	0.35	0/1837	0.59	0/2475
5	E	0.36	0/1800	0.59	0/2433
5	S	0.35	0/1800	0.59	0/2433
6	F	0.36	0/1932	0.56	0/2609
6	T	0.35	0/1932	0.56	0/2609
7	G	0.36	0/1945	0.58	0/2634
7	U	0.36	0/1945	0.57	0/2634
8	H	0.34	0/1750	0.60	1/2373 (0.0%)
8	V	0.34	0/1750	0.61	1/2373 (0.0%)
9	I	0.36	0/1611	0.59	0/2174
9	W	0.35	0/1611	0.59	0/2174
10	J	0.35	0/1589	0.61	0/2142
10	X	0.35	0/1589	0.62	0/2142
11	K	0.35	0/1681	0.62	1/2274 (0.0%)
11	Y	0.34	0/1681	0.63	1/2274 (0.0%)
12	L	0.36	0/1795	0.60	0/2420
12	Z	0.36	0/1795	0.59	0/2420
13	M	0.37	0/1821	0.64	0/2470
13	a	0.36	0/1846	0.64	0/2503
14	N	0.34	0/1541	0.60	1/2087 (0.0%)
14	b	0.34	0/1541	0.60	0/2087
All	All	0.35	0/50221	0.60	5/67907 (0.0%)

There are no bond length outliers.



All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	V	196	ARG	NE-CZ-NH1	5.39	122.99	120.30
8	H	196	ARG	NE-CZ-NH1	5.32	122.96	120.30
11	Y	4	LEU	CA-CB-CG	5.24	127.34	115.30
11	K	4	LEU	CA-CB-CG	5.13	127.10	115.30
14	N	36	ARG	NE-CZ-NH2	-5.03	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	1	0
1	O	1915	0	1929	3	0
2	B	1904	0	1904	7	0
2	P	1904	0	1904	5	0
3	C	1881	0	1895	7	0
3	Q	1881	0	1895	6	0
4	D	1813	0	1797	5	0
4	R	1813	0	1797	6	0
5	E	1773	0	1775	4	0
5	S	1773	0	1775	3	0
6	F	1892	0	1883	3	0
6	T	1892	0	1883	3	0
7	G	1907	0	1901	3	0
7	U	1907	0	1901	3	0
8	H	1719	0	1718	6	0
8	V	1719	0	1718	8	0
9	I	1581	0	1574	7	0
9	W	1581	0	1574	6	0
10	J	1561	0	1569	5	0
10	X	1561	0	1569	4	0
11	K	1644	0	1594	5	0
11	Y	1644	0	1594	3	0
12	L	1757	0	1711	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	Z	1757	0	1711	4	0
13	M	1790	0	1793	2	0
13	a	1815	0	1821	0	0
14	N	1512	0	1481	4	0
14	b	1512	0	1481	0	0
15	G	1	0	0	0	0
15	I	1	0	0	0	0
15	K	1	0	0	0	0
15	N	1	0	0	0	0
15	V	1	0	0	0	0
15	W	1	0	0	0	0
15	Y	1	0	0	0	0
15	Z	1	0	0	0	0
16	G	1	0	0	0	0
16	U	1	0	0	0	0
17	H	34	0	0	2	0
17	K	34	0	0	0	0
17	V	34	0	0	3	0
17	Y	34	0	0	1	0
18	A	10	0	0	0	0
18	B	17	0	0	2	0
18	C	12	0	0	0	0
18	D	5	0	0	0	0
18	E	9	0	0	1	0
18	F	14	0	0	0	0
18	G	7	0	0	0	0
18	H	13	0	0	0	0
18	I	5	0	0	0	0
18	J	13	0	0	0	0
18	K	6	0	0	0	0
18	L	21	0	0	0	0
18	M	18	0	0	0	0
18	N	11	0	0	0	0
18	O	5	0	0	0	0
18	P	14	0	0	1	0
18	Q	11	0	0	0	0
18	R	10	0	0	0	0
18	S	7	0	0	0	0
18	T	11	0	0	0	0
18	U	15	0	0	0	0
18	V	16	0	0	0	0
18	W	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	X	12	0	0	0	0
18	Y	9	0	0	0	0
18	Z	18	0	0	0	0
18	a	14	0	0	0	0
18	b	13	0	0	0	0
All	All	49792	0	49076	95	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 (95) 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)
17:H:901:QOE:C5	9:I:125:LEU:HD21	2.12	0.80
8:H:52:THR:O	8:H:56:THR:OG1	2.09	0.71
17:H:901:QOE:C4	9:I:125:LEU:HD21	2.21	0.70
8:V:52:THR:O	8:V:56:THR:OG1	2.11	0.68
11:Y:1:THR:O	11:Y:130:GLY:HA3	1.97	0.65
17:V:901:QOE:C4	9:W:125:LEU:HD21	2.28	0.64
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.65	0.61
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.65	0.60
2:P:93:HIS:HB3	18:P:301:HOH:O	2.01	0.60
2:B:93:HIS:HB3	18:B:301:HOH:O	2.07	0.55
17:V:901:QOE:C5	9:W:125:LEU:HD21	2.37	0.53
7:G:23:PHE:O	7:G:26:THR:HB	2.08	0.53
8:V:80:LEU:HD21	8:V:111:PHE:CG	2.43	0.53
8:H:80:LEU:HD21	8:H:111:PHE:CG	2.43	0.53
1:O:12:PHE:H	2:P:20:GLN:HE22	1.57	0.53
5:E:12:PHE:H	6:F:19:GLN:HE22	1.58	0.52
2:B:12:PHE:H	3:C:17:GLN:HE22	1.56	0.52
17:Y:901:QOE:N23	17:Y:901:QOE:C18	2.73	0.52
8:H:80:LEU:CD2	8:H:111:PHE:CG	2.93	0.51
7:U:23:PHE:O	7:U:26:THR:HB	2.10	0.51
8:V:80:LEU:CD2	8:V:111:PHE:CG	2.94	0.51
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	1.93	0.51
5:S:12:PHE:H	6:T:19:GLN:HE22	1.59	0.50
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.94	0.50
8:V:35:HIS:HB2	8:V:56:THR:HG21	1.95	0.49
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.95	0.49
8:H:35:HIS:HB2	8:H:56:THR:HG21	1.95	0.49
10:J:21:VAL:HG11	11:K:122:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:68:ARG:HH12	14:N:36:ARG:HH22	1.60	0.48
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.62	0.48
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.79	0.47
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.80	0.46
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.81	0.46
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.98	0.46
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.98	0.45
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.98	0.45
6:F:123:ASN:HD22	6:F:124:SER:N	2.13	0.45
8:H:84:LYS:HA	8:H:113:ILE:HD11	1.98	0.45
1:A:12:PHE:H	2:B:20:GLN:HE22	1.64	0.45
8:V:84:LYS:HA	8:V:113:ILE:HD11	1.99	0.45
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.51	0.45
11:K:1:THR:O	11:K:130:GLY:HA3	2.17	0.44
7:G:73:VAL:HG12	7:G:133:THR:HB	1.99	0.44
3:C:35:LYS:HG2	3:C:158:SER:O	2.18	0.44
9:I:141:ALA:HB2	9:I:177:ASP:HB2	2.00	0.44
6:T:123:ASN:HD22	6:T:124:SER:N	2.14	0.44
8:V:1:THR:N	17:V:901:QOE:C26	2.81	0.43
9:I:10:ILE:HG21	9:I:141:ALA:HB3	2.01	0.43
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.99	0.43
2:B:146:GLN:HG2	3:C:57:ILE:HG21	2.00	0.43
13:M:187:ARG:NH1	8:V:139:GLU:OE1	2.46	0.43
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.53	0.43
9:W:141:ALA:HB2	9:W:177:ASP:HB2	2.01	0.43
2:P:47:ALA:HB1	2:P:64:LYS:HD2	2.01	0.43
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.19	0.43
4:D:88:ALA:HA	4:D:99:ILE:HG21	2.02	0.42
10:J:50:ALA:O	11:K:91:LYS:NZ	2.52	0.42
9:W:10:ILE:HG21	9:W:141:ALA:HB3	2.00	0.42
3:C:201:VAL:O	3:C:202:GLN:CB	2.67	0.42
4:D:91:HIS:CD2	4:D:99:ILE:HG22	2.54	0.42
4:D:176:LEU:HD22	5:E:55:LEU:CD2	2.50	0.42
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.02	0.42
4:R:91:HIS:CD2	4:R:99:ILE:HG22	2.54	0.42
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.66	0.42
4:R:159:TYR:CE1	5:S:56:SER:HB3	2.55	0.42
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.19	0.42
14:N:35:THR:HG21	14:N:45:ARG:HE	1.85	0.42
7:U:73:VAL:HG12	7:U:133:THR:HB	2.01	0.42
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.50	0.42
8:H:80:LEU:CD2	8:H:111:PHE:CD2	3.03	0.42
2:B:47:ALA:HB1	2:B:64:LYS:HD2	2.01	0.41
11:K:20:ALA:HB2	11:K:31:VAL:HG21	2.01	0.41
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.50	0.41
8:V:80:LEU:CD2	8:V:111:PHE:CD2	3.03	0.41
2:B:113:ARG:NE	18:B:301:HOH:O	2.35	0.41
9:W:36:SER:HB2	10:X:126:VAL:HG11	2.03	0.41
13:M:27:LEU:HD21	13:M:34:LEU:HD22	2.02	0.41
12:L:31:THR:CG2	12:L:36:ASN:HD21	2.34	0.41
12:Z:31:THR:CG2	12:Z:36:ASN:HD21	2.33	0.41
6:F:123:ASN:HD22	6:F:123:ASN:C	2.24	0.41
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.19	0.41
10:X:3:ILE:HG23	10:X:18:SER:HB3	2.03	0.41
11:K:116:ASP:OD1	11:K:117:SER:N	2.54	0.41
12:Z:100:LYS:HE3	12:Z:103:PHE:O	2.22	0.41
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.68	0.40
6:T:123:ASN:HD22	6:T:123:ASN:C	2.25	0.40
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	2.03	0.40
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.57	0.40
3:C:51:LYS:O	3:C:52:LEU:HB2	2.19	0.40
3:C:9:PHE:H	4:D:15:GLN:HE22	1.68	0.40
5:E:147:GLN:NE2	18:E:301:HOH:O	2.55	0.40
9:I:36:SER:HB2	10:J:126:VAL:HG11	2.02	0.40
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.51	0.40
10:J:3:ILE:HG23	10:J:18:SER:HB3	2.03	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%)	241 (97%)	6 (2%)	1 (0%)	34	72
1	O	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	34	72
2	B	242/258 (94%)	234 (97%)	4 (2%)	4 (2%)	9	39
2	P	242/258 (94%)	234 (97%)	4 (2%)	4 (2%)	9	39
3	C	238/254 (94%)	233 (98%)	2 (1%)	3 (1%)	12	45
3	Q	238/254 (94%)	233 (98%)	2 (1%)	3 (1%)	12	45
4	D	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
4	R	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
5	E	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
5	S	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
6	F	241/288 (84%)	238 (99%)	3 (1%)	0	100	100
6	T	241/288 (84%)	238 (99%)	3 (1%)	0	100	100
7	G	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
7	U	239/252 (95%)	238 (100%)	1 (0%)	0	100	100
8	H	224/232 (97%)	219 (98%)	5 (2%)	0	100	100
8	V	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	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%)	207 (99%)	3 (1%)	0	100	100
11	Y	210/212 (99%)	207 (99%)	3 (1%)	0	100	100
12	L	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
12	Z	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
13	M	227/246 (92%)	220 (97%)	7 (3%)	0	100	100
13	a	230/246 (94%)	223 (97%)	6 (3%)	1 (0%)	34	72
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	6279/6614 (95%)	6139 (98%)	123 (2%)	17 (0%)	41	76

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR
2	B	51	VAL
2	B	221	ASP
3	C	202	GLN
1	O	2	THR
2	P	51	VAL
2	P	221	ASP
3	Q	202	GLN
2	B	218	GLY
2	B	220	ASN
2	P	218	GLY
2	P	220	ASN
3	C	205	ALA
3	Q	205	ALA
3	C	183	PRO
3	Q	183	PRO
13	a	229	GLY

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	206 (99%)	3 (1%)	67	88
1	O	209/209 (100%)	206 (99%)	3 (1%)	67	88
2	B	203/216 (94%)	197 (97%)	6 (3%)	41	75
2	P	203/216 (94%)	197 (97%)	6 (3%)	41	75
3	C	212/226 (94%)	201 (95%)	11 (5%)	23	59
3	Q	212/226 (94%)	201 (95%)	11 (5%)	23	59
4	D	194/215 (90%)	185 (95%)	9 (5%)	27	64
4	R	194/215 (90%)	184 (95%)	10 (5%)	23	59
5	E	190/193 (98%)	181 (95%)	9 (5%)	26	63
5	S	190/193 (98%)	181 (95%)	9 (5%)	26	63
6	F	201/239 (84%)	191 (95%)	10 (5%)	24	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	T	201/239 (84%)	191 (95%)	10 (5%)	24	60
7	G	206/210 (98%)	197 (96%)	9 (4%)	28	65
7	U	206/210 (98%)	197 (96%)	9 (4%)	28	65
8	H	185/190 (97%)	179 (97%)	6 (3%)	39	74
8	V	185/190 (97%)	179 (97%)	6 (3%)	39	74
9	I	172/173 (99%)	169 (98%)	3 (2%)	60	85
9	W	172/173 (99%)	169 (98%)	3 (2%)	60	85
10	J	173/175 (99%)	168 (97%)	5 (3%)	42	76
10	X	173/175 (99%)	168 (97%)	5 (3%)	42	76
11	K	169/169 (100%)	160 (95%)	9 (5%)	22	58
11	Y	169/169 (100%)	160 (95%)	9 (5%)	22	58
12	L	185/185 (100%)	178 (96%)	7 (4%)	33	69
12	Z	185/185 (100%)	178 (96%)	7 (4%)	33	69
13	M	195/208 (94%)	189 (97%)	6 (3%)	40	75
13	a	198/208 (95%)	192 (97%)	6 (3%)	41	75
14	N	162/162 (100%)	157 (97%)	5 (3%)	40	75
14	b	162/162 (100%)	157 (97%)	5 (3%)	40	75
All	All	5315/5540 (96%)	5118 (96%)	197 (4%)	34	70

All (197) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
2	B	50	LYS
2	B	79	LEU
2	B	113	ARG
2	B	186	ASP
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	49	THR
3	C	51	LYS
3	C	77	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	206	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	116	GLN
5	E	184	ASN
5	E	188	LEU
5	E	202	ASP
5	E	231	LYS
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	172	LEU
6	F	181	GLU
6	F	201	GLU
6	F	202	ASP
6	F	207	ASP
6	F	214	TRP
6	F	240	GLN
7	G	75	ASN
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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	G	236	LEU
8	H	30	ASN
8	H	34	LEU
8	H	56	THR
8	H	68	LEU
8	H	80	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	90	LYS
10	J	99	GLN
11	K	4	LEU
11	K	9	GLN
11	K	97	MET
11	K	104	TYR
11	K	107	LYS
11	K	116	ASP
11	K	131	SER
11	K	140	LEU
11	K	148	LEU
12	L	23	LEU
12	L	31	THR
12	L	49	ASN
12	L	106	TYR
12	L	130	SER
12	L	136	CYS
12	L	150	LEU
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
14	N	9	LYS
14	N	39	ASP
14	N	83	LYS
14	N	104	ASP
14	N	107	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	50	LYS
2	P	79	LEU
2	P	113	ARG
2	P	186	ASP
2	P	191	LEU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	50	LEU
3	Q	51	LYS
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	206	LYS
3	Q	240	GLU
4	R	40	LEU
4	R	99	ILE
4	R	125	LEU
4	R	143	ASP
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	55	LEU
5	S	71	LEU
5	S	116	GLN
5	S	184	ASN
5	S	188	LEU
5	S	202	ASP
5	S	231	LYS
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	T	172	LEU
6	T	181	GLU
6	T	201	GLU
6	T	202	ASP
6	T	207	ASP
6	T	214	TRP
6	T	240	GLN
7	U	75	ASN
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN
7	U	122	ARG
7	U	125	MET
7	U	208	GLU
7	U	235	ARG
7	U	236	LEU
8	V	30	ASN
8	V	34	LEU
8	V	56	THR
8	V	68	LEU
8	V	80	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	90	LYS
10	X	99	GLN
11	Y	4	LEU
11	Y	9	GLN
11	Y	97	MET
11	Y	104	TYR
11	Y	107	LYS
11	Y	116	ASP
11	Y	131	SER
11	Y	140	LEU
11	Y	148	LEU
12	Z	23	LEU
12	Z	31	THR
12	Z	49	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
12	Z	106	TYR
12	Z	130	SER
12	Z	136	CYS
12	Z	150	LEU
13	a	2	GLN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
14	b	9	LYS
14	b	39	ASP
14	b	83	LYS
14	b	104	ASP
14	b	107	LYS

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

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	100	ASN
4	D	146	GLN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	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	165	ASN
8	H	172	ASN
8	H	189	ASN
9	I	37	ASN
10	J	55	GLN
11	K	85	ASN
11	K	176	ASN
11	K	208	ASN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	79	HIS
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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	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
5	S	59	GLN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	151	ASN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
6	T	240	GLN
7	U	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	GLN
8	V	30	ASN
8	V	116	HIS
8	V	165	ASN
8	V	172	ASN
8	V	189	ASN
9	W	37	ASN

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Mol	Chain	Res	Type
10	X	55	GLN
10	X	86	GLN
11	Y	85	ASN
11	Y	176	ASN
11	Y	208	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	55	ASN
12	Z	70	ASN
12	Z	79	HIS
12	Z	158	ASN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	179	ASN
13	a	194	ASN
13	a	213	GLN
14	b	161	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 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	QOE	K	901	11	35,35,35	2.31	6 (17%)	44,46,46	1.26	3 (6%)
17	QOE	H	901	8	35,35,35	2.22	6 (17%)	44,46,46	1.15	4 (9%)
17	QOE	V	901	8	35,35,35	2.17	5 (14%)	44,46,46	1.35	7 (15%)
17	QOE	Y	901	11	35,35,35	2.18	4 (11%)	44,46,46	1.35	5 (11%)

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	QOE	K	901	11	-	15/44/44/44	0/1/2/2
17	QOE	H	901	8	-	5/44/44/44	0/1/2/2
17	QOE	V	901	8	-	5/44/44/44	0/1/2/2
17	QOE	Y	901	11	-	7/44/44/44	0/1/2/2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	901	QOE	C26-C24	-8.29	1.35	1.51
17	H	901	QOE	C26-C24	-8.16	1.35	1.51
17	V	901	QOE	C26-C24	-8.13	1.36	1.51
17	Y	901	QOE	C17-C31	-7.13	1.34	1.52
17	Y	901	QOE	C26-C24	-7.10	1.37	1.51
17	K	901	QOE	C17-C31	-6.91	1.34	1.52
17	H	901	QOE	C17-C31	-6.78	1.35	1.52
17	V	901	QOE	C17-C31	-6.22	1.36	1.52
17	Y	901	QOE	C2-C3	-4.99	1.37	1.51
17	K	901	QOE	C2-C3	-4.76	1.37	1.51
17	H	901	QOE	C2-C3	-4.60	1.38	1.51
17	V	901	QOE	C2-C3	-4.42	1.38	1.51
17	V	901	QOE	C27-C28	-3.09	1.48	1.53
17	H	901	QOE	C18-C19	-2.51	1.46	1.52
17	K	901	QOE	C24-N23	2.49	1.39	1.33
17	Y	901	QOE	C24-N23	2.38	1.38	1.33
17	H	901	QOE	O20-C19	-2.14	1.37	1.43
17	H	901	QOE	C24-N23	2.12	1.38	1.33
17	V	901	QOE	C34-C14	-2.12	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	901	QOE	C27-C28	-2.10	1.49	1.53
17	K	901	QOE	O35-C34	-2.06	1.37	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Y	901	QOE	C26-C27-C28	-4.21	107.54	114.02
17	V	901	QOE	C26-C27-C28	-3.81	108.16	114.02
17	K	901	QOE	C22-N23-C24	3.34	129.03	122.84
17	K	901	QOE	C26-C27-C28	-3.20	109.10	114.02
17	V	901	QOE	C15-C14-N13	-3.04	102.08	110.36
17	Y	901	QOE	C22-N23-C24	2.94	128.30	122.84
17	V	901	QOE	C34-C14-N13	-2.85	104.43	111.72
17	H	901	QOE	C34-C14-N13	-2.53	105.24	111.72
17	V	901	QOE	O35-C34-C14	-2.38	104.35	109.13
17	K	901	QOE	C36-C34-C14	-2.27	107.70	112.29
17	Y	901	QOE	C31-C17-N16	-2.26	105.00	111.16
17	H	901	QOE	C34-C14-C15	-2.26	106.30	111.28
17	H	901	QOE	C18-C19-C21	-2.25	107.67	112.51
17	H	901	QOE	C26-C27-C28	-2.25	110.56	114.02
17	V	901	QOE	C29-C28-C27	-2.25	107.22	111.47
17	Y	901	QOE	C27-C26-C24	2.20	117.96	113.04
17	V	901	QOE	O32-C31-N30	-2.19	118.88	122.93
17	Y	901	QOE	C1-C2-C3	2.15	120.55	112.70
17	V	901	QOE	C18-C19-C21	-2.05	108.11	112.51

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	H	901	QOE	N16-C17-C18-C19
17	H	901	QOE	C24-C26-C27-C28
17	K	901	QOE	N16-C17-C18-C19
17	K	901	QOE	O20-C19-C21-C22
17	K	901	QOE	C18-C19-C21-C22
17	K	901	QOE	C17-C18-C19-C21
17	K	901	QOE	C17-C18-C19-O20
17	K	901	QOE	C15-C14-C34-O35
17	K	901	QOE	N13-C14-C34-O35
17	V	901	QOE	N16-C17-C18-C19
17	V	901	QOE	O20-C19-C21-C22
17	V	901	QOE	C24-C26-C27-C28

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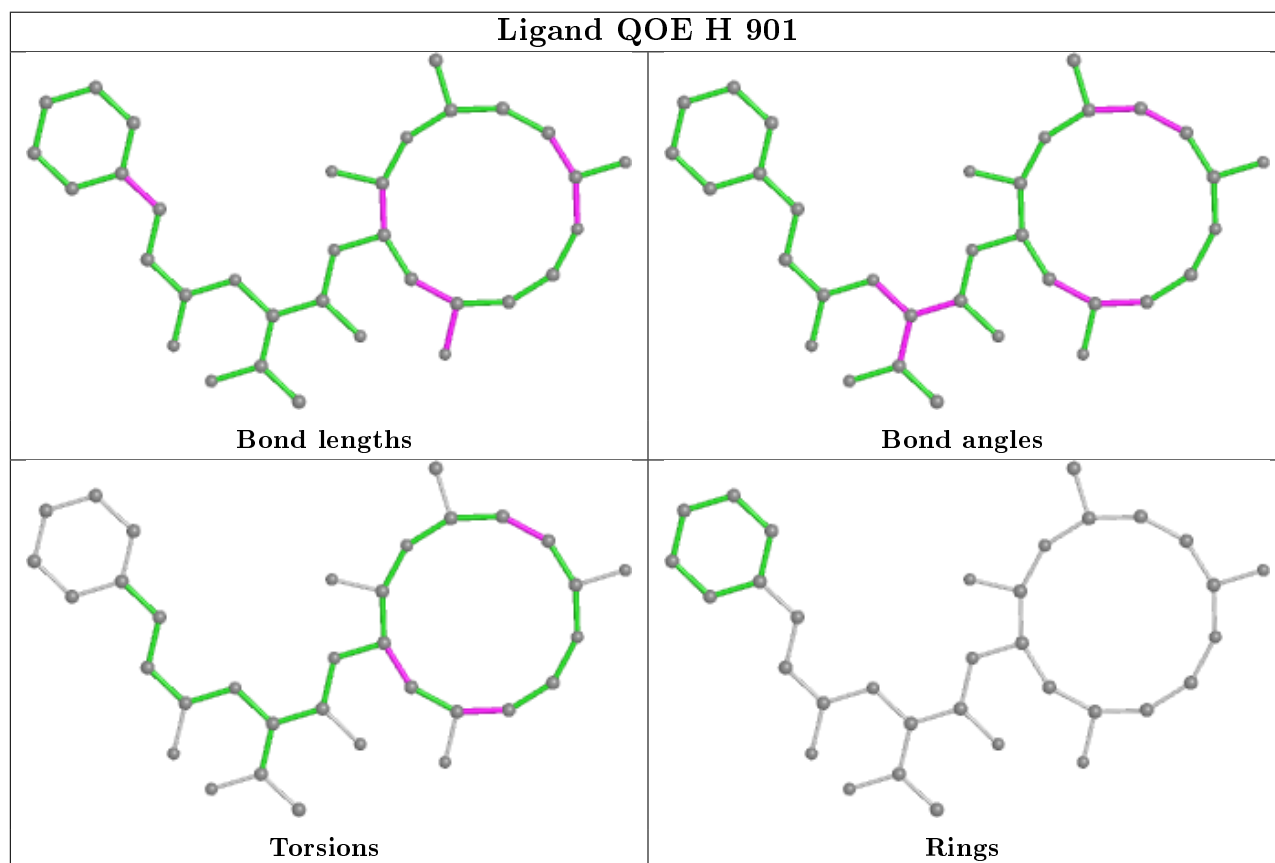
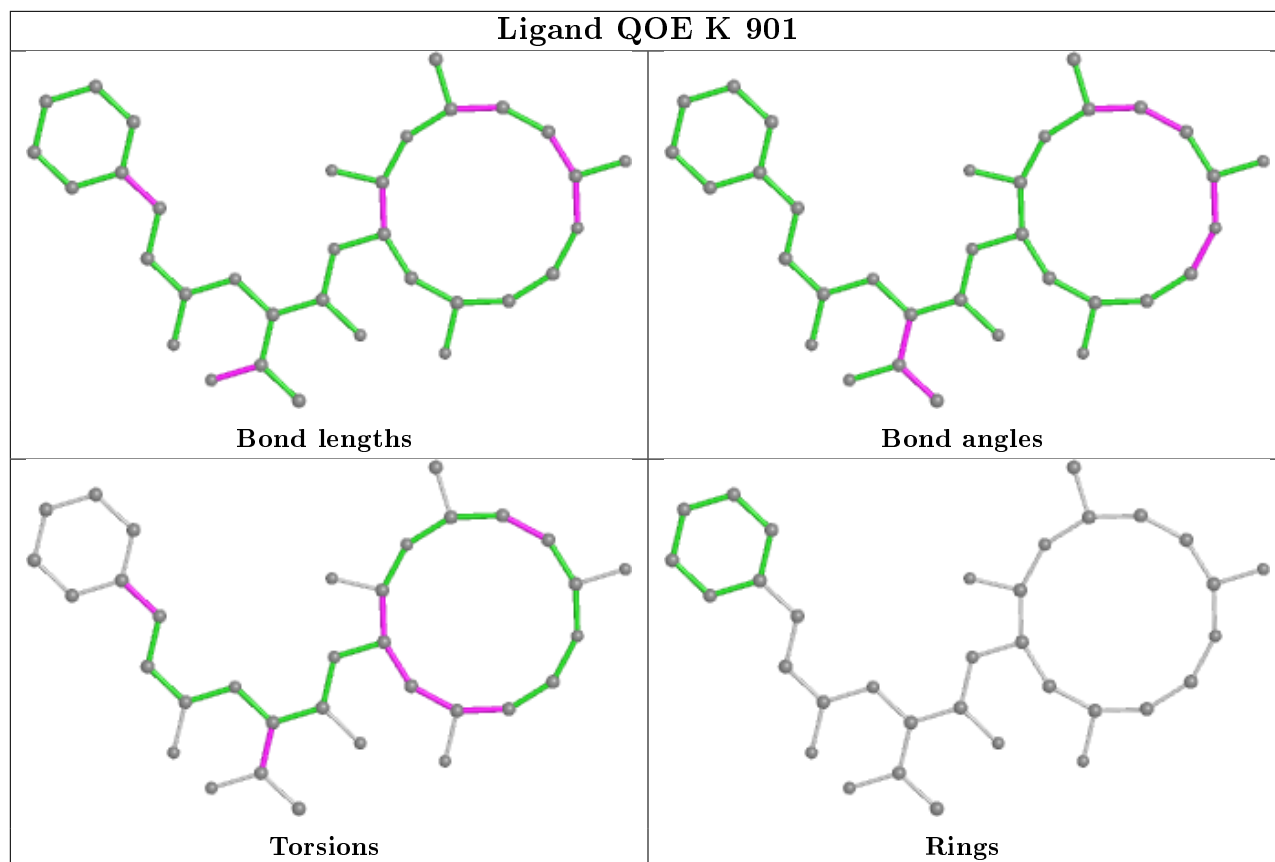
Mol	Chain	Res	Type	Atoms
17	Y	901	QOE	N16-C17-C18-C19
17	Y	901	QOE	O20-C19-C21-C22
17	Y	901	QOE	C18-C19-C21-C22
17	H	901	QOE	C31-C17-C18-C19
17	K	901	QOE	C31-C17-C18-C19
17	V	901	QOE	C31-C17-C18-C19
17	Y	901	QOE	C31-C17-C18-C19
17	Y	901	QOE	C17-C18-C19-O20
17	Y	901	QOE	C17-C18-C19-C21
17	Y	901	QOE	C24-C26-C27-C28
17	K	901	QOE	N13-C14-C34-C36
17	K	901	QOE	C15-C14-C34-C36
17	H	901	QOE	C18-C19-C21-C22
17	V	901	QOE	C18-C19-C21-C22
17	H	901	QOE	O20-C19-C21-C22
17	K	901	QOE	C24-C26-C27-C28
17	K	901	QOE	C1-C2-C3-C8
17	K	901	QOE	C1-C2-C3-C4
17	K	901	QOE	N16-C17-C31-O32
17	K	901	QOE	N16-C17-C31-N30

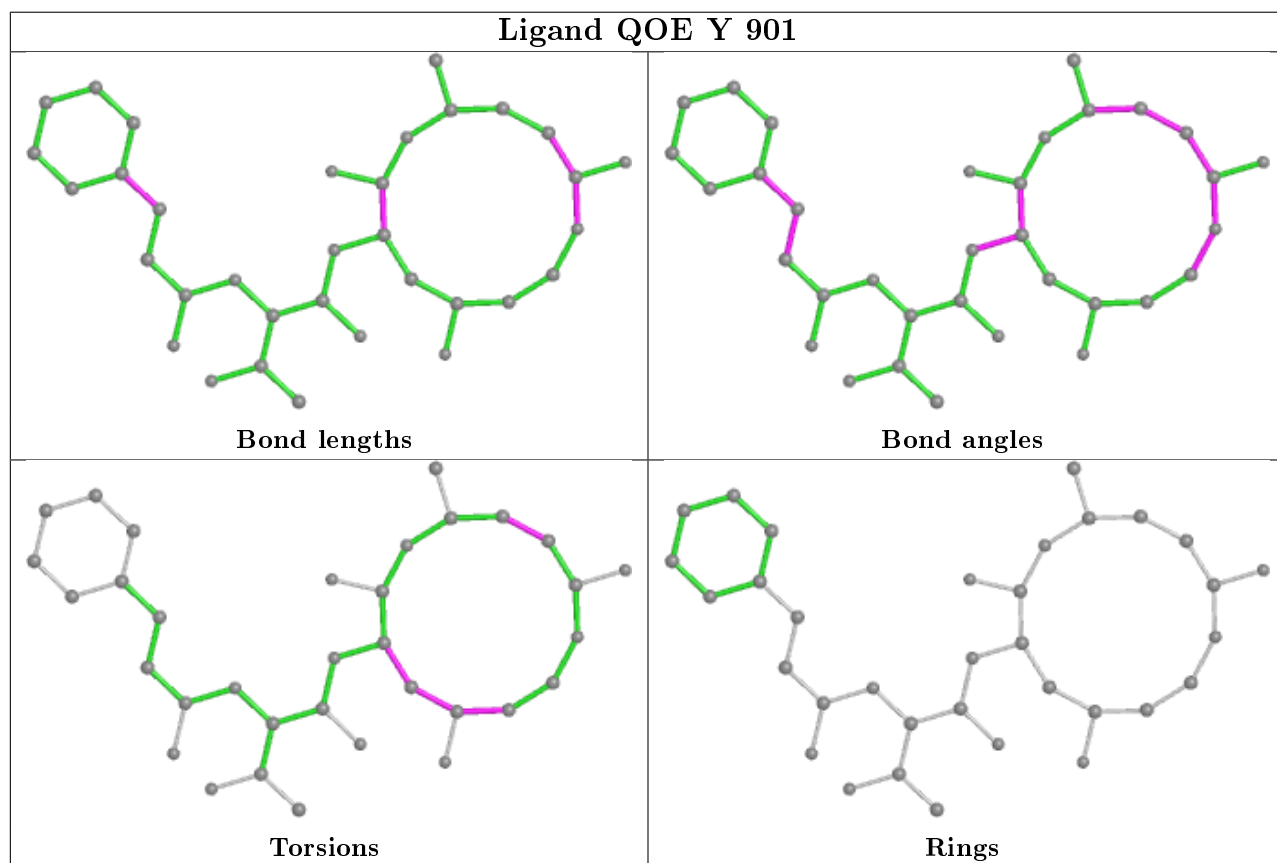
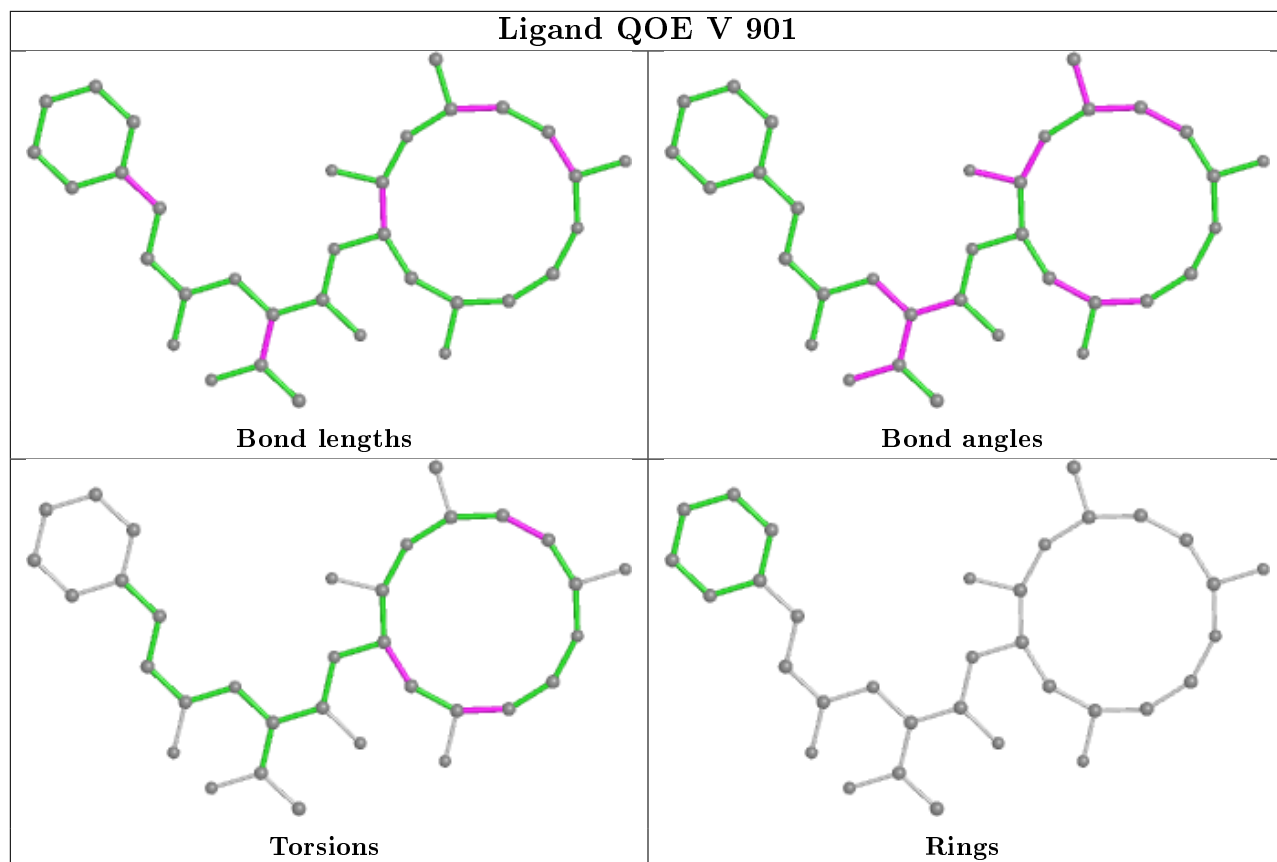
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	H	901	QOE	2	0
17	V	901	QOE	3	0
17	Y	901	QOE	1	0

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	250/250 (100%)	-0.62	3 (1%) 79 54	44, 58, 93, 135	0
1	O	250/250 (100%)	-0.62	1 (0%) 92 79	46, 64, 107, 135	0
2	B	244/258 (94%)	-0.57	4 (1%) 72 44	43, 62, 107, 163	0
2	P	244/258 (94%)	-0.51	6 (2%) 57 29	49, 67, 109, 159	0
3	C	240/254 (94%)	-0.49	5 (2%) 63 34	43, 67, 127, 148	0
3	Q	240/254 (94%)	-0.34	7 (2%) 51 23	52, 79, 158, 182	0
4	D	235/260 (90%)	-0.63	1 (0%) 92 79	49, 69, 102, 140	0
4	R	235/260 (90%)	-0.58	0 100 100	50, 74, 114, 147	0
5	E	231/234 (98%)	-0.54	2 (0%) 84 63	52, 72, 111, 152	0
5	S	231/234 (98%)	-0.44	1 (0%) 92 79	52, 80, 128, 169	0
6	F	243/288 (84%)	-0.67	1 (0%) 92 79	42, 63, 114, 140	0
6	T	243/288 (84%)	-0.63	0 100 100	42, 71, 128, 159	0
7	G	241/252 (95%)	-0.70	0 100 100	38, 58, 92, 138	0
7	U	241/252 (95%)	-0.66	2 (0%) 86 65	44, 60, 95, 139	0
8	H	226/232 (97%)	-0.63	6 (2%) 54 26	39, 55, 94, 159	0
8	V	226/232 (97%)	-0.59	6 (2%) 54 26	44, 57, 94, 176	0
9	I	204/205 (99%)	-0.82	0 100 100	40, 56, 86, 111	0
9	W	204/205 (99%)	-0.82	1 (0%) 91 75	42, 56, 90, 113	0
10	J	195/198 (98%)	-0.74	1 (0%) 91 75	40, 57, 81, 133	0
10	X	195/198 (98%)	-0.71	2 (1%) 82 59	42, 59, 83, 148	0
11	K	212/212 (100%)	-0.69	1 (0%) 91 75	42, 59, 87, 108	0
11	Y	212/212 (100%)	-0.73	1 (0%) 91 75	46, 59, 89, 108	0
12	L	222/222 (100%)	-0.70	1 (0%) 91 75	42, 58, 96, 127	0
12	Z	222/222 (100%)	-0.73	1 (0%) 91 75	42, 57, 95, 126	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	229/246 (93%)	-0.76	1 (0%) 92 79	38, 57, 82, 98	0
13	a	232/246 (94%)	-0.73	1 (0%) 92 79	38, 56, 81, 93	0
14	N	196/196 (100%)	-0.81	0 100 100	39, 51, 82, 105	0
14	b	196/196 (100%)	-0.78	1 (0%) 91 75	39, 52, 81, 117	0
All	All	6339/6614 (95%)	-0.65	56 (0%) 84 63	38, 62, 108, 182	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	49	THR	6.6
8	V	224	GLN	5.7
8	V	226	GLU	4.9
8	V	225	GLU	4.8
2	B	221	ASP	4.6
5	E	202	ASP	4.5
2	P	220	ASN	4.4
8	V	222	ASP	4.4
2	P	221	ASP	4.2
8	H	224	GLN	3.7
2	B	220	ASN	3.7
3	C	206	LYS	3.6
3	Q	50	LEU	3.6
2	B	51	VAL	3.6
3	Q	206	LYS	3.5
10	X	1	MET	3.4
8	V	223	ILE	3.3
8	V	221	CYS	3.2
8	H	222	ASP	3.2
2	P	219	ALA	3.1
8	H	226	GLU	3.1
5	S	202	ASP	3.1
2	P	222	GLY	3.0
3	C	49	THR	2.9
9	W	1	SER	2.9
10	J	1	MET	2.7
10	X	194	ASP	2.7
1	A	2	THR	2.7
8	H	221	CYS	2.7
1	O	2	THR	2.6
11	Y	212	GLY	2.6
3	Q	236	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
8	H	223	ILE	2.5
1	A	249	ALA	2.5
14	b	195	GLN	2.4
3	C	202	GLN	2.4
3	Q	239	GLN	2.4
3	Q	240	GLU	2.4
8	H	225	GLU	2.4
12	Z	174	TYR	2.4
11	K	212	GLY	2.4
5	E	54	GLU	2.3
2	P	51	VAL	2.3
2	P	59	ASP	2.2
3	Q	238	LYS	2.2
7	U	222	ASP	2.2
3	C	236	GLN	2.2
12	L	174	TYR	2.1
3	C	238	LYS	2.1
6	F	244	ASN	2.1
13	M	216	ASN	2.1
7	U	242	GLN	2.1
13	a	232	LYS	2.0
2	B	222	GLY	2.0
4	D	242	GLU	2.0
1	A	1	MET	2.0

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

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

## 6.3 Carbohydrates [i](#)

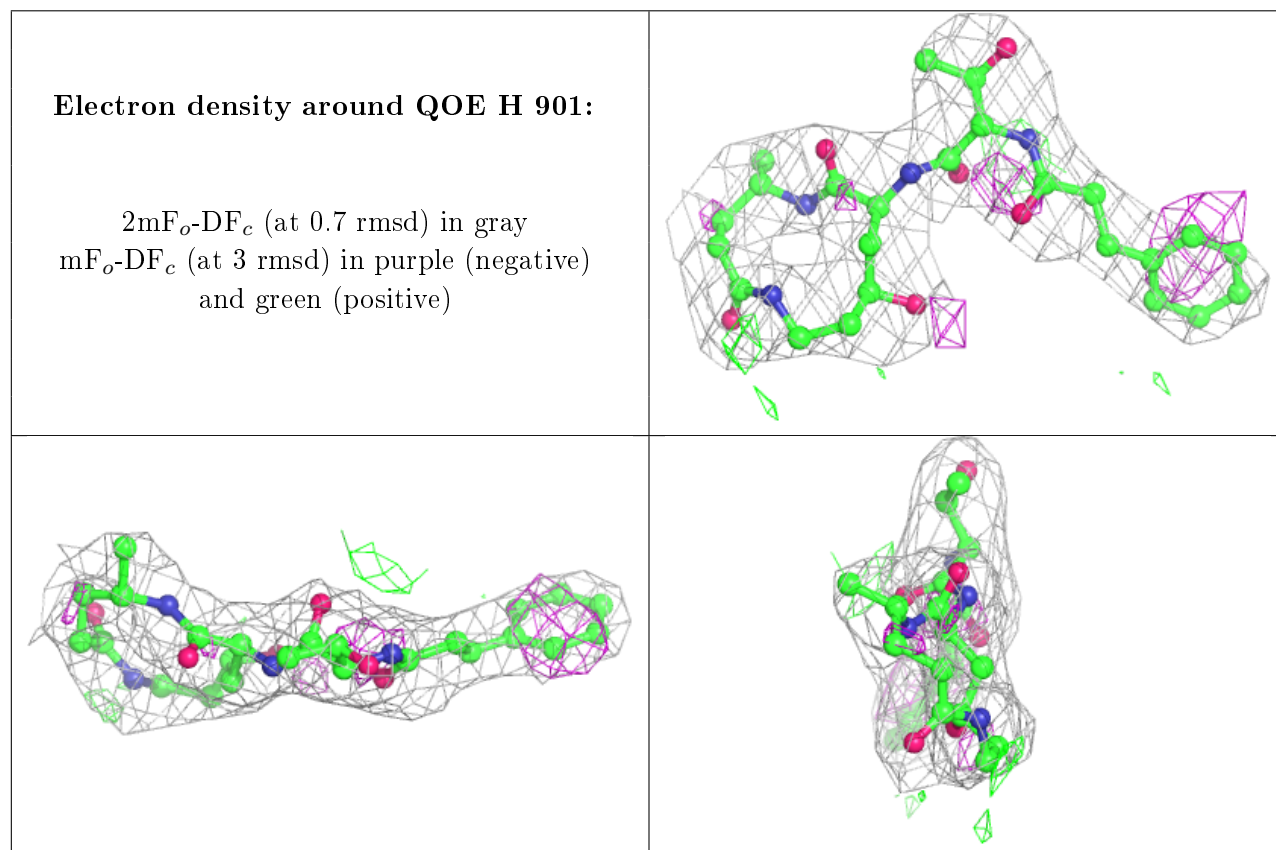
There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

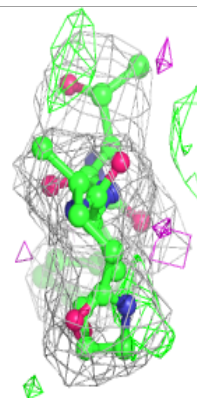
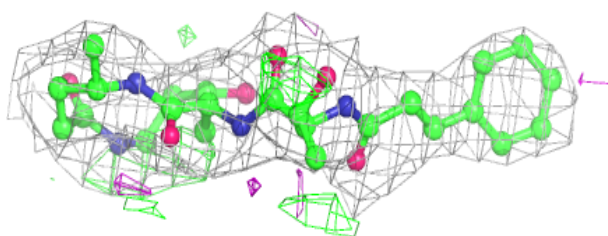
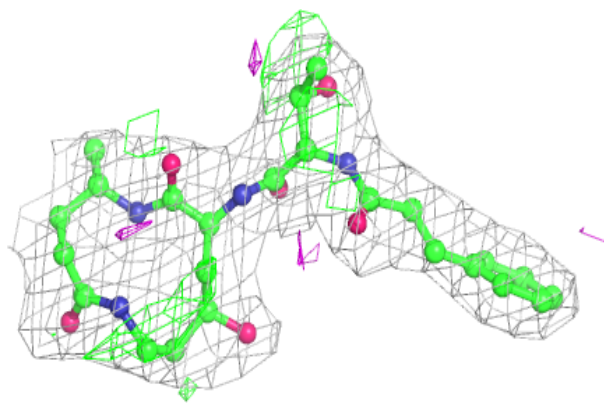
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
17	QOE	H	901	34/34	0.94	0.22	42,51,60,61	0
17	QOE	K	901	34/34	0.94	0.18	49,54,59,60	0
17	QOE	V	901	34/34	0.94	0.22	41,50,60,63	0
17	QOE	Y	901	34/34	0.94	0.20	48,54,58,63	0
15	MG	I	301	1/1	0.96	0.52	77,77,77,77	0
15	MG	V	902	1/1	0.96	0.13	78,78,78,78	0
15	MG	K	902	1/1	0.97	0.08	68,68,68,68	0
15	MG	Z	301	1/1	0.97	0.31	56,56,56,56	0
15	MG	W	301	1/1	0.98	0.40	70,70,70,70	0
15	MG	Y	902	1/1	0.98	0.12	68,68,68,68	0
15	MG	N	201	1/1	0.98	0.07	36,36,36,36	0
16	CL	U	301	1/1	0.98	0.26	54,54,54,54	0
16	CL	G	302	1/1	0.99	0.14	42,42,42,42	0
15	MG	G	301	1/1	0.99	0.08	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.

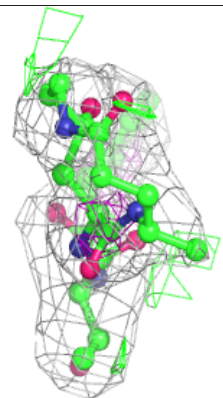
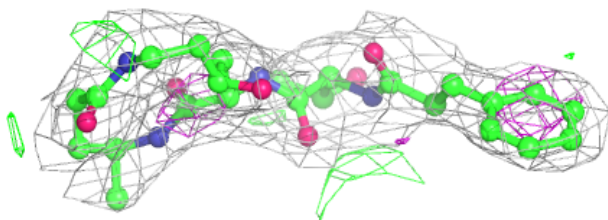
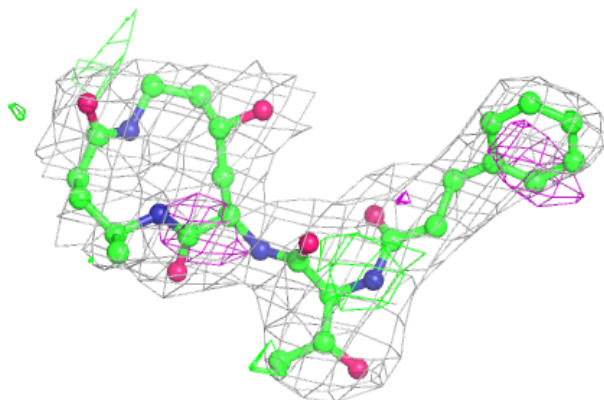


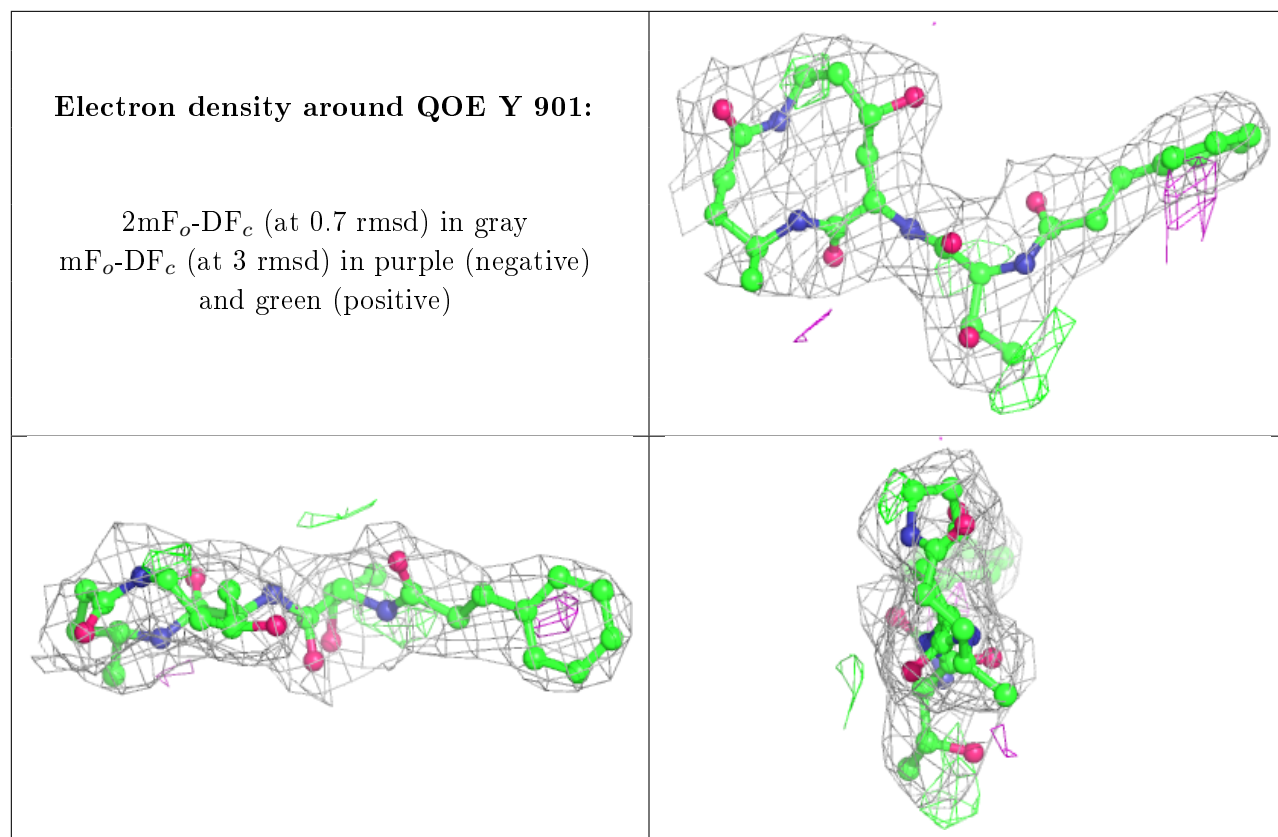
**Electron density around QOE K 901:**

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

**Electron density around QOE V 901:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.