



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 16, 2024 – 03:41 am GMT

PDB ID : 6HWF  
Title : Yeast 20S proteasome beta2-G45A mutant in complex with ONX 0914  
Authors : Huber, E.M.; Groll, M.  
Deposited on : 2018-10-11  
Resolution : 2.50 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.

The types of validation reports are described at

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

---

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

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

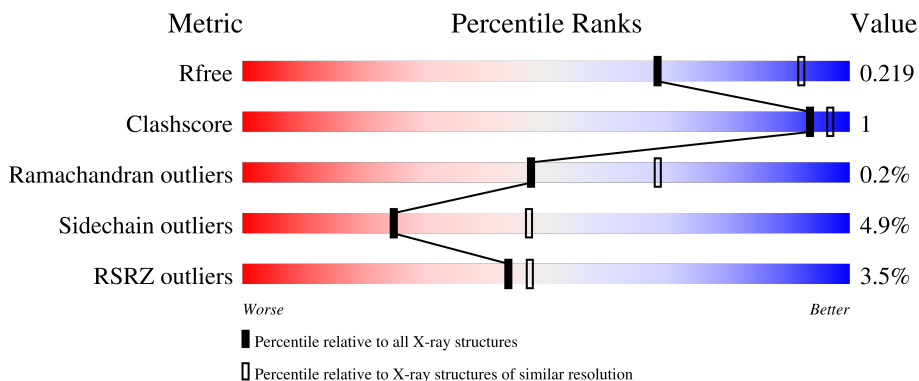
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

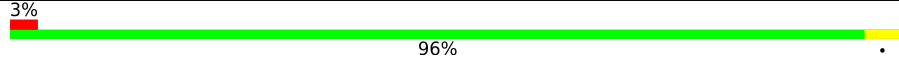
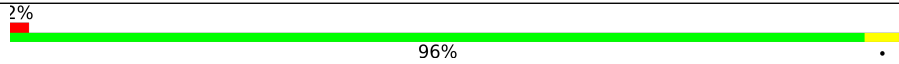
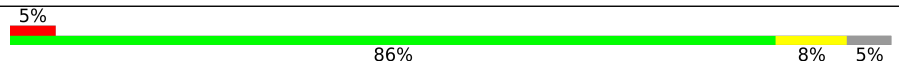

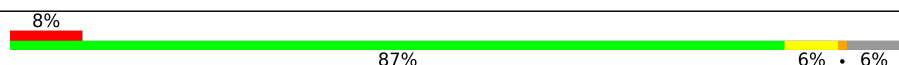
The reported resolution of this entry is 2.50 Å.

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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	 3% 96%
1	O	250	 2% 96%
2	B	258	 5% 86% 8% 5%
2	P	258	 5% 87% 7% 5%
3	C	254	 8% 87% 6% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	Q	254	13% 87% 6% • 6%
4	D	260	2% 82% 8% 10%
4	R	260	3% 82% 8% 10%
5	E	234	4% 89% 9% ..
5	S	234	7% 90% 8% ..
6	F	288	5% 79% 5% • 16%
6	T	288	5% 79% 5% • 16%
7	G	252	3% 90% 5% ..
7	U	252	2% 90% 5% ..
8	H	232	3% 92% • •
8	V	232	3% 91% 6% ..
9	I	205	% 95% •
9	W	205	% 96% •
10	J	198	2% 90% 8% ..
10	X	198	2% 90% 8% ..
11	K	212	% 95% 5%
11	Y	212	% 95% 5%
12	L	222	% 89% 8% •
12	Z	222	% 89% 8% •
13	M	246	4% 89% 6% 5%
13	a	246	3% 91% • 5%
14	N	196	% 94% 5% •
14	b	196	% 97% •

## 2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 50758 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 1720	C 1083	N 298	O 332	S 7	0	0	0
8	V	226	Total 1720	C 1083	N 298	O 332	S 7	0	0	0

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
			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
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			

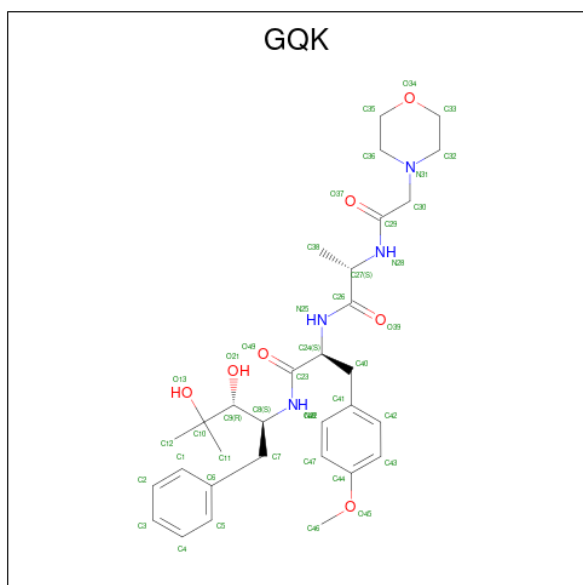
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

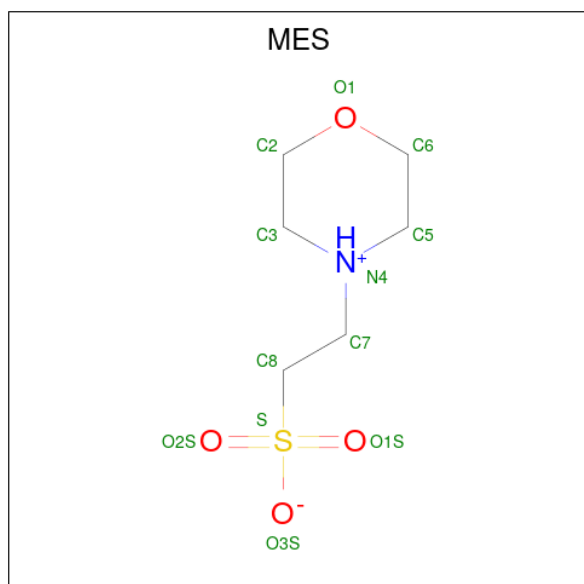
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total Cl 1 1	0	0
16	U	1	Total Cl 1 1	0	0

- Molecule 17 is (2 {S})-3-(4-methoxyphenyl)- {N}-[(2 {S},3 {R})-4-methyl-3,4-bis(oxidanyl)-1-phenyl-pentan-2-yl]-2-[[[(2 {S})-2-(2-morpholin-4-ylethanoylamino)propanoyl]amino]prop anamide (three-letter code: GQK) (formula: C<sub>31</sub>H<sub>44</sub>N<sub>4</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	H	1	Total	C	N	O	0	0
			42	31	4	7		
17	K	1	Total	C	N	O	0	0
			42	31	4	7		
17	N	1	Total	C	N	O	0	0
			42	31	4	7		
17	V	1	Total	C	N	O	0	0
			42	31	4	7		
17	Y	1	Total	C	N	O	0	0
			42	31	4	7		
17	b	1	Total	C	N	O	0	0
			42	31	4	7		

- Molecule 18 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



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: SO<sub>4</sub>) (formula: O<sub>4</sub>S).





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	49	Total	O	0	0
			49	49		
20	B	41	Total	O	0	0
			41	41		
20	C	35	Total	O	0	0
			35	35		
20	D	25	Total	O	0	0
			25	25		
20	E	19	Total	O	0	0
			19	19		
20	F	32	Total	O	0	0
			32	32		
20	G	47	Total	O	0	0
			47	47		
20	H	42	Total	O	0	0
			42	42		
20	I	36	Total	O	0	0
			36	36		
20	J	48	Total	O	0	0
			48	48		

*Continued on next page...*

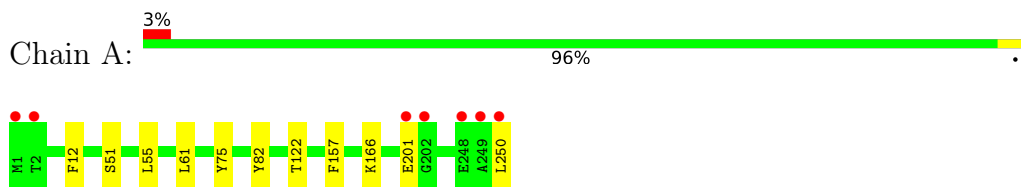
*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	K	64	Total O 64 64	0	0
20	L	52	Total O 52 52	0	0
20	M	41	Total O 41 41	0	0
20	N	35	Total O 35 35	0	0
20	O	25	Total O 25 25	0	0
20	P	25	Total O 25 25	0	0
20	Q	22	Total O 22 22	0	0
20	R	16	Total O 16 16	0	0
20	S	21	Total O 21 21	0	0
20	T	32	Total O 32 32	0	0
20	U	39	Total O 39 39	0	0
20	V	43	Total O 43 43	0	0
20	W	35	Total O 35 35	0	0
20	X	43	Total O 43 43	0	0
20	Y	53	Total O 53 53	0	0
20	Z	47	Total O 47 47	0	0
20	a	64	Total O 64 64	0	0
20	b	39	Total O 39 39	0	0

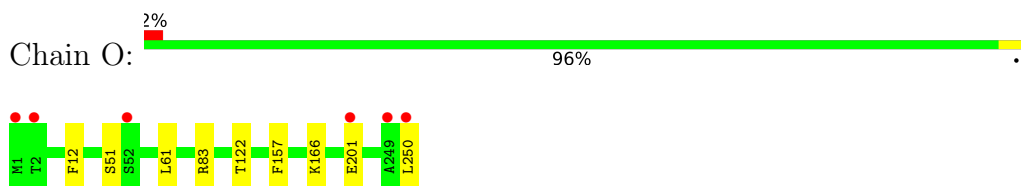
### 3 Residue-property plots [i](#)

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.

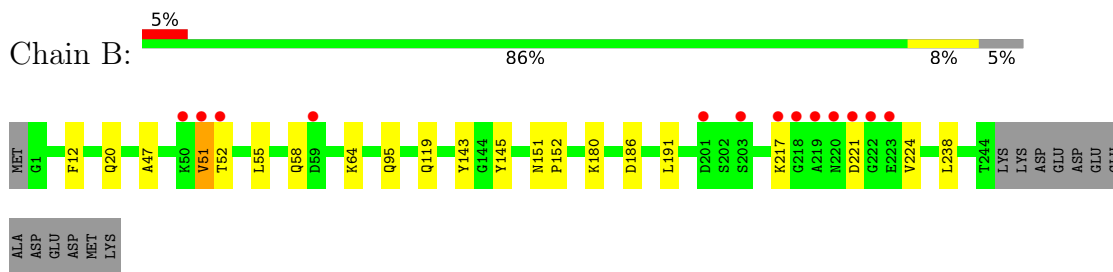
- Molecule 1: Proteasome subunit alpha type-2



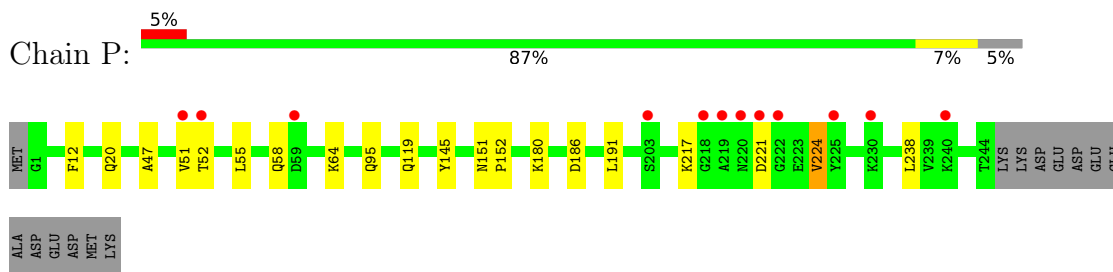
- Molecule 1: Proteasome subunit alpha type-2



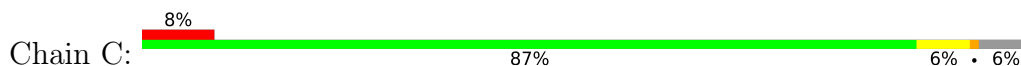
- Molecule 2: Proteasome subunit alpha type-3

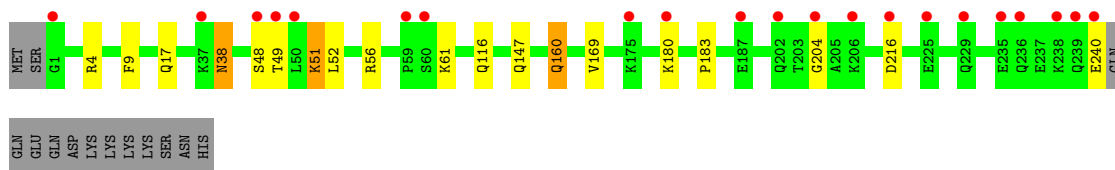


- Molecule 2: Proteasome subunit alpha type-3

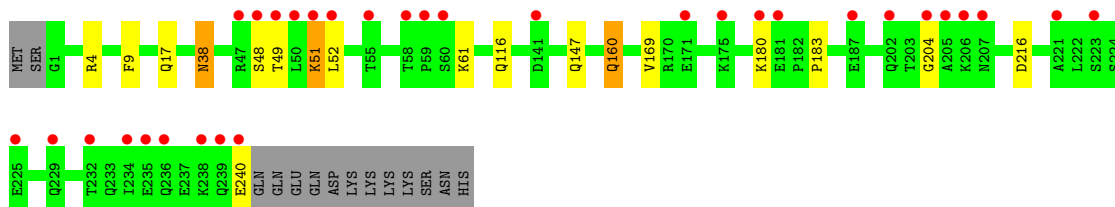
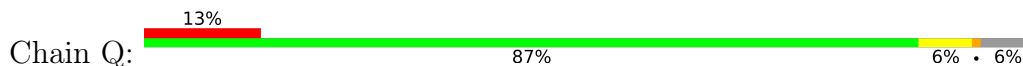


- Molecule 3: Proteasome subunit alpha type-4

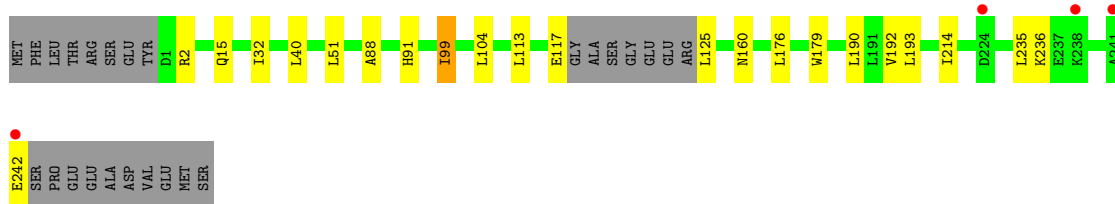
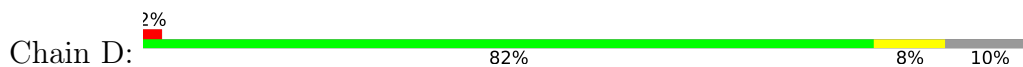




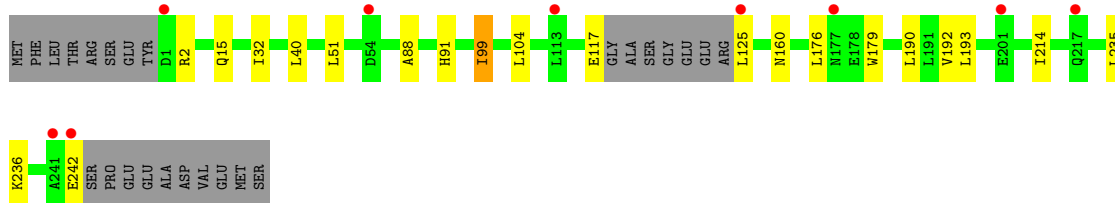
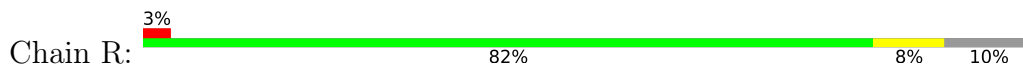
• Molecule 3: Proteasome subunit alpha type-4



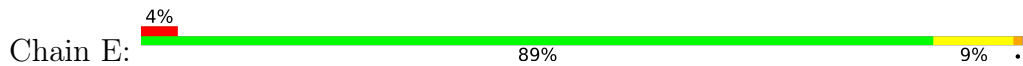
• Molecule 4: Proteasome subunit alpha type-5



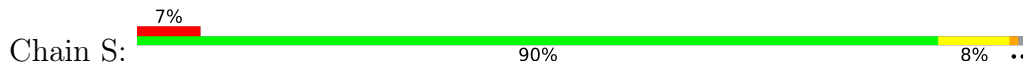
• Molecule 4: Proteasome subunit alpha type-5

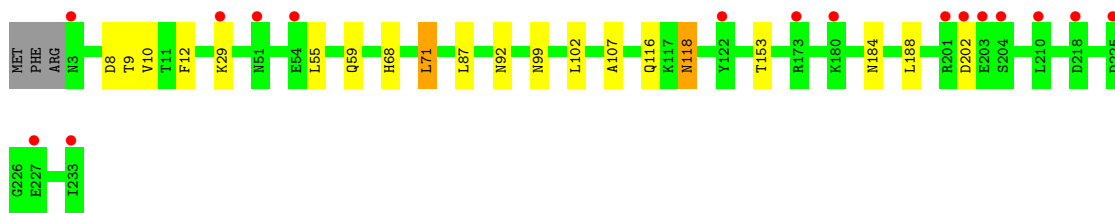


• Molecule 5: Proteasome subunit alpha type-6

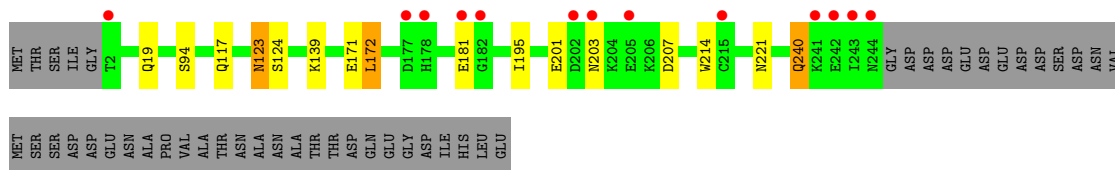
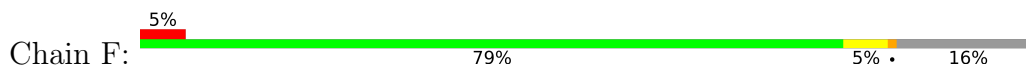


• Molecule 5: Proteasome subunit alpha type-6

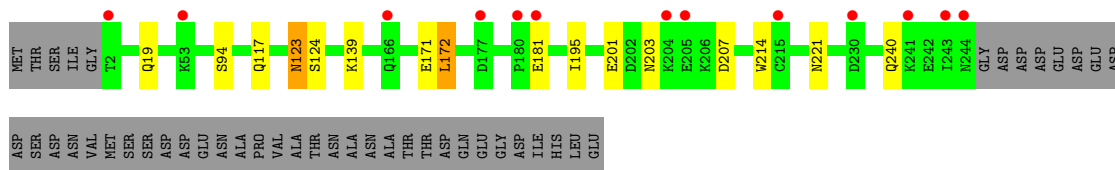
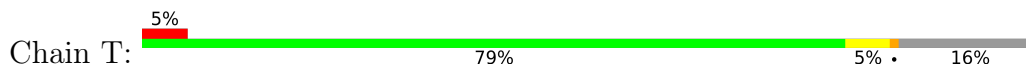




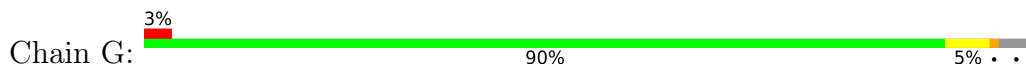
● Molecule 6: Probable proteasome subunit alpha type-7



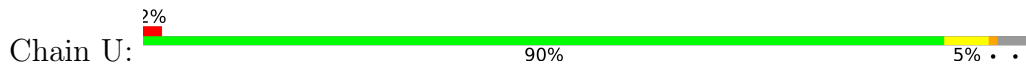
● Molecule 6: Probable proteasome subunit alpha type-7



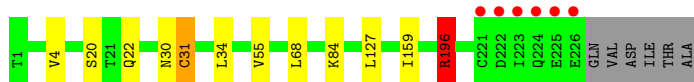
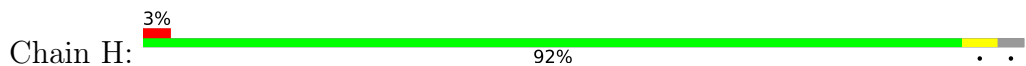
● Molecule 7: Proteasome subunit alpha type-1



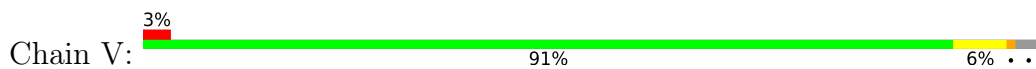
● Molecule 7: Proteasome subunit alpha type-1



● Molecule 8: Proteasome subunit beta type-2



● Molecule 8: Proteasome subunit beta type-2



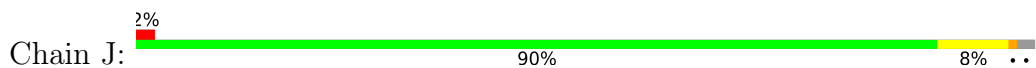
- Molecule 9: Proteasome subunit beta type-3



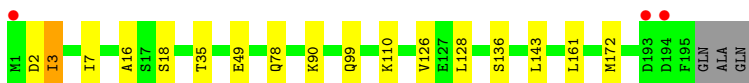
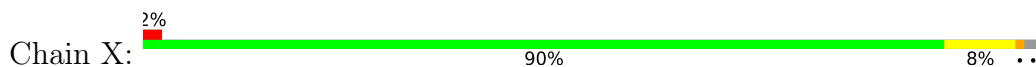
- Molecule 9: Proteasome subunit beta type-3



- Molecule 10: Proteasome subunit beta type-4



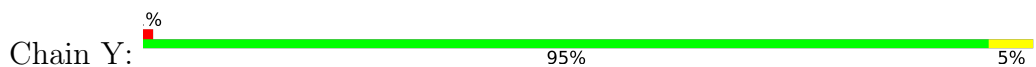
- Molecule 10: Proteasome subunit beta type-4




- Molecule 11: Proteasome subunit beta type-5



- Molecule 11: Proteasome subunit beta type-5




- Molecule 12: Proteasome subunit beta type-6

Chain L:  89% 8%

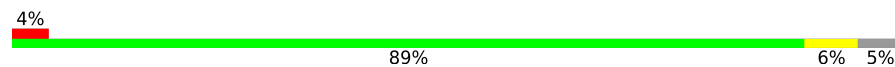


- Molecule 12: Proteasome subunit beta type-6

Chain Z:  89% 8%

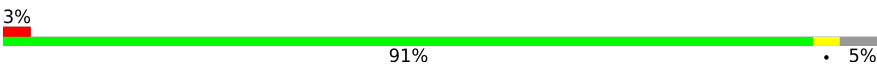


- Molecule 13: Proteasome subunit beta type-7

Chain M:  89% 6% 5% 4%

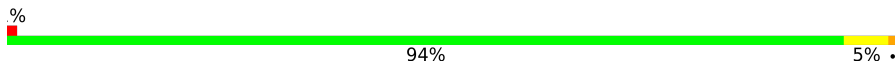


- Molecule 13: Proteasome subunit beta type-7

Chain a:  91% 5% 3%



- Molecule 14: Proteasome subunit beta type-1

Chain N:  94% 5%



- 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, $\alpha$ , $\beta$ , $\gamma$	136.63Å 299.66Å 145.15Å 90.00° 113.39° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 15.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.2 (15.00-2.50) 97.6 (15.00-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.47 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.189 , 0.216 0.194 , 0.219	Depositor DCC
$R_{free}$ test set	17869 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.4	Xtrriage
Anisotropy	0.363	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 33.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	50758	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG, MES, CL, GQK, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.37	0/1952	0.61	0/2642
1	O	0.37	0/1952	0.61	0/2642
2	B	0.39	0/1934	0.69	2/2618 (0.1%)
2	P	0.38	0/1934	0.69	2/2618 (0.1%)
3	C	0.38	0/1910	0.67	0/2586
3	Q	0.38	0/1910	0.67	0/2586
4	D	0.37	0/1837	0.65	0/2475
4	R	0.37	0/1837	0.65	0/2475
5	E	0.38	0/1800	0.63	1/2433 (0.0%)
5	S	0.38	0/1800	0.63	1/2433 (0.0%)
6	F	0.38	0/1932	0.61	0/2609
6	T	0.38	0/1932	0.61	0/2609
7	G	0.37	0/1945	0.62	0/2634
7	U	0.37	0/1945	0.62	0/2634
8	H	0.34	0/1751	0.62	1/2375 (0.0%)
8	V	0.35	0/1751	0.63	1/2375 (0.0%)
9	I	0.36	0/1611	0.63	0/2174
9	W	0.36	0/1611	0.63	0/2174
10	J	0.36	0/1589	0.65	0/2142
10	X	0.36	0/1589	0.65	0/2142
11	K	0.35	0/1681	0.86	3/2274 (0.1%)
11	Y	0.34	0/1681	0.85	3/2274 (0.1%)
12	L	0.37	0/1795	0.66	0/2420
12	Z	0.37	0/1795	0.66	0/2420
13	M	0.38	0/1855	0.68	0/2514
13	a	0.38	0/1855	0.68	0/2514
14	N	0.34	0/1541	0.61	0/2087
14	b	0.34	0/1541	0.61	0/2087
All	All	0.37	0/50266	0.66	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
12	L	0	1
12	Z	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-NH1	18.40	129.50	120.30
11	K	73	ARG	NE-CZ-NH2	-18.18	111.21	120.30
11	Y	73	ARG	NE-CZ-NH2	17.76	129.18	120.30
11	Y	73	ARG	NE-CZ-NH1	-17.75	111.43	120.30
11	Y	73	ARG	CD-NE-CZ	10.76	138.66	123.60
11	K	73	ARG	CD-NE-CZ	10.36	138.11	123.60
2	B	51	VAL	CG1-CB-CG2	5.79	120.16	110.90
5	S	71	LEU	CA-CB-CG	5.61	128.20	115.30
5	E	71	LEU	CA-CB-CG	5.59	128.16	115.30
2	P	224	VAL	CG1-CB-CG2	5.56	119.79	110.90
8	H	196	ARG	NE-CZ-NH1	5.46	123.03	120.30
8	V	196	ARG	NE-CZ-NH1	5.41	123.00	120.30
2	B	224	VAL	CG1-CB-CG2	5.33	119.44	110.90
2	P	51	VAL	CG1-CB-CG2	5.23	119.26	110.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	L	135	GLN	Peptide
12	Z	135	GLN	Peptide

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	3	0
1	O	1915	0	1929	3	0
2	B	1904	0	1904	10	0
2	P	1904	0	1904	8	0
3	C	1881	0	1895	6	0
3	Q	1881	0	1895	5	0
4	D	1813	0	1797	7	0
4	R	1813	0	1797	6	0
5	E	1773	0	1775	8	0
5	S	1773	0	1775	7	0
6	F	1892	0	1883	5	0
6	T	1892	0	1883	4	0
7	G	1907	0	1901	5	0
7	U	1907	0	1901	5	0
8	H	1720	0	1719	3	0
8	V	1720	0	1719	4	0
9	I	1581	0	1574	5	0
9	W	1581	0	1574	4	0
10	J	1561	0	1569	4	0
10	X	1561	0	1569	4	0
11	K	1644	0	1593	4	0
11	Y	1644	0	1593	4	0
12	L	1757	0	1711	14	0
12	Z	1757	0	1711	14	0
13	M	1824	0	1832	6	0
13	a	1824	0	1832	0	0
14	N	1512	0	1479	4	0
14	b	1512	0	1479	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	42	0	0	0	0
17	K	42	0	0	2	0
17	N	42	0	0	0	0
17	V	42	0	0	0	0
17	Y	42	0	0	2	0
17	b	42	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

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	49	0	0	0	0
20	B	41	0	0	0	0
20	C	35	0	0	0	0
20	D	25	0	0	0	0
20	E	19	0	0	0	0
20	F	32	0	0	0	0
20	G	47	0	0	0	0
20	H	42	0	0	0	0
20	I	36	0	0	0	0
20	J	48	0	0	0	0
20	K	64	0	0	0	0
20	L	52	0	0	0	0
20	M	41	0	0	1	0
20	N	35	0	0	0	0
20	O	25	0	0	0	0
20	P	25	0	0	0	0
20	Q	22	0	0	0	0
20	R	16	0	0	0	0
20	S	21	0	0	0	0
20	T	32	0	0	0	0
20	U	39	0	0	0	0
20	V	43	0	0	0	0
20	W	35	0	0	0	0
20	X	43	0	0	0	0
20	Y	53	0	0	0	0
20	Z	47	0	0	0	0
20	a	64	0	0	0	0
20	b	39	0	0	0	0
All	All	50758	0	49174	125	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 (125) 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)
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.50	0.76
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.51	0.75
5:S:12:PHE:H	6:T:19:GLN:HE22	1.37	0.73
2:B:12:PHE:H	3:C:17:GLN:HE22	1.37	0.70
5:E:12:PHE:H	6:F:19:GLN:HE22	1.38	0.69
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.39	0.68
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.59	0.68
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.59	0.67
2:P:95:GLN:HE22	9:W:71:ASN:HD22	1.42	0.67
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.78	0.66
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.77	0.66
5:S:92:ASN:HD21	12:Z:70:ASN:HD21	1.44	0.65
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.45	0.63
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.82	0.61
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.82	0.61
5:E:92:ASN:HD21	12:L:70:ASN:HD21	1.49	0.61
12:Z:42:LYS:HD2	12:Z:55:ASN:HD22	1.66	0.60
12:L:42:LYS:HD2	12:L:55:ASN:HD22	1.67	0.60
2:P:145:TYR:OH	2:P:217:LYS:N	2.37	0.58
1:O:12:PHE:H	2:P:20:GLN:HE22	1.50	0.58
4:R:99:ILE:HD11	4:R:104:LEU:HB2	1.86	0.58
2:B:145:TYR:OH	2:B:217:LYS:N	2.37	0.57
7:G:23:PHE:O	7:G:26:THR:HB	2.04	0.57
7:U:23:PHE:O	7:U:26:THR:HB	2.04	0.57
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.88	0.56
4:D:99:ILE:HD11	4:D:104:LEU:HB2	1.88	0.56
2:P:95:GLN:NE2	9:W:71:ASN:HD22	2.04	0.55
4:R:32:ILE:HD12	4:R:192:VAL:HG23	1.88	0.55
1:A:12:PHE:H	2:B:20:GLN:HE22	1.55	0.54
11:K:176:ASN:ND2	11:K:190:ASN:HD22	2.06	0.54
4:D:32:ILE:HD12	4:D:192:VAL:HG23	1.88	0.54
2:B:95:GLN:NE2	9:I:71:ASN:HD22	2.06	0.54
13:M:156:ARG:HH11	8:V:165:ASN:HD22	1.56	0.54
5:S:92:ASN:ND2	12:Z:70:ASN:HD21	2.06	0.54
11:Y:176:ASN:ND2	11:Y:190:ASN:HD22	2.05	0.53
9:W:36:SER:HB2	10:X:126:VAL:HG11	1.90	0.53
12:Z:31:THR:CG2	12:Z:36:ASN:HD21	2.21	0.53
3:C:9:PHE:H	4:D:15:GLN:HE22	1.56	0.52
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.57	0.52
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.92	0.52
12:Z:23:LEU:HD13	12:Z:43:VAL:HG13	1.91	0.52
12:L:23:LEU:HD13	12:L:43:VAL:HG13	1.90	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:155:ILE:HB	14:N:175:MET:HE3	1.91	0.52
13:M:27:LEU:HD21	13:M:34:LEU:HD22	1.92	0.51
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.92	0.51
6:T:123:ASN:HD22	6:T:124:SER:N	2.07	0.51
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.92	0.51
6:F:123:ASN:HD22	6:F:124:SER:N	2.08	0.51
8:V:20:SER:HB3	8:V:31:CYS:SG	2.51	0.51
12:L:31:THR:CG2	12:L:36:ASN:HD21	2.21	0.50
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.92	0.50
5:E:118:ASN:HD22	5:E:118:ASN:N	2.10	0.50
5:S:92:ASN:HD21	12:Z:70:ASN:ND2	2.08	0.50
7:G:83:ASN:C	7:G:83:ASN:HD22	2.16	0.49
11:K:176:ASN:HD21	11:K:190:ASN:HD22	1.59	0.49
5:S:118:ASN:N	5:S:118:ASN:HD22	2.11	0.49
12:Z:136:CYS:SG	12:Z:150:LEU:HB3	2.52	0.49
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.93	0.49
6:T:123:ASN:HD22	6:T:123:ASN:C	2.17	0.48
11:Y:176:ASN:HD21	11:Y:190:ASN:HD22	1.60	0.48
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.49	0.47
12:L:8:ASN:HA	12:L:30:ILE:O	2.14	0.47
12:L:136:CYS:SG	12:L:150:LEU:HB3	2.55	0.47
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.14	0.47
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.50	0.47
2:B:145:TYR:HH	2:B:217:LYS:N	2.12	0.47
8:H:20:SER:HB3	8:H:31:CYS:SG	2.54	0.47
5:E:92:ASN:ND2	12:L:70:ASN:HD21	2.11	0.47
14:N:22:THR:OG1	14:N:27:ALA:HB2	2.14	0.47
7:U:83:ASN:C	7:U:83:ASN:HD22	2.18	0.46
14:N:55:ILE:HD11	14:N:93:LEU:HD13	1.96	0.46
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.45	0.46
5:E:92:ASN:HD21	12:L:70:ASN:ND2	2.14	0.46
6:F:123:ASN:HD22	6:F:123:ASN:C	2.19	0.46
2:P:145:TYR:OH	2:P:217:LYS:HB2	2.16	0.46
12:Z:3:ASN:HD22	12:Z:4:PRO:HD2	1.81	0.46
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.46	0.45
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.46	0.45
13:M:127:LEU:HG	13:M:142:LEU:HD12	1.99	0.45
7:G:167:GLN:HE21	7:G:171:THR:HG23	1.82	0.45
12:L:3:ASN:HD22	12:L:4:PRO:HD2	1.82	0.45
12:Z:146:ILE:HG22	12:Z:150:LEU:HD22	1.99	0.45
8:H:196:ARG:NH2	9:I:150:GLU:O	2.49	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:113:LEU:HD12	5:E:78:PRO:HB2	2.00	0.44
2:B:143:TYR:O	3:C:56:ARG:NH1	2.46	0.44
2:B:145:TYR:OH	2:B:217:LYS:HB2	2.17	0.44
7:U:167:GLN:HE21	7:U:171:THR:HG23	1.83	0.44
12:L:146:ILE:HG22	12:L:150:LEU:HD22	1.99	0.44
1:O:83:ARG:HE	7:U:114:ASN:ND2	2.15	0.43
13:M:179:ASN:HD22	13:M:182:ARG:HH11	1.65	0.43
3:Q:38:ASN:HD22	3:Q:38:ASN:C	2.22	0.43
3:C:51:LYS:O	3:C:52:LEU:HB2	2.18	0.43
9:I:10:ILE:HG21	9:I:141:ALA:HB3	2.01	0.43
11:K:31:VAL:HG11	17:K:301:GQK:C3	2.49	0.43
10:J:3:ILE:HG23	10:J:18:SER:HB3	2.01	0.42
11:K:31:VAL:HG11	17:K:301:GQK:C4	2.50	0.42
1:A:55:LEU:HD12	7:G:170:THR:HG23	2.02	0.42
10:J:126:VAL:HG12	10:J:128:LEU:HG	2.01	0.42
6:T:172:LEU:HD13	6:T:195:ILE:HD13	2.01	0.42
10:X:3:ILE:HG23	10:X:18:SER:HB3	2.01	0.42
13:M:179:ASN:HD22	13:M:182:ARG:NH1	2.17	0.42
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.46	0.42
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.19	0.42
5:S:68:HIS:HE1	5:S:102:LEU:O	2.02	0.42
8:V:4:VAL:HG22	8:V:159:ILE:HD11	2.01	0.42
13:M:2:GLN:NE2	20:M:301:HOH:O	2.52	0.42
1:O:83:ARG:HE	7:U:114:ASN:HD21	1.67	0.41
10:X:126:VAL:HG12	10:X:128:LEU:HG	2.01	0.41
11:Y:31:VAL:HG11	17:Y:301:GQK:C3	2.50	0.41
3:C:38:ASN:C	3:C:38:ASN:HD22	2.22	0.41
6:F:172:LEU:HD13	6:F:195:ILE:HD13	2.01	0.41
9:W:10:ILE:HG21	9:W:141:ALA:HB3	2.02	0.41
12:Z:18:GLU:HG3	12:Z:174:TYR:CD2	2.55	0.41
2:B:47:ALA:HB1	2:B:64:LYS:HD2	2.02	0.41
7:G:83:ASN:C	7:G:83:ASN:ND2	2.74	0.41
8:H:4:VAL:HG22	8:H:159:ILE:HD11	2.01	0.41
12:L:18:GLU:HG3	12:L:174:TYR:CD2	2.56	0.41
2:P:47:ALA:HB1	2:P:64:LYS:HD2	2.02	0.41
6:F:240:GLN:HE21	6:F:240:GLN:HA	1.85	0.41
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.51	0.41
8:V:112:SER:HB3	8:V:125:LEU:HD13	2.03	0.41
5:E:68:HIS:HE1	5:E:102:LEU:O	2.03	0.41
11:Y:31:VAL:HG11	17:Y:301:GQK:C4	2.51	0.41
1:A:75:TYR:HB3	1:A:82:TYR:CD1	2.56	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.51	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	54
1	O	248/250 (99%)	241 (97%)	6 (2%)	1 (0%)	34	54
2	B	242/258 (94%)	233 (96%)	8 (3%)	1 (0%)	34	54
2	P	242/258 (94%)	233 (96%)	8 (3%)	1 (0%)	34	54
3	C	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	19	35
3	Q	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	19	35
4	D	231/260 (89%)	225 (97%)	5 (2%)	1 (0%)	34	54
4	R	231/260 (89%)	226 (98%)	4 (2%)	1 (0%)	34	54
5	E	229/234 (98%)	220 (96%)	9 (4%)	0	100	100
5	S	229/234 (98%)	220 (96%)	9 (4%)	0	100	100
6	F	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
6	T	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
7	G	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
7	U	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
8	H	224/232 (97%)	220 (98%)	4 (2%)	0	100	100
8	V	224/232 (97%)	220 (98%)	4 (2%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
10	J	193/198 (98%)	190 (98%)	3 (2%)	0	100	100

Continued on next page...



Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	X	193/198 (98%)	190 (98%)	3 (2%)	0	100	100
11	K	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
11	Y	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
12	L	220/222 (99%)	212 (96%)	7 (3%)	1 (0%)	29	48
12	Z	220/222 (99%)	212 (96%)	7 (3%)	1 (0%)	29	48
13	M	231/246 (94%)	221 (96%)	9 (4%)	1 (0%)	34	54
13	a	231/246 (94%)	221 (96%)	9 (4%)	1 (0%)	34	54
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	6284/6614 (95%)	6116 (97%)	154 (2%)	14 (0%)	47	68

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	221	ASP
4	D	2	ARG
2	P	221	ASP
4	R	2	ARG
1	A	166	LYS
1	O	166	LYS
3	C	183	PRO
3	Q	183	PRO
13	M	229	GLY
13	a	229	GLY
12	L	166	GLY
12	Z	166	GLY
3	C	204	GLY
3	Q	204	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%)	203 (97%)	6 (3%)	42	69
1	O	209/209 (100%)	203 (97%)	6 (3%)	42	69
2	B	203/216 (94%)	194 (96%)	9 (4%)	28	52
2	P	203/216 (94%)	194 (96%)	9 (4%)	28	52
3	C	212/226 (94%)	199 (94%)	13 (6%)	18	36
3	Q	212/226 (94%)	199 (94%)	13 (6%)	18	36
4	D	194/215 (90%)	182 (94%)	12 (6%)	18	35
4	R	194/215 (90%)	182 (94%)	12 (6%)	18	35
5	E	190/193 (98%)	175 (92%)	15 (8%)	12	24
5	S	190/193 (98%)	176 (93%)	14 (7%)	13	27
6	F	201/239 (84%)	188 (94%)	13 (6%)	17	33
6	T	201/239 (84%)	188 (94%)	13 (6%)	17	33
7	G	206/210 (98%)	196 (95%)	10 (5%)	25	47
7	U	206/210 (98%)	196 (95%)	10 (5%)	25	47
8	H	185/190 (97%)	176 (95%)	9 (5%)	25	47
8	V	185/190 (97%)	176 (95%)	9 (5%)	25	47
9	I	172/173 (99%)	168 (98%)	4 (2%)	50	76
9	W	172/173 (99%)	168 (98%)	4 (2%)	50	76
10	J	173/175 (99%)	161 (93%)	12 (7%)	15	30
10	X	173/175 (99%)	161 (93%)	12 (7%)	15	30
11	K	169/169 (100%)	163 (96%)	6 (4%)	35	61
11	Y	169/169 (100%)	163 (96%)	6 (4%)	35	61
12	L	185/185 (100%)	174 (94%)	11 (6%)	19	37
12	Z	185/185 (100%)	174 (94%)	11 (6%)	19	37
13	M	199/208 (96%)	192 (96%)	7 (4%)	36	62
13	a	199/208 (96%)	192 (96%)	7 (4%)	36	62
14	N	162/162 (100%)	157 (97%)	5 (3%)	40	67
14	b	162/162 (100%)	157 (97%)	5 (3%)	40	67
All	All	5320/5540 (96%)	5057 (95%)	263 (5%)	25	47

All (263) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	SER
1	A	61	LEU
1	A	122	THR
1	A	157	PHE
1	A	201	GLU
1	A	250	LEU
2	B	51	VAL
2	B	52	THR
2	B	55	LEU
2	B	58	GLN
2	B	119	GLN
2	B	180	LYS
2	B	186	ASP
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	48	SER
3	C	49	THR
3	C	51	LYS
3	C	61	LYS
3	C	116	GLN
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	216	ASP
3	C	240	GLU
4	D	40	LEU
4	D	51	LEU
4	D	99	ILE
4	D	117	GLU
4	D	125	LEU
4	D	176	LEU
4	D	190	LEU
4	D	193	LEU
4	D	214	ILE
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	8	ASP
5	E	9	THR
5	E	10	VAL

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	E	29	LYS
5	E	55	LEU
5	E	59	GLN
5	E	71	LEU
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	153	THR
5	E	184	ASN
5	E	188	LEU
5	E	202	ASP
5	E	211	SER
6	F	94	SER
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	171	GLU
6	F	172	LEU
6	F	181	GLU
6	F	201	GLU
6	F	203	ASN
6	F	207	ASP
6	F	214	TRP
6	F	221	ASN
6	F	240	GLN
7	G	13	GLU
7	G	26	THR
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	22	GLN
8	H	30	ASN
8	H	31	CYS
8	H	34	LEU
8	H	55	VAL
8	H	68	LEU
8	H	84	LYS

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	H	127	LEU
8	H	196	ARG
9	I	31	GLN
9	I	37	ASN
9	I	171	LEU
9	I	182	TRP
10	J	2	ASP
10	J	3	ILE
10	J	7	ILE
10	J	35	THR
10	J	49	GLU
10	J	78	GLN
10	J	90	LYS
10	J	99	GLN
10	J	110	LYS
10	J	136	SER
10	J	143	LEU
10	J	172	MET
11	K	9	GLN
11	K	41	LEU
11	K	118	ASP
11	K	148	LEU
11	K	177	LEU
11	K	209	ASN
12	L	13	LEU
12	L	18	GLU
12	L	23	LEU
12	L	31	THR
12	L	49	ASN
12	L	106	TYR
12	L	136	CYS
12	L	150	LEU
12	L	172	LEU
12	L	173	LYS
12	L	179	GLU
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
13	M	212	LEU

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
14	N	9	LYS
14	N	22	THR
14	N	83	LYS
14	N	119	VAL
14	N	178	LEU
1	O	51	SER
1	O	61	LEU
1	O	122	THR
1	O	157	PHE
1	O	201	GLU
1	O	250	LEU
2	P	52	THR
2	P	55	LEU
2	P	58	GLN
2	P	119	GLN
2	P	180	LYS
2	P	186	ASP
2	P	191	LEU
2	P	224	VAL
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	48	SER
3	Q	49	THR
3	Q	51	LYS
3	Q	61	LYS
3	Q	116	GLN
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	216	ASP
3	Q	240	GLU
4	R	40	LEU
4	R	51	LEU
4	R	99	ILE
4	R	117	GLU
4	R	125	LEU
4	R	176	LEU
4	R	190	LEU
4	R	193	LEU
4	R	214	ILE

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	8	ASP
5	S	9	THR
5	S	10	VAL
5	S	29	LYS
5	S	55	LEU
5	S	59	GLN
5	S	71	LEU
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	153	THR
5	S	184	ASN
5	S	188	LEU
5	S	202	ASP
6	T	94	SER
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	171	GLU
6	T	172	LEU
6	T	181	GLU
6	T	201	GLU
6	T	203	ASN
6	T	207	ASP
6	T	214	TRP
6	T	221	ASN
6	T	240	GLN
7	U	13	GLU
7	U	26	THR
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	22	GLN
8	V	30	ASN

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	V	31	CYS
8	V	34	LEU
8	V	55	VAL
8	V	68	LEU
8	V	84	LYS
8	V	127	LEU
8	V	196	ARG
9	W	31	GLN
9	W	37	ASN
9	W	171	LEU
9	W	182	TRP
10	X	2	ASP
10	X	3	ILE
10	X	7	ILE
10	X	35	THR
10	X	49	GLU
10	X	78	GLN
10	X	90	LYS
10	X	99	GLN
10	X	110	LYS
10	X	136	SER
10	X	143	LEU
10	X	172	MET
11	Y	9	GLN
11	Y	41	LEU
11	Y	118	ASP
11	Y	148	LEU
11	Y	177	LEU
11	Y	209	ASN
12	Z	13	LEU
12	Z	18	GLU
12	Z	23	LEU
12	Z	31	THR
12	Z	49	ASN
12	Z	106	TYR
12	Z	136	CYS
12	Z	150	LEU
12	Z	172	LEU
12	Z	173	LYS
12	Z	179	GLU
13	a	2	GLN
13	a	48	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
13	a	212	LEU
14	b	9	LYS
14	b	22	THR
14	b	83	LYS
14	b	119	VAL
14	b	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (137) 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	100	ASN
4	D	198	GLN
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
6	F	86	ASN
6	F	117	GLN

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	F	123	ASN
6	F	191	GLN
6	F	240	GLN
7	G	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	167	GLN
7	G	175	ASN
8	H	30	ASN
8	H	66	HIS
8	H	165	ASN
8	H	172	ASN
8	H	189	ASN
9	I	37	ASN
10	J	55	GLN
10	J	118	GLN
10	J	191	GLN
11	K	85	ASN
11	K	143	ASN
11	K	176	ASN
11	K	209	ASN
12	L	3	ASN
12	L	36	ASN
12	L	49	ASN
12	L	70	ASN
12	L	76	HIS
12	L	80	ASN
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	53	GLN
14	N	69	GLN
14	N	161	GLN
1	O	94	HIS

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	P	20	GLN
2	P	58	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	155	ASN
2	P	176	GLN
3	Q	17	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	100	ASN
4	R	225	ASN
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	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
7	U	167	GLN
7	U	175	ASN
8	V	30	ASN
8	V	35	HIS
8	V	165	ASN
8	V	172	ASN
8	V	189	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
9	W	37	ASN
10	X	55	GLN
10	X	86	GLN
10	X	118	GLN
10	X	146	HIS
10	X	191	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	70	ASN
12	Z	76	HIS
12	Z	80	ASN
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 [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

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	GQK	b	201	14	44,44,44	1.35	5 (11%)	59,60,60	1.28	7 (11%)
18	MES	V	302	-	12,12,12	2.16	1 (8%)	14,16,16	1.58	2 (14%)
18	MES	Y	302	-	12,12,12	2.23	1 (8%)	14,16,16	1.59	2 (14%)
18	MES	K	303	-	12,12,12	2.26	1 (8%)	14,16,16	1.53	2 (14%)
17	GQK	Y	301	11	44,44,44	1.40	6 (13%)	59,60,60	1.41	7 (11%)
19	SO4	N	203	-	4,4,4	0.34	0	6,6,6	0.08	0
19	SO4	b	202	-	4,4,4	0.32	0	6,6,6	0.13	0
17	GQK	V	301	8	44,44,44	1.43	6 (13%)	59,60,60	1.46	8 (13%)
17	GQK	H	301	8	44,44,44	1.47	7 (15%)	59,60,60	1.50	8 (13%)
18	MES	H	302	-	12,12,12	2.17	1 (8%)	14,16,16	1.49	2 (14%)
17	GQK	K	301	11	44,44,44	1.39	6 (13%)	59,60,60	1.44	7 (11%)
17	GQK	N	201	14	44,44,44	1.33	6 (13%)	59,60,60	1.29	8 (13%)

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	GQK	b	201	14	-	5/44/52/52	0/3/3/3
18	MES	V	302	-	-	5/6/14/14	0/1/1/1
18	MES	Y	302	-	-	3/6/14/14	0/1/1/1
18	MES	K	303	-	-	2/6/14/14	0/1/1/1
17	GQK	Y	301	11	-	3/44/52/52	0/3/3/3
17	GQK	V	301	8	-	10/44/52/52	0/3/3/3
17	GQK	H	301	8	-	10/44/52/52	0/3/3/3
18	MES	H	302	-	-	1/6/14/14	0/1/1/1

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	GQK	K	301	11	-	3/44/52/52	0/3/3/3
17	GQK	N	201	14	-	6/44/52/52	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	K	303	MES	C8-S	-7.63	1.66	1.77
18	Y	302	MES	C8-S	-7.45	1.66	1.77
18	H	302	MES	C8-S	-7.22	1.67	1.77
18	V	302	MES	C8-S	-7.19	1.67	1.77
17	K	301	GQK	C40-C41	-5.02	1.39	1.51
17	Y	301	GQK	C40-C41	-5.00	1.39	1.51
17	b	201	GQK	C40-C41	-4.97	1.39	1.51
17	H	301	GQK	C40-C41	-4.91	1.39	1.51
17	N	201	GQK	C40-C41	-4.83	1.39	1.51
17	V	301	GQK	C40-C41	-4.72	1.40	1.51
17	V	301	GQK	C7-C6	-3.97	1.41	1.51
17	H	301	GQK	C7-C6	-3.94	1.41	1.51
17	K	301	GQK	C7-C6	-3.59	1.42	1.51
17	b	201	GQK	C7-C6	-3.55	1.42	1.51
17	Y	301	GQK	C7-C6	-3.52	1.42	1.51
17	H	301	GQK	C10-C9	3.46	1.61	1.54
17	b	201	GQK	C11-C10	3.43	1.58	1.52
17	N	201	GQK	C7-C6	-3.38	1.43	1.51
17	V	301	GQK	C11-C10	3.26	1.57	1.52
17	Y	301	GQK	C11-C10	3.16	1.57	1.52
17	V	301	GQK	C10-C9	3.12	1.60	1.54
17	N	201	GQK	C11-C10	3.10	1.57	1.52
17	H	301	GQK	C11-C10	2.91	1.57	1.52
17	Y	301	GQK	C10-C9	2.82	1.60	1.54
17	K	301	GQK	C10-C9	2.80	1.60	1.54
17	K	301	GQK	C12-C10	2.73	1.57	1.52
17	K	301	GQK	C11-C10	2.72	1.57	1.52
17	H	301	GQK	C12-C10	2.61	1.56	1.52
17	Y	301	GQK	C12-C10	2.61	1.56	1.52
17	V	301	GQK	C12-C10	2.50	1.56	1.52
17	b	201	GQK	C9-C8	2.33	1.56	1.53
17	N	201	GQK	C9-C8	2.30	1.56	1.53
17	N	201	GQK	C10-C9	2.27	1.59	1.54
17	K	301	GQK	C9-C8	2.26	1.56	1.53
17	b	201	GQK	C10-C9	2.18	1.59	1.54
17	Y	301	GQK	C9-C8	2.15	1.56	1.53

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	H	301	GQK	C30-C29	2.09	1.55	1.52
17	N	201	GQK	C30-C29	2.04	1.55	1.52
17	H	301	GQK	C9-C8	2.04	1.56	1.53
17	V	301	GQK	C9-C8	2.00	1.56	1.53

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	H	301	GQK	C12-C10-C11	-7.14	100.36	110.56
17	V	301	GQK	C12-C10-C11	-6.89	100.71	110.56
17	K	301	GQK	C12-C10-C11	-4.48	104.15	110.56
18	Y	302	MES	O3S-S-C8	4.44	112.95	105.77
17	K	301	GQK	C11-C10-C9	4.18	119.11	111.28
17	Y	301	GQK	C11-C10-C9	4.08	118.91	111.28
17	Y	301	GQK	C12-C10-C11	-3.88	105.01	110.56
17	K	301	GQK	C30-N31-C36	-3.80	105.20	111.09
17	Y	301	GQK	C30-N31-C36	-3.80	105.20	111.09
18	V	302	MES	O3S-S-C8	3.56	111.53	105.77
18	K	303	MES	O1S-S-C8	3.53	111.17	106.92
18	V	302	MES	O1S-S-C8	3.45	111.07	106.92
18	H	302	MES	O1S-S-C8	3.31	110.90	106.92
18	K	303	MES	O3S-S-C8	3.17	110.89	105.77
17	H	301	GQK	C46-O45-C44	3.12	124.28	117.51
18	H	302	MES	O2S-S-C8	3.08	110.62	106.92
17	K	301	GQK	C46-O45-C44	3.02	124.06	117.51
17	V	301	GQK	C46-O45-C44	3.01	124.03	117.51
17	Y	301	GQK	C46-O45-C44	2.91	123.82	117.51
17	b	201	GQK	C46-O45-C44	2.90	123.80	117.51
17	N	201	GQK	C11-C10-C9	2.86	116.64	111.28
17	b	201	GQK	C11-C10-C9	2.83	116.58	111.28
17	N	201	GQK	C7-C6-C5	2.81	126.48	120.91
17	N	201	GQK	C46-O45-C44	2.78	123.54	117.51
17	H	301	GQK	C12-C10-C9	2.78	116.47	111.28
17	b	201	GQK	C7-C6-C5	2.74	126.35	120.91
17	V	301	GQK	C7-C6-C5	2.67	126.21	120.91
17	N	201	GQK	C29-C30-N31	-2.66	107.18	113.36
17	H	301	GQK	C11-C10-C9	2.65	116.25	111.28
17	b	201	GQK	C29-C30-N31	-2.65	107.21	113.36
17	H	301	GQK	C7-C6-C5	2.62	126.12	120.91
17	V	301	GQK	C12-C10-C9	2.62	116.19	111.28
17	V	301	GQK	C7-C6-C1	-2.55	115.85	120.91
17	Y	301	GQK	C7-C6-C5	2.55	125.97	120.91

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	K	301	GQK	C7-C6-C5	2.53	125.94	120.91
17	H	301	GQK	C7-C6-C1	-2.53	115.89	120.91
17	V	301	GQK	C11-C10-C9	2.44	115.85	111.28
17	Y	301	GQK	O34-C35-C36	-2.44	106.43	111.80
17	H	301	GQK	C6-C7-C8	2.37	117.45	113.33
17	N	201	GQK	O13-C10-C11	-2.36	102.82	107.90
17	K	301	GQK	O34-C35-C36	-2.33	106.66	111.80
18	Y	302	MES	O1S-S-C8	2.31	109.70	106.92
17	V	301	GQK	C6-C7-C8	2.27	117.28	113.33
17	H	301	GQK	O34-C35-C36	-2.26	106.82	111.80
17	N	201	GQK	O34-C35-C36	-2.25	106.84	111.80
17	K	301	GQK	C7-C6-C1	-2.22	116.49	120.91
17	Y	301	GQK	C7-C6-C1	-2.22	116.50	120.91
17	b	201	GQK	C7-C6-C1	-2.18	116.58	120.91
17	V	301	GQK	O34-C35-C36	-2.16	107.03	111.80
17	N	201	GQK	C7-C6-C1	-2.14	116.66	120.91
17	b	201	GQK	C35-C36-N31	2.14	113.34	110.10
17	b	201	GQK	O34-C35-C36	-2.12	107.12	111.80
17	N	201	GQK	C35-C36-N31	2.12	113.31	110.10

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	H	301	GQK	C11-C10-C9-C8
17	H	301	GQK	C11-C10-C9-O21
17	H	301	GQK	C12-C10-C9-C8
17	H	301	GQK	C12-C10-C9-O21
17	H	301	GQK	O13-C10-C9-C8
17	H	301	GQK	O13-C10-C9-O21
17	V	301	GQK	C11-C10-C9-C8
17	V	301	GQK	C11-C10-C9-O21
17	V	301	GQK	C12-C10-C9-C8
17	V	301	GQK	C12-C10-C9-O21
17	V	301	GQK	O13-C10-C9-C8
17	V	301	GQK	O13-C10-C9-O21
18	H	302	MES	N4-C7-C8-S
18	V	302	MES	C7-C8-S-O2S
18	Y	302	MES	C7-C8-S-O2S
17	b	201	GQK	C5-C6-C7-C8
18	V	302	MES	C7-C8-S-O3S
18	Y	302	MES	C7-C8-S-O3S

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	N	201	GQK	C5-C6-C7-C8
17	b	201	GQK	C1-C6-C7-C8
17	N	201	GQK	C1-C6-C7-C8
17	Y	301	GQK	C5-C6-C7-C8
17	K	301	GQK	C5-C6-C7-C8
17	H	301	GQK	N28-C29-C30-N31
17	V	301	GQK	N28-C29-C30-N31
17	Y	301	GQK	C1-C6-C7-C8
17	K	301	GQK	C1-C6-C7-C8
17	H	301	GQK	C5-C6-C7-C8
17	V	301	GQK	C5-C6-C7-C8
17	V	301	GQK	C1-C6-C7-C8
17	H	301	GQK	C1-C6-C7-C8
17	N	201	GQK	N28-C29-C30-N31
17	b	201	GQK	N28-C29-C30-N31
17	H	301	GQK	O37-C29-C30-N31
17	N	201	GQK	O37-C29-C30-N31
17	V	301	GQK	O37-C29-C30-N31
17	b	201	GQK	O37-C29-C30-N31
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
18	V	302	MES	C7-C8-S-O1S
18	Y	302	MES	C7-C8-S-O1S
17	b	201	GQK	N25-C24-C40-C41
17	N	201	GQK	N25-C24-C40-C41
17	K	301	GQK	C12-C10-C9-C8
17	Y	301	GQK	C12-C10-C9-C8
17	N	201	GQK	C23-C24-C40-C41

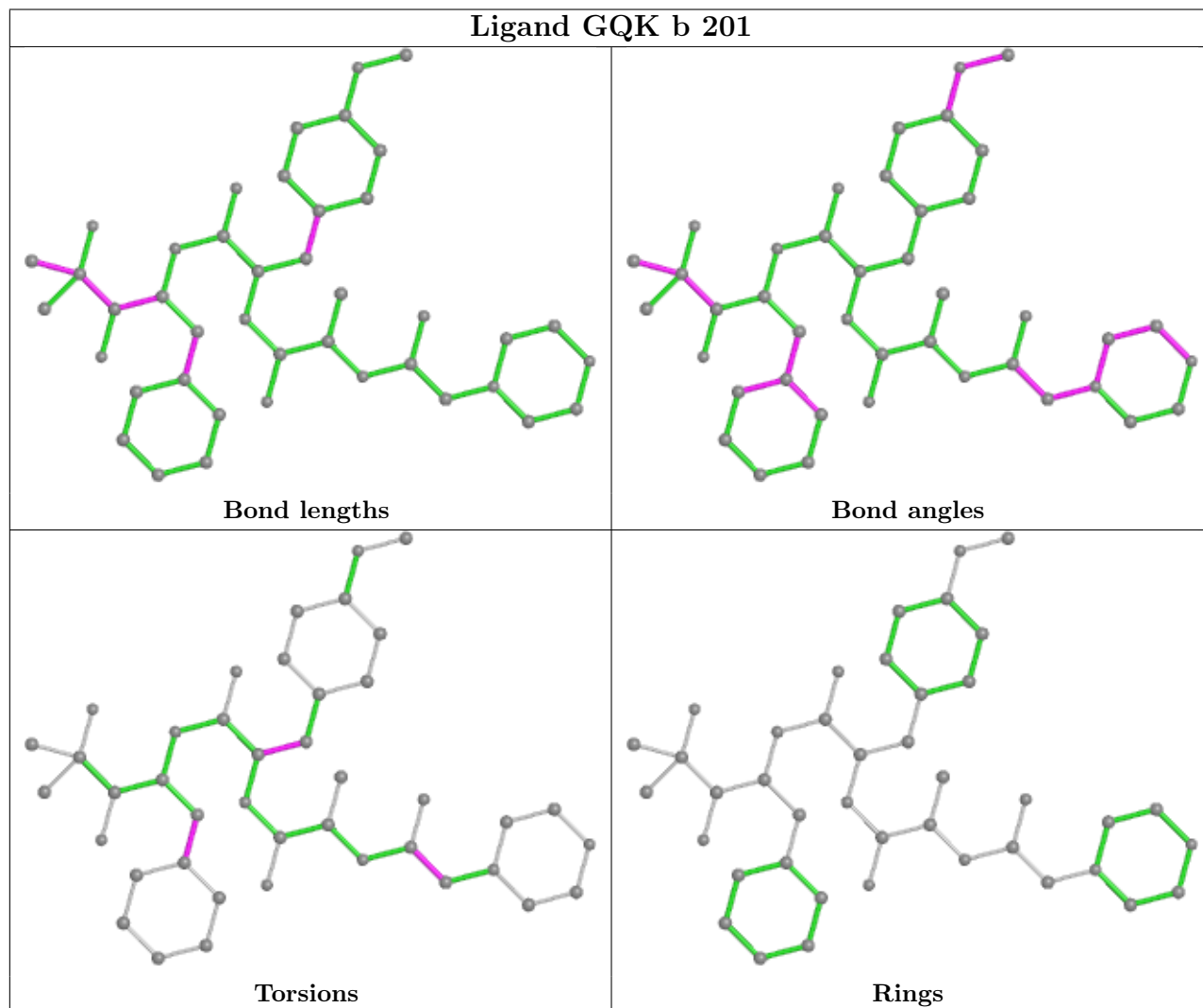
There are no ring outliers.

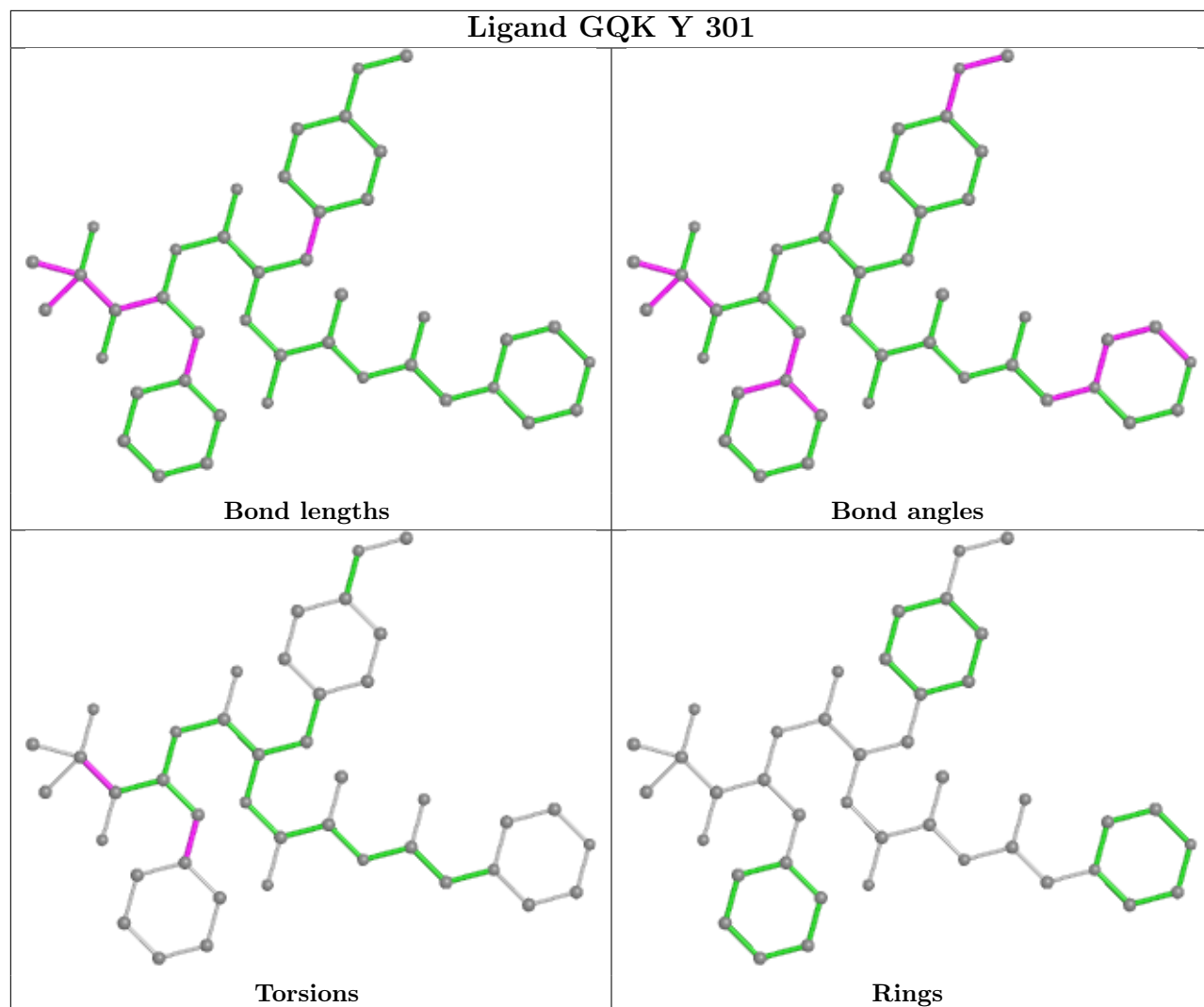
2 monomers are involved in 4 short contacts:

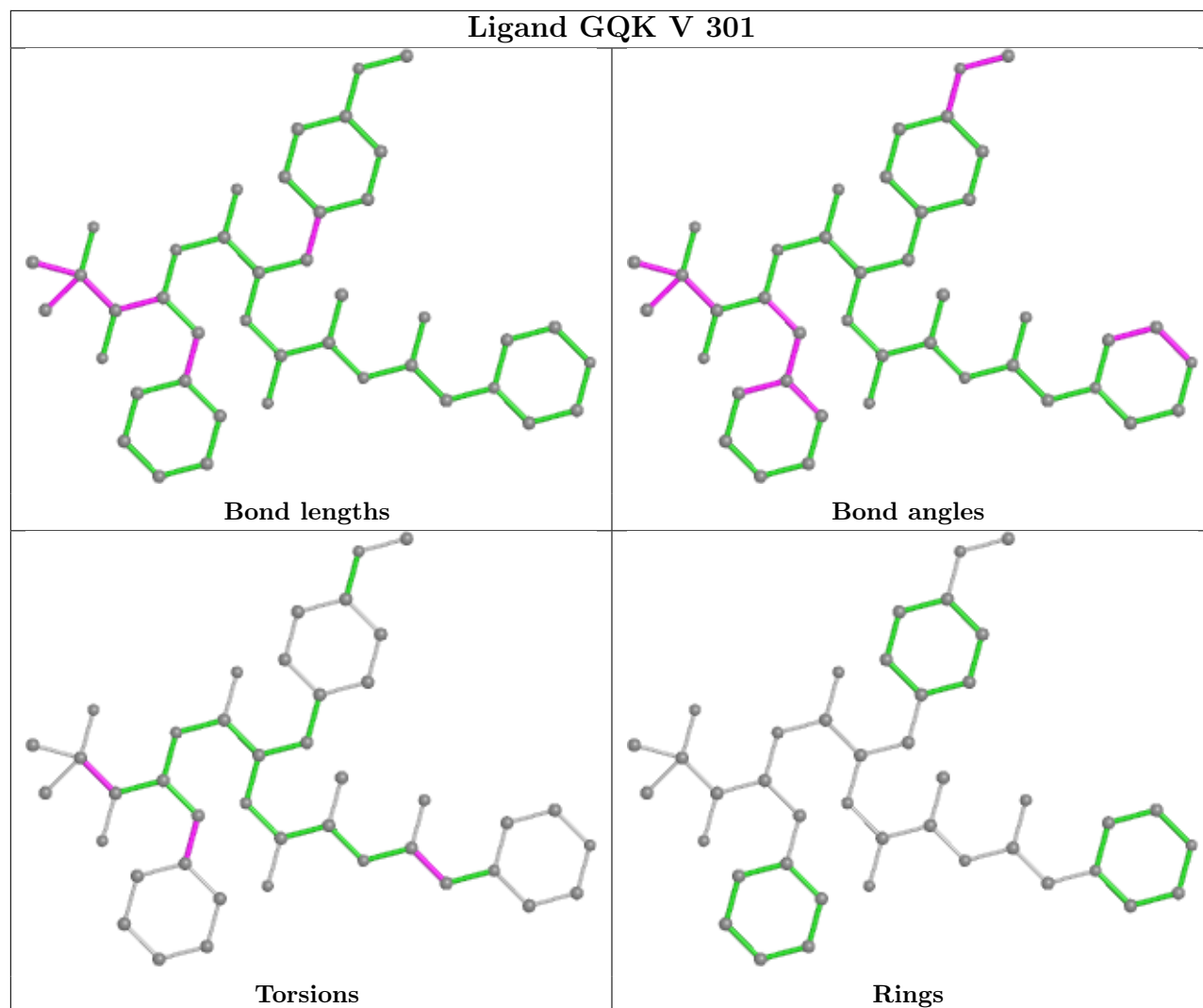
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	Y	301	GQK	2	0
17	K	301	GQK	2	0

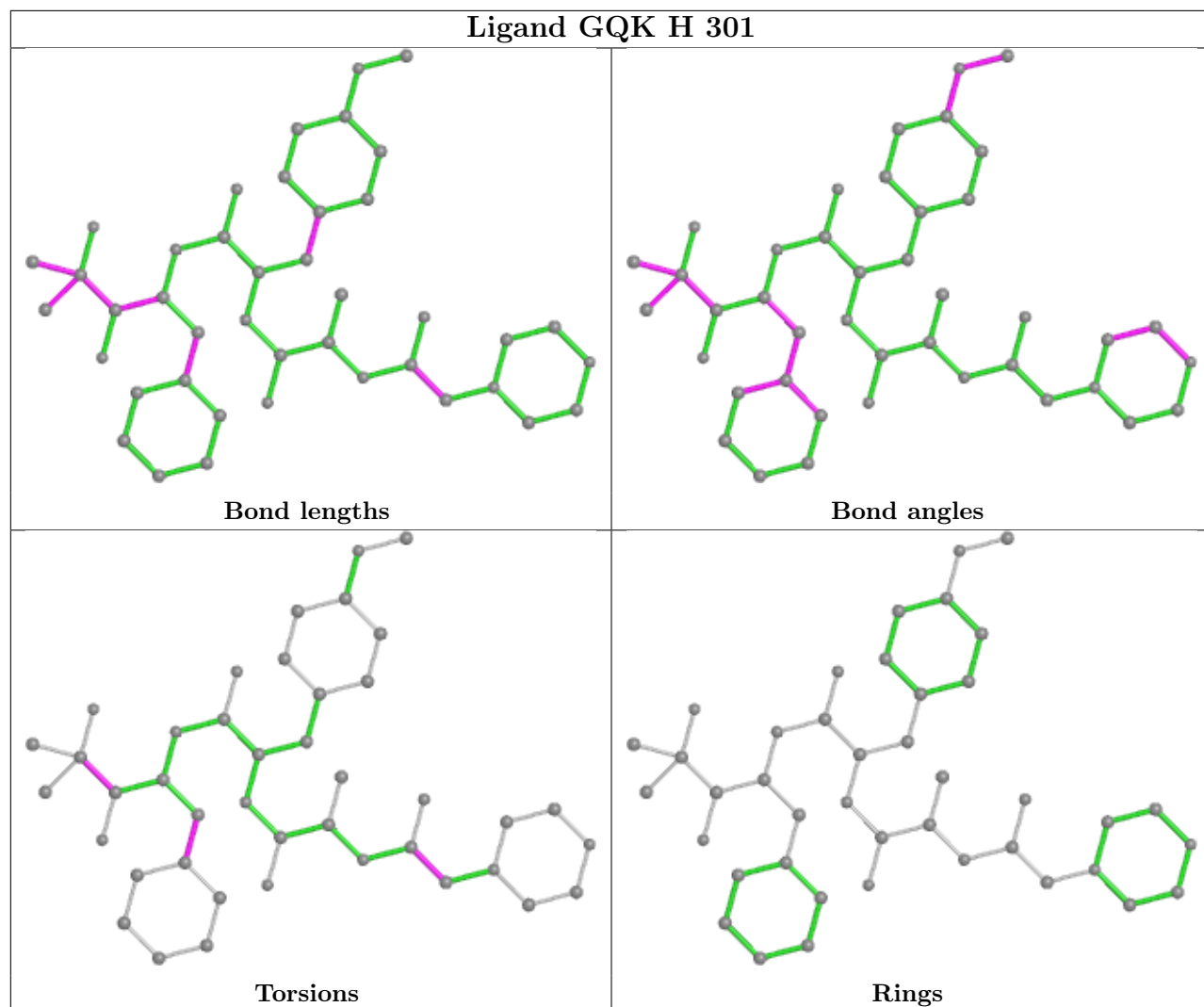
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

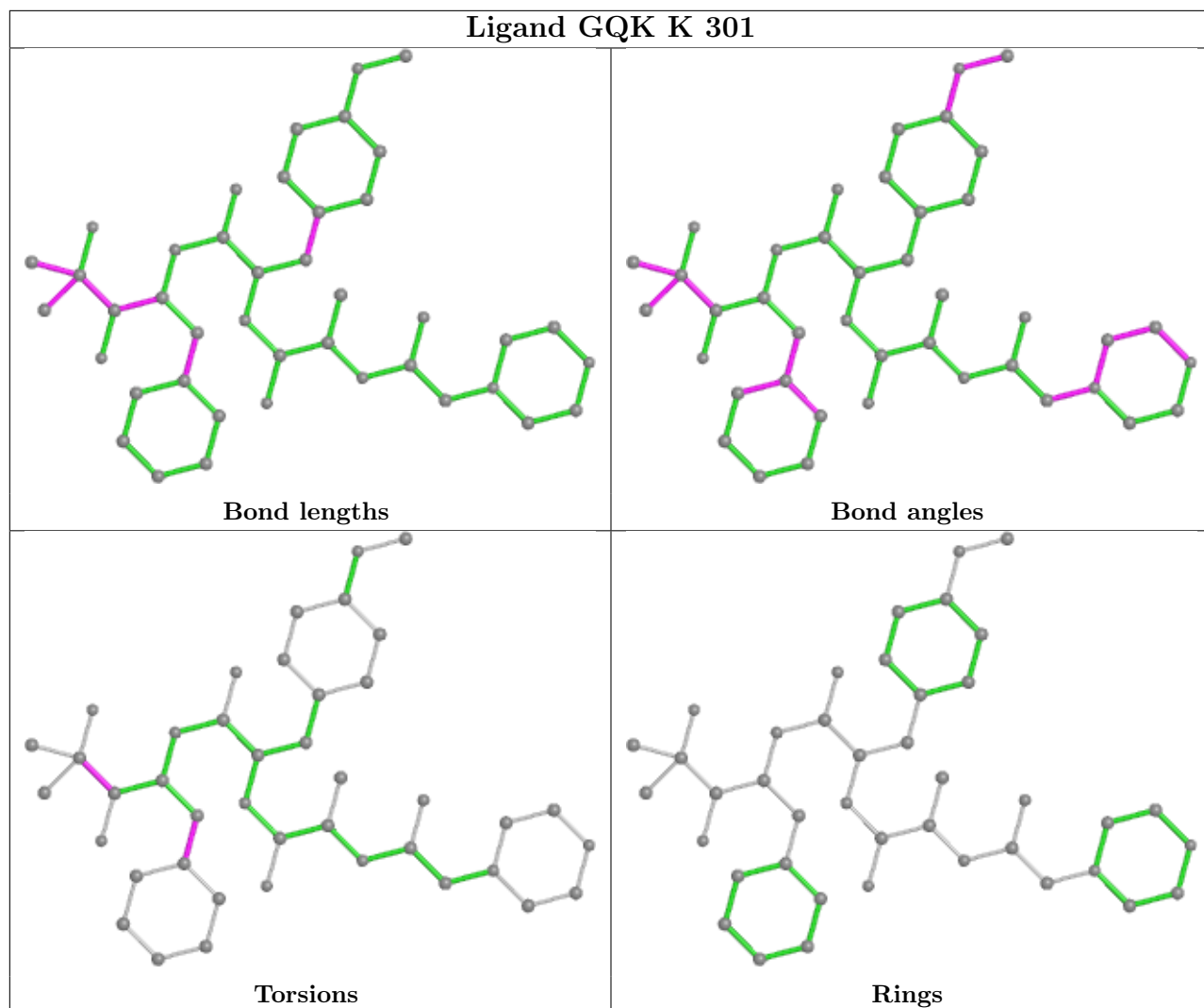
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

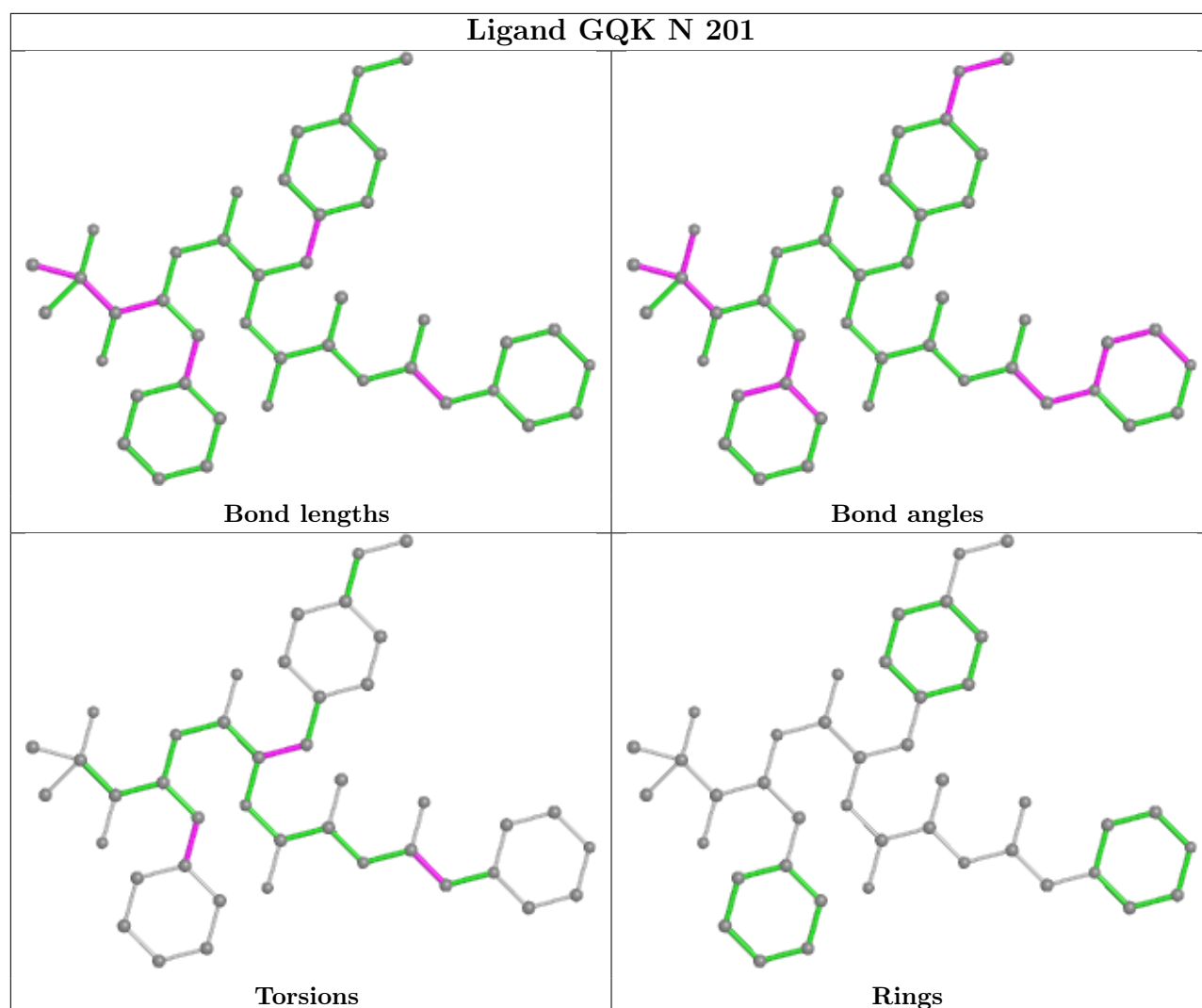












## 5.7 Other polymers [i](#)

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%)	-0.28	7 (2%) 53 56	35, 51, 84, 131	0
1	O	250/250 (100%)	-0.19	6 (2%) 59 62	36, 56, 96, 135	0
2	B	244/258 (94%)	-0.04	13 (5%) 26 28	35, 55, 108, 164	0
2	P	244/258 (94%)	-0.03	12 (4%) 29 31	41, 60, 105, 168	0
3	C	240/254 (94%)	0.10	21 (8%) 10 10	38, 61, 122, 146	0
3	Q	240/254 (94%)	0.42	32 (13%) 3 2	40, 74, 153, 183	0
4	D	235/260 (90%)	-0.19	4 (1%) 70 72	40, 60, 91, 133	0
4	R	235/260 (90%)	-0.07	9 (3%) 40 43	39, 63, 98, 132	0
5	E	231/234 (98%)	-0.06	10 (4%) 35 38	42, 63, 99, 134	0
5	S	231/234 (98%)	0.05	16 (6%) 16 17	41, 67, 109, 138	0
6	F	243/288 (84%)	-0.21	13 (5%) 26 28	36, 56, 103, 132	0
6	T	243/288 (84%)	-0.16	13 (5%) 26 28	37, 58, 109, 139	0
7	G	241/252 (95%)	-0.26	8 (3%) 46 50	35, 52, 86, 131	0
7	U	241/252 (95%)	-0.25	6 (2%) 57 61	35, 52, 87, 115	0
8	H	226/232 (97%)	-0.26	6 (2%) 54 58	35, 49, 76, 147	0
8	V	226/232 (97%)	-0.15	8 (3%) 44 47	36, 51, 82, 175	0
9	I	204/205 (99%)	-0.52	2 (0%) 82 84	32, 46, 74, 95	0
9	W	204/205 (99%)	-0.50	2 (0%) 82 84	28, 49, 76, 106	0
10	J	195/198 (98%)	-0.37	4 (2%) 63 66	34, 47, 74, 121	0
10	X	195/198 (98%)	-0.38	3 (1%) 73 75	34, 50, 76, 140	0
11	K	212/212 (100%)	-0.44	1 (0%) 91 91	29, 47, 73, 104	0
11	Y	212/212 (100%)	-0.42	3 (1%) 75 77	28, 49, 73, 105	0
12	L	222/222 (100%)	-0.49	1 (0%) 91 91	33, 49, 74, 93	0
12	Z	222/222 (100%)	-0.45	2 (0%) 84 86	34, 48, 75, 101	0

*Continued on next page...*



Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	233/246 (94%)	-0.26	10 (4%) 35 38	33, 48, 88, 149	0
13	a	233/246 (94%)	-0.35	8 (3%) 45 48	30, 46, 85, 136	0
14	N	196/196 (100%)	-0.45	2 (1%) 82 84	29, 46, 73, 104	0
14	b	196/196 (100%)	-0.42	1 (0%) 91 91	30, 47, 75, 100	0
All	All	6344/6614 (95%)	-0.23	223 (3%) 44 47	28, 53, 99, 183	0

All (223) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	219	ALA	9.6
3	Q	49	THR	8.7
2	B	220	ASN	7.7
3	Q	50	LEU	7.5
2	B	219	ALA	7.2
2	B	221	ASP	7.2
8	V	222	ASP	7.2
8	V	226	GLU	7.0
2	P	220	ASN	6.8
8	V	224	GLN	6.7
3	C	238	LYS	6.7
13	a	233	ILE	6.6
5	E	202	ASP	6.6
13	M	233	ILE	6.4
3	C	49	THR	6.3
3	Q	206	LYS	5.9
2	P	221	ASP	5.9
10	X	194	ASP	5.6
5	S	202	ASP	5.6
3	C	202	GLN	5.5
3	Q	202	GLN	5.4
3	Q	48	SER	5.4
8	H	224	GLN	5.3
10	J	1	MET	5.3
3	Q	239	GLN	5.2
13	M	230	THR	5.1
8	H	226	GLU	5.1
8	V	225	GLU	5.0
8	V	223	ILE	5.0
3	Q	238	LYS	5.0
6	T	241	LYS	4.8
2	B	218	GLY	4.7

Continued on next page...

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	51	VAL	4.7
10	X	1	MET	4.7
13	a	230	THR	4.7
8	H	222	ASP	4.7
13	M	228	TYR	4.6
8	V	221	CYS	4.6
3	C	180	LYS	4.5
13	M	229	GLY	4.5
10	J	194	ASP	4.4
3	Q	236	GLN	4.4
8	H	221	CYS	4.4
4	D	242	GLU	4.4
3	Q	223	SER	4.2
6	T	181	GLU	4.2
3	Q	240	GLU	4.1
1	A	250	LEU	4.0
6	F	243	ILE	3.9
3	Q	204	GLY	3.8
6	T	244	ASN	3.8
3	C	239	GLN	3.8
6	F	241	LYS	3.8
7	U	2	GLY	3.7
6	F	205	GLU	3.7
2	P	59	ASP	3.7
3	C	48	SER	3.7
13	M	232	LYS	3.7
3	Q	221	ALA	3.6
14	N	195	GLN	3.6
2	P	51	VAL	3.6
8	H	225	GLU	3.5
6	T	2	THR	3.5
3	Q	180	LYS	3.5
13	a	232	LYS	3.5
7	U	242	GLN	3.5
9	W	192	ASP	3.5
11	Y	106	ARG	3.5
1	O	249	ALA	3.5
7	G	3	TYR	3.4
3	Q	205	ALA	3.4
6	F	244	ASN	3.4
2	B	203	SER	3.3
4	D	241	ALA	3.3

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
5	E	227	GLU	3.3
3	C	236	GLN	3.3
7	U	203	ASP	3.3
3	C	240	GLU	3.3
2	B	222	GLY	3.3
5	S	203	GLU	3.3
3	Q	59	PRO	3.2
7	G	242	GLN	3.2
6	F	181	GLU	3.2
2	B	217	LYS	3.2
3	C	206	LYS	3.2
13	a	229	GLY	3.2
2	P	222	GLY	3.1
10	J	174	MET	3.1
5	E	54	GLU	3.1
2	P	52	THR	3.1
2	P	218	GLY	3.0
7	G	240	ALA	3.0
5	E	201	ARG	3.0
11	Y	212	GLY	3.0
6	T	53	LYS	3.0
1	O	250	LEU	3.0
13	a	1	THR	3.0
3	C	204	GLY	3.0
3	Q	51	LYS	2.9
7	G	222	ASP	2.9
10	X	193	ASP	2.9
5	E	173	ARG	2.9
1	A	249	ALA	2.9
14	b	195	GLN	2.9
4	R	242	GLU	2.9
1	A	1	MET	2.9
2	B	52	THR	2.8
6	T	205	GLU	2.8
1	O	52	SER	2.8
4	R	217	GLN	2.8
4	R	113	LEU	2.8
2	P	203	SER	2.8
3	C	60	SER	2.8
5	S	225	ASP	2.8
1	A	248	GLU	2.8
3	Q	225	GLU	2.8

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	Q	58	THR	2.8
3	Q	181	GLU	2.7
3	Q	55	THR	2.7
11	K	212	GLY	2.7
5	S	54	GLU	2.7
5	S	173	ARG	2.7
7	G	241	GLU	2.7
14	N	105	LYS	2.7
3	Q	187	GLU	2.7
3	C	50	LEU	2.7
13	M	227	GLY	2.7
3	C	216	ASP	2.7
3	C	37	LYS	2.6
4	R	125	LEU	2.6
7	G	2	GLY	2.6
6	F	178	HIS	2.6
5	S	51	ASN	2.6
3	C	235	GLU	2.6
3	Q	141	ASP	2.6
4	D	224	ASP	2.6
1	A	201	GLU	2.6
3	Q	229	GLN	2.6
4	R	241	ALA	2.6
5	E	225	ASP	2.6
7	U	222	ASP	2.6
1	O	2	THR	2.6
2	B	201	ASP	2.6
3	Q	171	GLU	2.6
3	Q	235	GLU	2.6
12	Z	165	ASN	2.6
5	E	233	ILE	2.6
3	Q	175	LYS	2.6
5	S	29	LYS	2.6
4	R	1	ASP	2.6
4	R	177	ASN	2.5
5	S	204	SER	2.5
1	A	2	THR	2.5
6	T	243	ILE	2.5
6	T	204	LYS	2.5
3	Q	60	SER	2.5
3	Q	207	ASN	2.5
6	F	215	CYS	2.5

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
6	T	215	CYS	2.4
7	G	179	LYS	2.4
3	Q	234	ILE	2.4
6	T	180	PRO	2.4
3	Q	232	THR	2.4
7	U	230	GLU	2.4
5	S	210	LEU	2.4
2	P	240	LYS	2.4
8	V	145	ASP	2.4
12	L	165	ASN	2.4
6	T	177	ASP	2.4
10	J	193	ASP	2.4
4	R	54	ASP	2.4
5	S	3	ASN	2.3
9	I	1	SER	2.3
8	V	219	ASN	2.3
6	F	202	ASP	2.3
13	a	231	GLN	2.3
13	a	216	ASN	2.3
9	W	1	SER	2.3
3	C	229	GLN	2.3
5	E	3	ASN	2.3
13	M	216	ASN	2.3
3	C	187	GLU	2.3
9	I	192	ASP	2.2
5	S	227	GLU	2.2
13	M	1	THR	2.2
6	F	203	ASN	2.2
6	F	2	THR	2.2
2	B	223	GLU	2.2
1	O	1	MET	2.2
7	G	188	GLU	2.2
1	O	201	GLU	2.2
8	H	223	ILE	2.2
7	U	181	LYS	2.1
12	Z	210	ASP	2.1
3	C	1	GLY	2.1
3	C	175	LYS	2.1
11	Y	202	GLU	2.1
13	a	224	ASP	2.1
5	S	180	LYS	2.1
6	T	166	GLN	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
5	S	201	ARG	2.1
5	S	218	ASP	2.1
6	F	182	GLY	2.1
3	C	225	GLU	2.1
6	F	177	ASP	2.1
6	T	230	ASP	2.1
4	D	238	LYS	2.1
2	P	225	TYR	2.1
3	Q	52	LEU	2.1
1	A	202	GLY	2.1
3	Q	47	ARG	2.1
13	M	82	ASP	2.0
5	S	122	TYR	2.0
4	R	201	GLU	2.0
2	P	230	LYS	2.0
5	E	217	LYS	2.0
3	C	59	PRO	2.0
2	B	50	LYS	2.0
2	B	59	ASP	2.0
6	F	242	GLU	2.0
5	E	180	LYS	2.0
5	S	233	ILE	2.0
13	M	47	ASP	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.

*Continued on next page...*

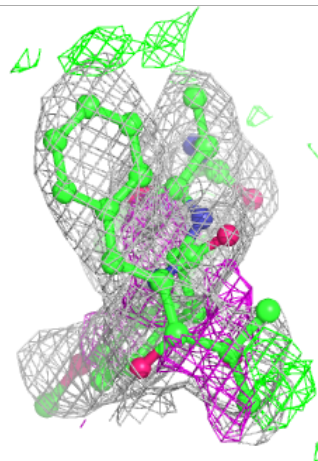
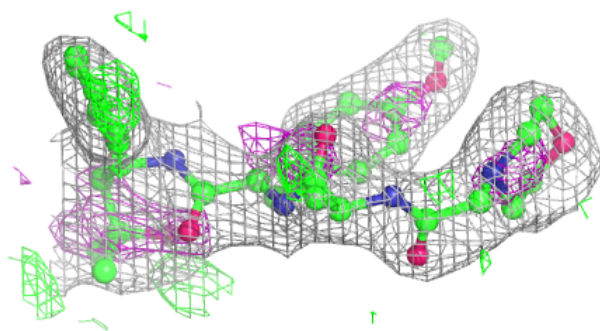
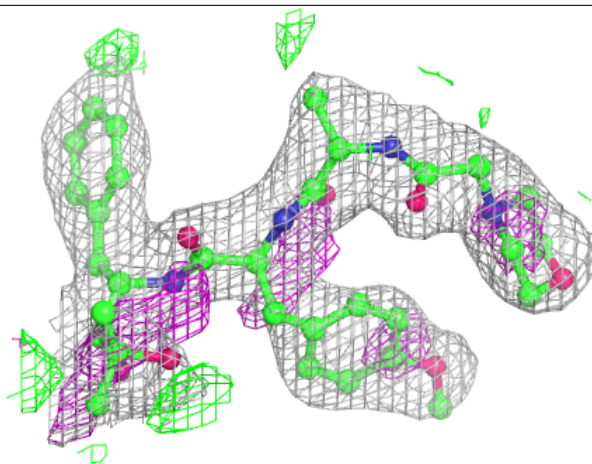
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
17	GQK	N	201	42/42	0.90	0.21	31,47,66,69	0
17	GQK	H	301	42/42	0.91	0.17	35,41,67,68	0
15	MG	G	301	1/1	0.92	0.11	52,52,52,52	0
17	GQK	b	201	42/42	0.92	0.15	27,48,71,74	0
18	MES	V	302	12/12	0.92	0.19	58,67,71,71	12
17	GQK	V	301	42/42	0.94	0.16	36,40,74,74	0
15	MG	W	301	1/1	0.95	0.30	57,57,57,57	0
17	GQK	Y	301	42/42	0.95	0.12	24,38,55,57	0
17	GQK	K	301	42/42	0.95	0.12	25,39,53,54	0
18	MES	H	302	12/12	0.95	0.17	51,62,72,72	12
15	MG	Z	301	1/1	0.95	0.18	70,70,70,70	0
19	SO4	N	203	5/5	0.95	0.24	53,60,69,70	5
15	MG	N	202	1/1	0.96	0.07	51,51,51,51	0
19	SO4	b	202	5/5	0.96	0.21	50,58,66,67	5
15	MG	I	301	1/1	0.97	0.23	59,59,59,59	0
18	MES	Y	302	12/12	0.98	0.14	38,41,41,43	12
18	MES	K	303	12/12	0.98	0.13	35,39,39,43	12
15	MG	K	302	1/1	0.98	0.07	58,58,58,58	0
15	MG	L	301	1/1	0.99	0.04	54,54,54,54	0
15	MG	I	302	1/1	0.99	0.12	59,59,59,59	0
16	CL	G	302	1/1	0.99	0.06	43,43,43,43	0
16	CL	U	301	1/1	0.99	0.09	47,47,47,47	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 GQK N 201:**

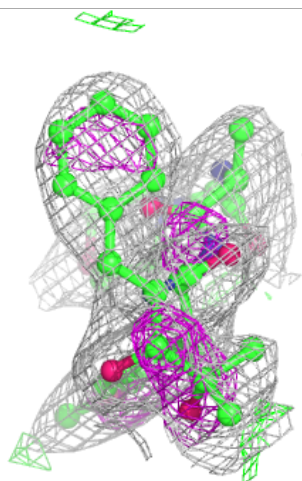
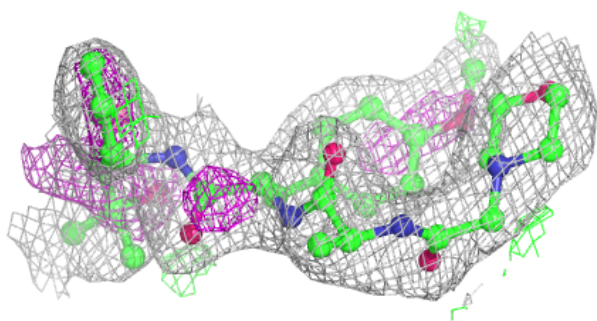
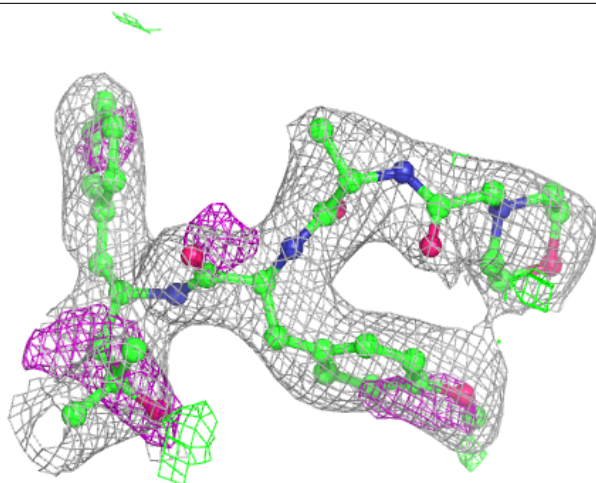
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

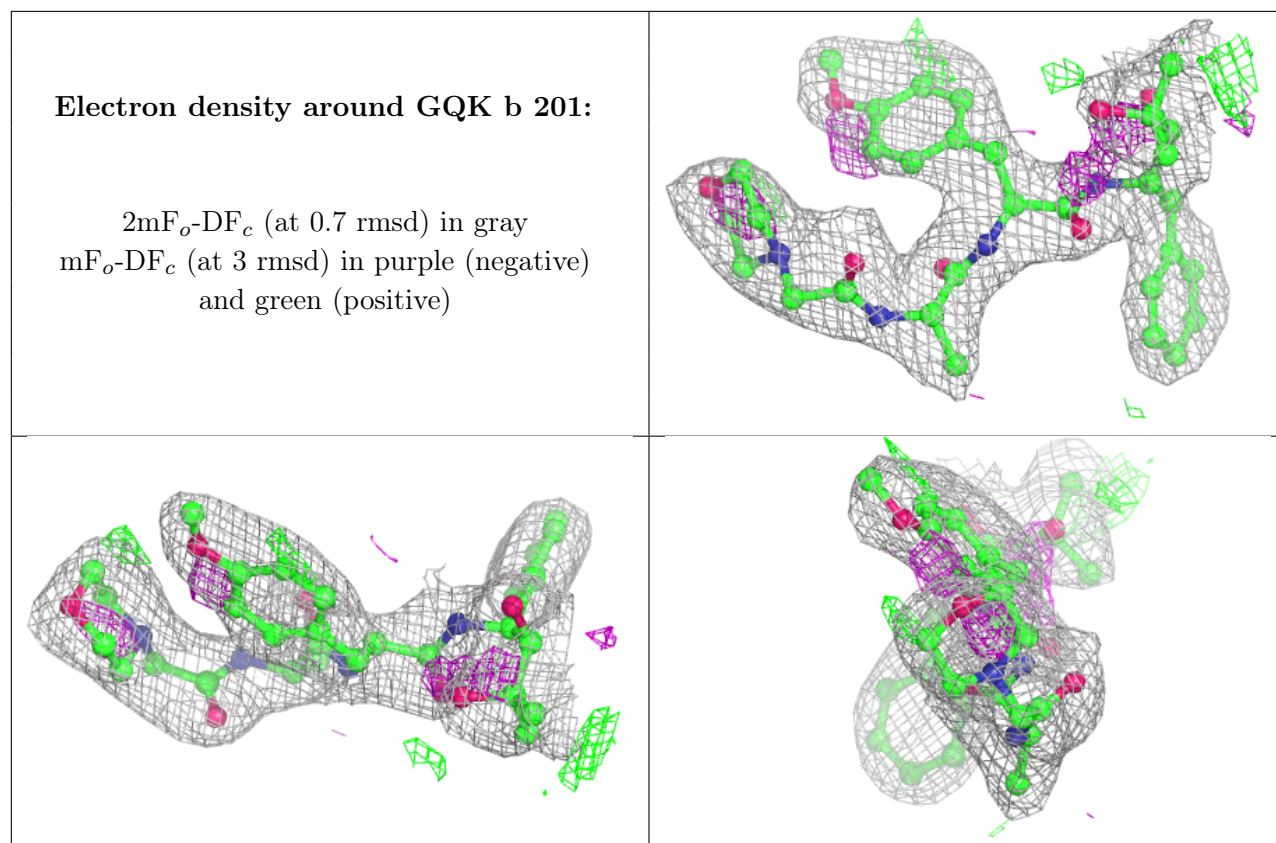




**Electron density around GQK H 301:**

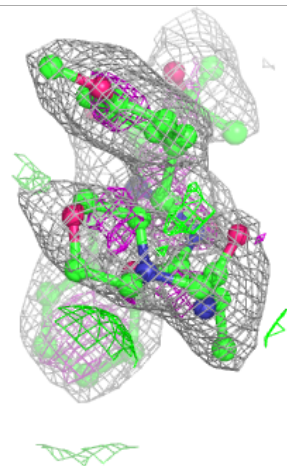
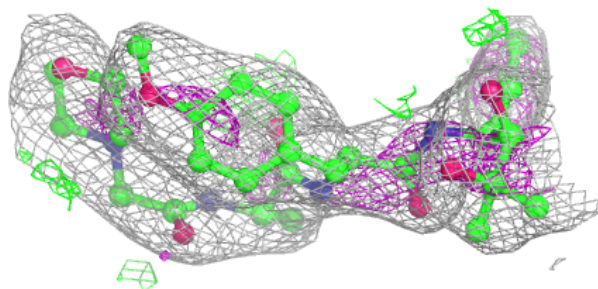
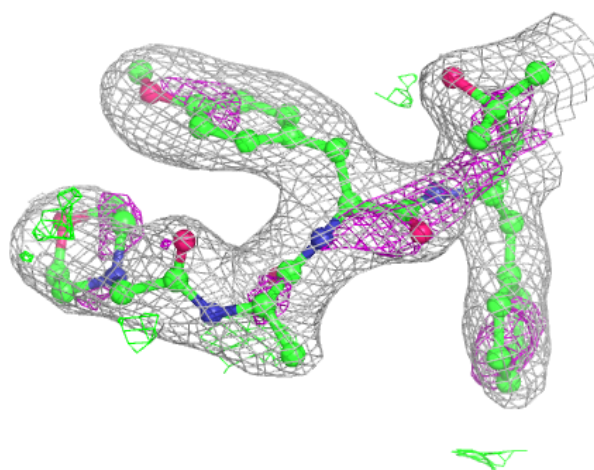
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





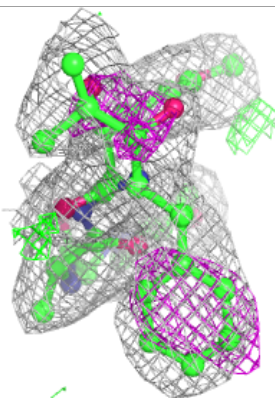
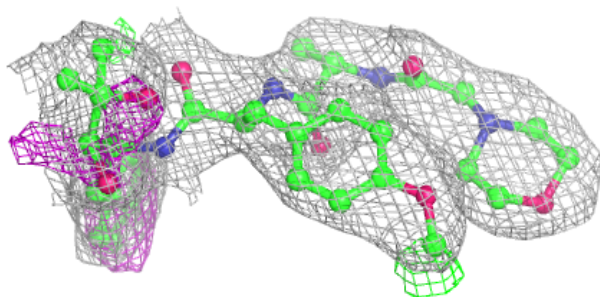
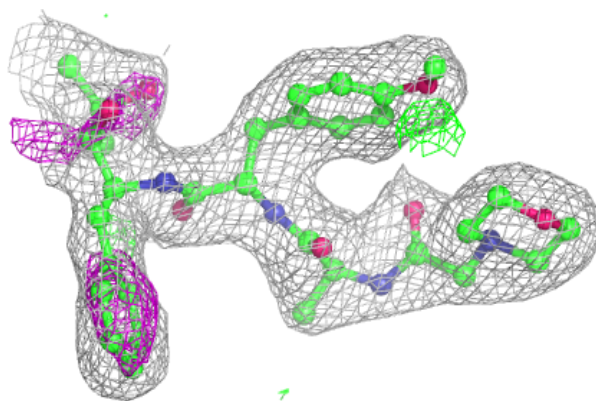
**Electron density around GQK V 301:**

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

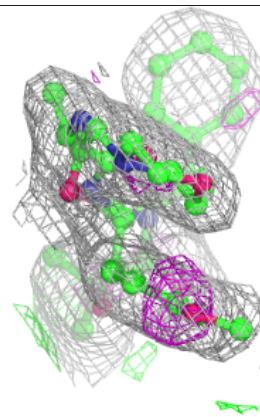
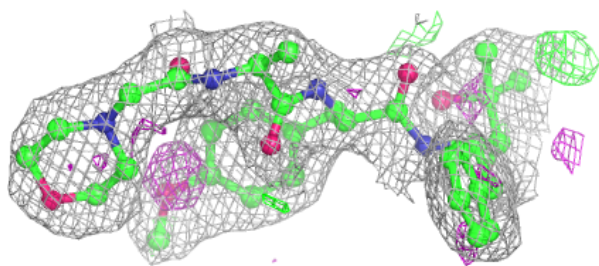
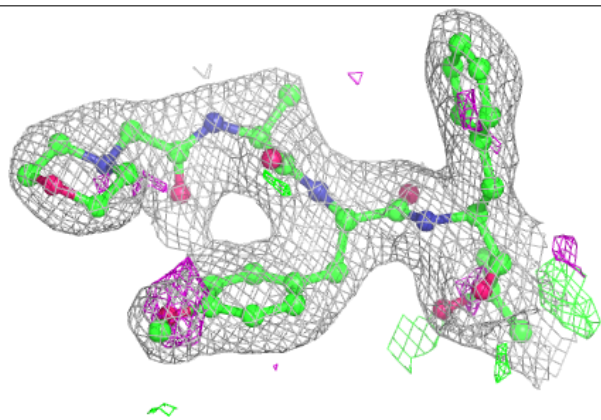


**Electron density around GQK Y 301:**

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

**Electron density around GQK 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 [i](#)

There are no such residues in this entry.