Full wwPDB X-ray Structure Validation Report ⓘ

Jun 26, 2024 – 10:32 AM EDT

PDB ID	:	6ZOU
Title	:	Yeast 20S proteasome in complex with glidobactin-like natural product HB333
Authors	:	Zhao, L.; Le Chapelain, C.; Brachmann, A.O.; Kaiser, M.; Groll, M.; Bode, H.B.
Deposited on	:	2020-07-07
Resolution	:	2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The 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:

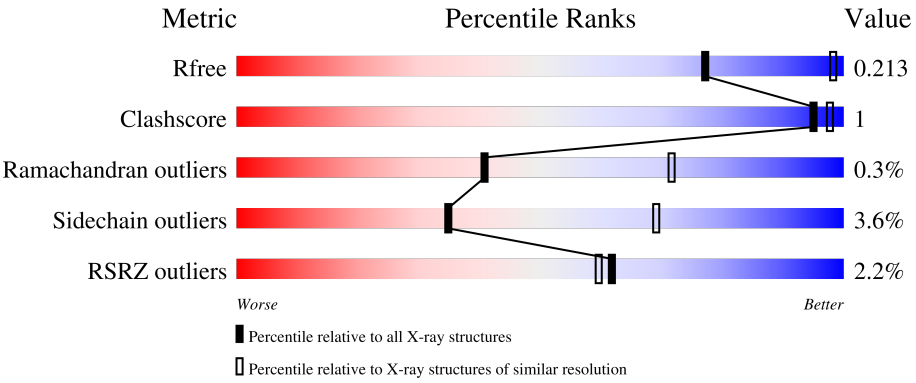
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	2% 98% ·
1	O	250	% 98% ·
2	B	258	4% 88% 6% 5%
2	P	258	5% 89% 5% 5%
3	C	254	6% 87% 6% · 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	6% 88% 6% 6%
4	D	260	85% 5% 10%
4	R	260	85% 5% 10%
5	E	234	92% 6%
5	S	234	3% 92% 6%
6	F	288	2% 80% 16%
6	T	288	80% 16%
7	G	252	3% 88% 8%
7	U	252	88% 6%
8	H	232	3% 91%
8	V	232	3% 92%
9	I	205	94% 5%
9	W	205	95%
10	J	198	93% 5%
10	X	198	2% 93% 5%
11	K	212	93% 7%
11	Y	212	93% 6%
12	L	222	3% 93% 7%
12	Z	222	2% 93% 6%
13	M	246	90% 7%
13	a	246	91% 6%
14	N	196	95%
14	b	196	97%

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 49808 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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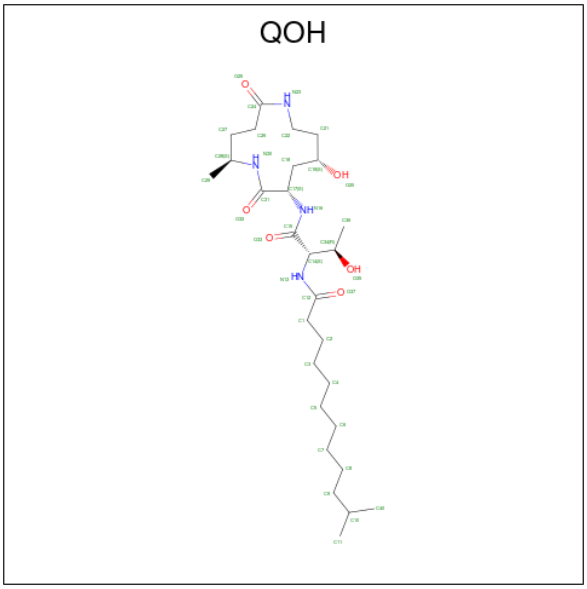
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	K	1	Total Mg 1 1	0	0
15	N	1	Total Mg 1 1	0	0
15	V	1	Total Mg 1 1	0	0
15	W	1	Total Mg 1 1	0	0
15	Y	1	Total Mg 1 1	0	0
15	Z	1	Total Mg 1 1	0	0

- 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 11-methyl- {N}-[(2 {S},3 {R})-1-[[(5 {S},8 {S},10 {S})-5-methyl-10-oxidanyl -2,7-bis(oxidanylidene)-1,6-diazacyclododec-8-yl]amino]-3-oxidanyl-1-oxidanylidene-butan-2-yl]dodecanamide (three-letter code: QOH) (formula: $C_{28}H_{52}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	H	1	Total 38	C 28	N 4	O 6	0	0
17	K	1	Total 38	C 28	N 4	O 6	0	0
17	V	1	Total 38	C 28	N 4	O 6	0	0
17	Y	1	Total 38	C 28	N 4	O 6	0	0

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	10	Total 10	O 10	0	0
18	B	12	Total 12	O 12	0	0
18	C	8	Total 8	O 8	0	0
18	D	6	Total 6	O 6	0	0
18	E	8	Total 8	O 8	0	0
18	F	6	Total 6	O 6	0	0
18	G	11	Total 11	O 11	0	0
18	H	9	Total 9	O 9	0	0
18	I	8	Total 8	O 8	0	0
18	J	14	Total 14	O 14	0	0
18	K	13	Total 13	O 13	0	0
18	L	17	Total 17	O 17	0	0
18	M	19	Total 19	O 19	0	0
18	N	16	Total 16	O 16	0	0
18	O	6	Total 6	O 6	0	0
18	P	6	Total 6	O 6	0	0

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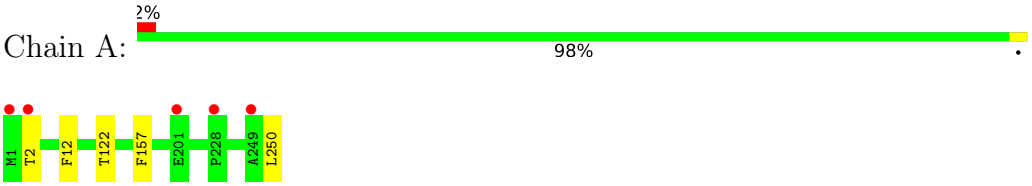
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	Q	15	Total O 15 15	0	0
18	R	9	Total O 9 9	0	0
18	S	4	Total O 4 4	0	0
18	T	9	Total O 9 9	0	0
18	U	13	Total O 13 13	0	0
18	V	15	Total O 15 15	0	0
18	W	9	Total O 9 9	0	0
18	X	11	Total O 11 11	0	0
18	Y	12	Total O 12 12	0	0
18	Z	16	Total O 16 16	0	0
18	a	25	Total O 25 25	0	0
18	b	16	Total O 16 16	0	0

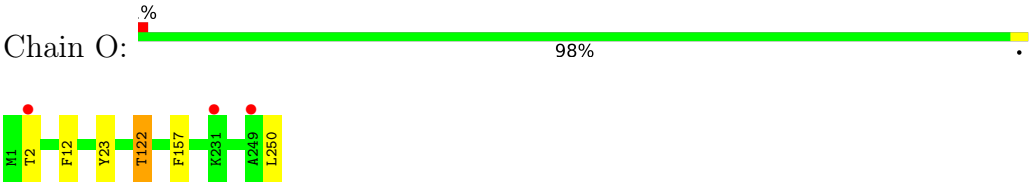
3 Residue-property plots (i)

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.

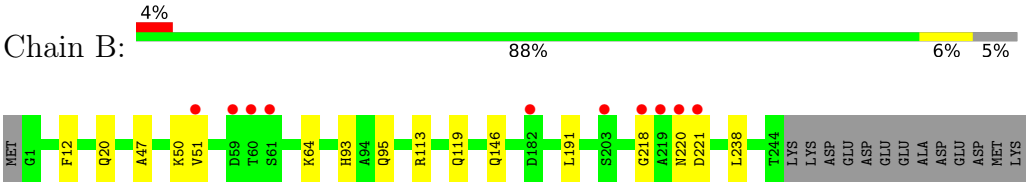
• Molecule 1: Proteasome subunit alpha type-2



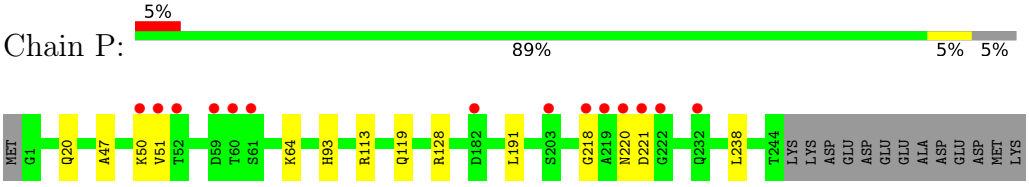
• Molecule 1: Proteasome subunit alpha type-2



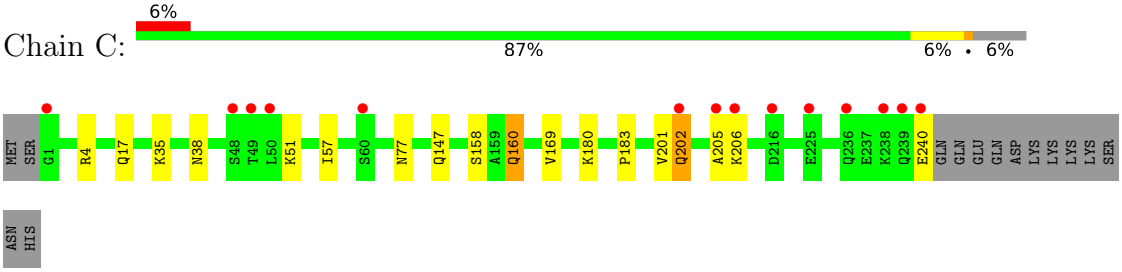
• Molecule 2: Proteasome subunit alpha type-3



• Molecule 2: Proteasome subunit alpha type-3

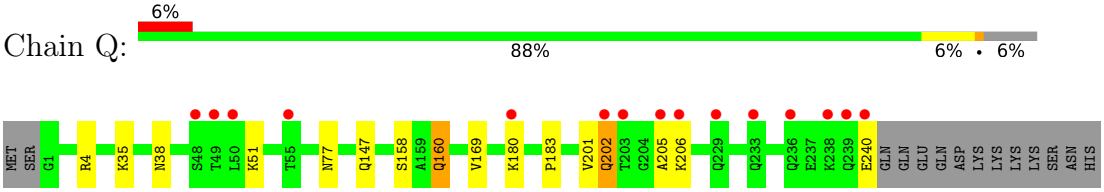


• Molecule 3: Proteasome subunit alpha type-4



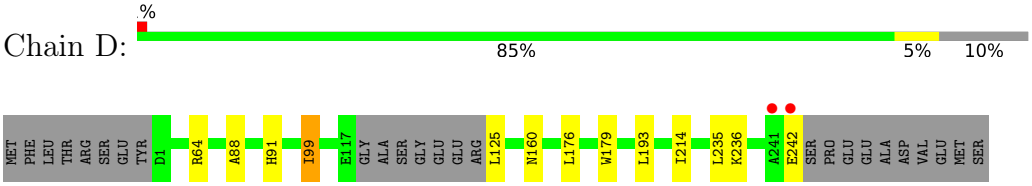
• Molecule 3: Proteasome subunit alpha type-4

Chain Q:



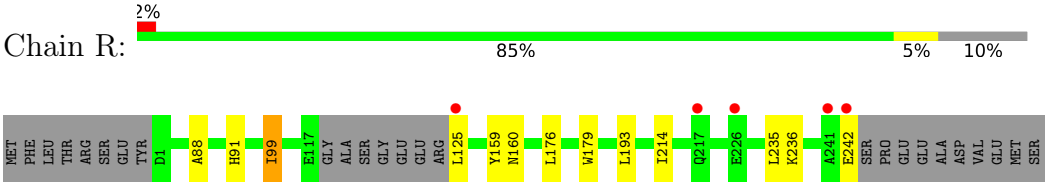
• Molecule 4: Proteasome subunit alpha type-5

Chain D:



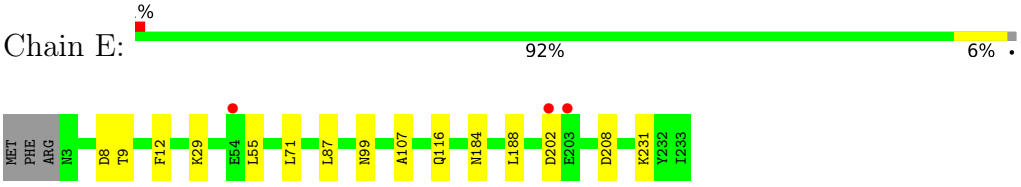
• Molecule 4: Proteasome subunit alpha type-5

Chain R:



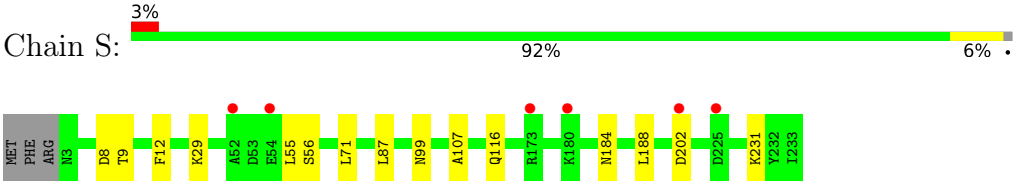
• Molecule 5: Proteasome subunit alpha type-6

Chain E:



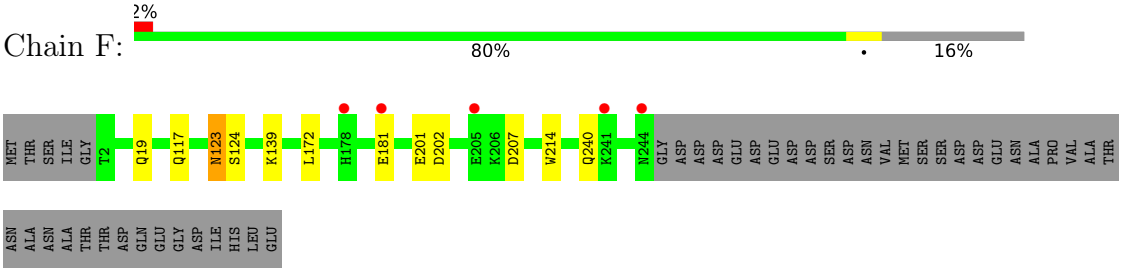
• Molecule 5: Proteasome subunit alpha type-6

Chain S:



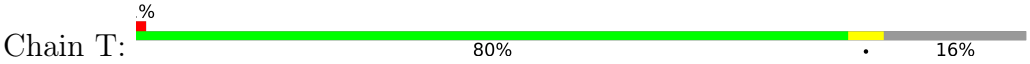
• Molecule 6: Probable proteasome subunit alpha type-7

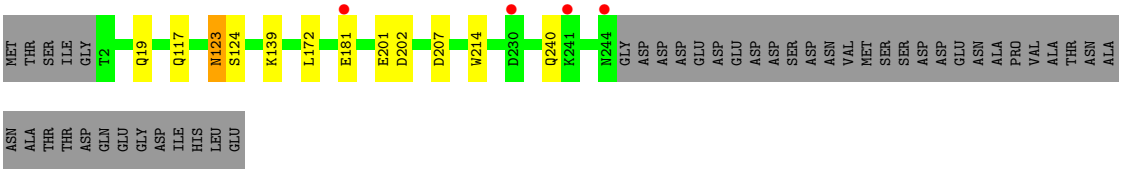
Chain F:



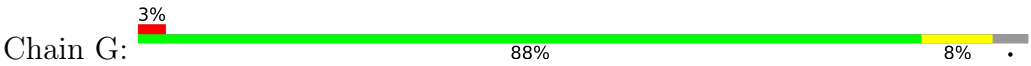
• Molecule 6: Probable proteasome subunit alpha type-7

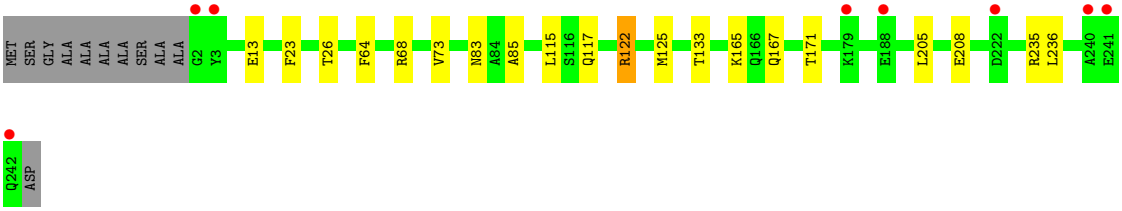
Chain T:



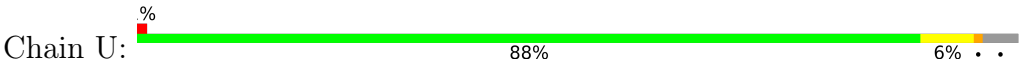


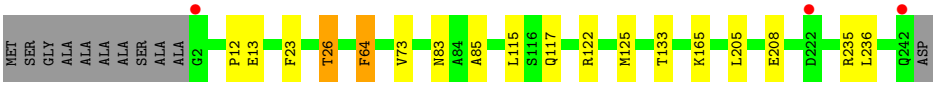
• Molecule 7: Proteasome subunit alpha type-1



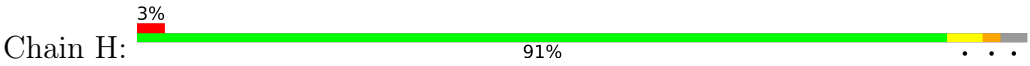


• Molecule 7: Proteasome subunit alpha type-1

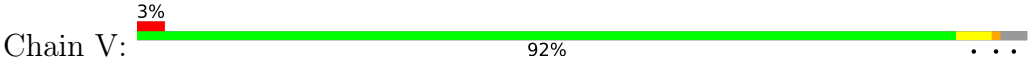




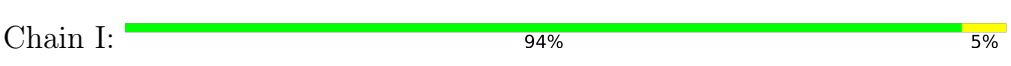
• Molecule 8: Proteasome subunit beta type-2



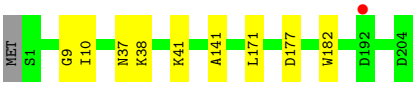
• Molecule 8: Proteasome subunit beta type-2



• Molecule 9: Proteasome subunit beta type-3

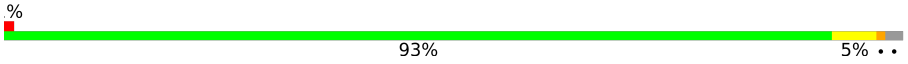


• Molecule 9: Proteasome subunit beta type-3



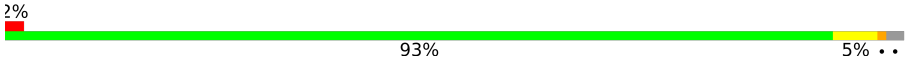
• Molecule 10: Proteasome subunit beta type-4

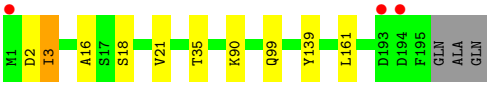
Chain J:



• Molecule 10: Proteasome subunit beta type-4

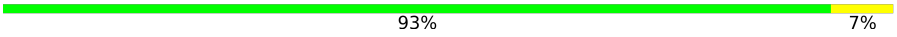
Chain X:





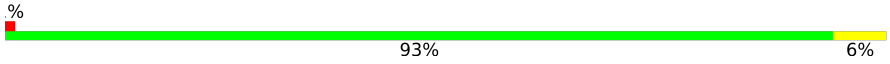
• Molecule 11: Proteasome subunit beta type-5

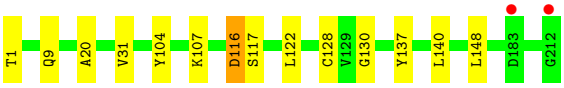
Chain K:



• Molecule 11: Proteasome subunit beta type-5

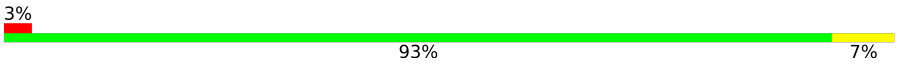
Chain Y:

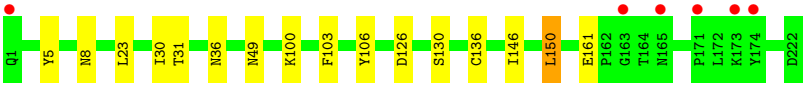




• Molecule 12: Proteasome subunit beta type-6

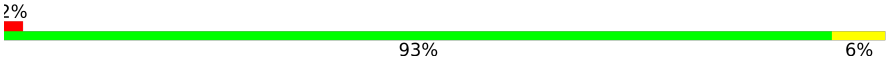
Chain L:





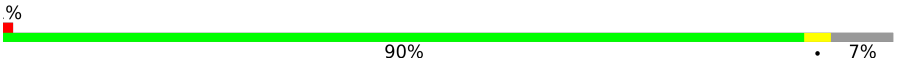
• Molecule 12: Proteasome subunit beta type-6

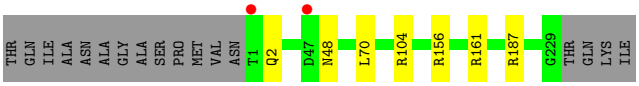
Chain Z:



• Molecule 13: Proteasome subunit beta type-7

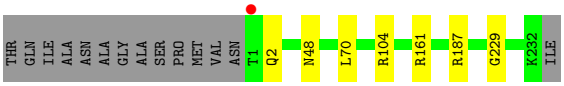
Chain M:





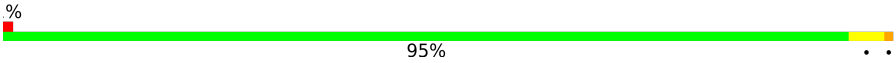
• Molecule 13: Proteasome subunit beta type-7

Chain a:



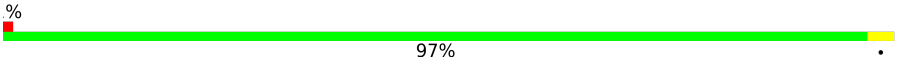
• Molecule 14: Proteasome subunit beta type-1

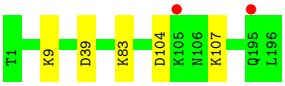
Chain N:



• Molecule 14: Proteasome subunit beta type-1

Chain b:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	136.78Å 300.24Å 145.74Å 90.00° 113.32° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 15.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.5 (15.00-2.90) 97.2 (15.00-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.75 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.172 , 0.212 0.177 , 0.213	Depositor DCC
R_{free} test set	11470 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	64.4	Xtriage
Anisotropy	0.427	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 32.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	49808	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CL, MG, QOH

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	0.58	0/2642
1	O	0.36	0/1952	0.58	0/2642
2	B	0.38	0/1934	0.62	0/2618
2	P	0.38	0/1934	0.62	0/2618
3	C	0.37	0/1910	0.64	0/2586
3	Q	0.37	0/1910	0.64	0/2586
4	D	0.36	0/1837	0.60	0/2475
4	R	0.36	0/1837	0.60	0/2475
5	E	0.36	0/1800	0.58	0/2433
5	S	0.36	0/1800	0.58	0/2433
6	F	0.36	0/1932	0.57	0/2609
6	T	0.36	0/1932	0.56	0/2609
7	G	0.37	0/1945	0.59	0/2634
7	U	0.37	0/1945	0.59	1/2634 (0.0%)
8	H	0.36	0/1750	0.60	1/2373 (0.0%)
8	V	0.35	0/1750	0.60	1/2373 (0.0%)
9	I	0.36	0/1611	0.59	0/2174
9	W	0.36	0/1611	0.59	0/2174
10	J	0.36	0/1589	0.62	0/2142
10	X	0.36	0/1589	0.61	0/2142
11	K	0.37	0/1681	0.62	0/2274
11	Y	0.35	0/1681	0.62	0/2274
12	L	0.37	0/1795	0.61	0/2420
12	Z	0.36	0/1795	0.60	0/2420
13	M	0.37	0/1821	0.65	0/2470
13	a	0.37	0/1846	0.64	0/2503
14	N	0.35	0/1541	0.60	1/2087 (0.0%)
14	b	0.34	0/1541	0.60	0/2087
All	All	0.36	0/50221	0.60	4/67907 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	V	196	ARG	NE-CZ-NH1	5.34	122.97	120.30
8	H	196	ARG	NE-CZ-NH1	5.24	122.92	120.30
14	N	36	ARG	NE-CZ-NH2	-5.05	117.77	120.30
7	U	64	PHE	CB-CG-CD1	5.02	124.31	120.80

There are no chirality outliers.

There are no planarity outliers.

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	1	0
1	O	1915	0	1929	3	0
2	B	1904	0	1904	6	0
2	P	1904	0	1904	4	0
3	C	1881	0	1895	5	0
3	Q	1881	0	1895	3	0
4	D	1813	0	1797	4	0
4	R	1813	0	1797	4	0
5	E	1773	0	1775	2	0
5	S	1773	0	1775	3	0
6	F	1892	0	1883	3	0
6	T	1892	0	1883	2	0
7	G	1907	0	1901	9	0
7	U	1907	0	1901	8	0
8	H	1719	0	1718	14	0
8	V	1719	0	1718	7	0
9	I	1581	0	1574	6	0
9	W	1581	0	1574	4	0
10	J	1561	0	1569	5	0
10	X	1561	0	1569	4	0
11	K	1644	0	1594	8	0
11	Y	1644	0	1594	6	0
12	L	1757	0	1711	6	0
12	Z	1757	0	1711	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	M	1790	0	1793	1	0
13	a	1815	0	1821	0	0
14	N	1512	0	1481	3	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	38	0	0	0	0
17	K	38	0	0	1	0
17	V	38	0	0	0	0
17	Y	38	0	0	3	0
18	A	10	0	0	0	0
18	B	12	0	0	1	0
18	C	8	0	0	0	0
18	D	6	0	0	1	0
18	E	8	0	0	0	0
18	F	6	0	0	0	0
18	G	11	0	0	1	0
18	H	9	0	0	0	0
18	I	8	0	0	0	0
18	J	14	0	0	0	0
18	K	13	0	0	0	0
18	L	17	0	0	0	0
18	M	19	0	0	0	0
18	N	16	0	0	0	0
18	O	6	0	0	0	0
18	P	6	0	0	1	0
18	Q	15	0	0	0	0
18	R	9	0	0	0	0
18	S	4	0	0	0	0
18	T	9	0	0	0	0
18	U	13	0	0	0	0
18	V	15	0	0	0	0
18	W	9	0	0	0	0
18	X	11	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	Y	12	0	0	0	0
18	Z	16	0	0	0	0
18	a	25	0	0	0	0
18	b	16	0	0	0	0
All	All	49808	0	49076	112	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 (112) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:14:ILE:HD13	8:H:101:ALA:HB3	1.69	0.74
8:H:14:ILE:HD13	8:H:101:ALA:CB	2.18	0.73
11:Y:1:THR:O	11:Y:130:GLY:HA3	1.92	0.70
8:H:4:VAL:HG13	8:H:159:ILE:HD11	1.75	0.68
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.63	0.63
7:G:64:PHE:CD2	7:G:85:ALA:HB2	2.34	0.63
7:U:64:PHE:CD2	7:U:85:ALA:HB2	2.34	0.63
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.62	0.62
8:H:14:ILE:HD11	8:H:99:ILE:HG22	1.82	0.61
2:P:93:HIS:HB3	18:P:301:HOH:O	2.04	0.57
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.87	0.56
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.69	0.56
8:H:4:VAL:HG13	8:H:159:ILE:CD1	2.35	0.56
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.87	0.55
7:G:23:PHE:O	7:G:26:THR:HB	2.07	0.55
2:B:93:HIS:HB3	18:B:301:HOH:O	2.06	0.54
12:Z:100:LYS:HE3	12:Z:103:PHE:O	2.08	0.54
7:G:64:PHE:HD2	7:G:85:ALA:HB2	1.73	0.54
12:L:100:LYS:HE3	12:L:103:PHE:O	2.08	0.53
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.73	0.53
7:U:64:PHE:HD2	7:U:85:ALA:HB2	1.71	0.53
7:U:23:PHE:O	7:U:26:THR:HB	2.10	0.51
1:O:12:PHE:H	2:P:20:GLN:HE22	1.57	0.51
17:Y:301:QOH:N23	17:Y:301:QOH:C18	2.73	0.51
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.93	0.51
17:Y:301:QOH:C9	12:Z:106:TYR:CE1	2.94	0.51
2:B:12:PHE:H	3:C:17:GLN:HE22	1.59	0.50
11:K:128:CYS:HB2	11:K:137:TYR:CZ	2.47	0.49
8:H:3:ILE:HG13	8:H:99:ILE:HD12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:80:LEU:HD22	8:H:111:PHE:CD2	2.47	0.49
5:S:12:PHE:H	6:T:19:GLN:HE22	1.60	0.49
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.94	0.49
7:G:68:ARG:HH12	14:N:36:ARG:HH22	1.61	0.49
11:Y:128:CYS:HB2	11:Y:137:TYR:CZ	2.48	0.49
8:V:80:LEU:HD22	8:V:111:PHE:CD2	2.48	0.48
2:B:146:GLN:HG2	3:C:57:ILE:HG21	1.95	0.48
8:V:113:ILE:HG13	8:V:119:THR:HG22	1.96	0.48
8:H:4:VAL:CG1	8:H:159:ILE:CD1	2.92	0.48
5:E:12:PHE:H	6:F:19:GLN:HE22	1.62	0.47
11:K:4:LEU:C	11:K:4:LEU:HD12	2.35	0.47
8:H:14:ILE:HD13	8:H:101:ALA:HB2	1.94	0.47
17:K:301:QOH:O35	12:L:126:ASP:OD2	2.33	0.47
1:A:12:PHE:H	2:B:20:GLN:HE22	1.63	0.46
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	1.96	0.46
8:H:113:ILE:HG13	8:H:119:THR:HG22	1.97	0.46
2:P:47:ALA:HB1	2:P:64:LYS:HD2	1.98	0.46
8:V:4:VAL:HG13	8:V:159:ILE:CD1	2.45	0.46
2:B:47:ALA:HB1	2:B:64:LYS:HD2	1.97	0.46
8:V:80:LEU:HD21	8:V:111:PHE:CG	2.50	0.46
11:K:116:ASP:OD1	11:K:116:ASP:C	2.54	0.45
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.97	0.45
8:H:80:LEU:HD21	8:H:111:PHE:CG	2.52	0.45
4:R:159:TYR:CE1	5:S:56:SER:HB3	2.52	0.45
7:U:73:VAL:HG12	7:U:133:THR:HB	1.99	0.45
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.98	0.44
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.00	0.44
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.98	0.44
8:V:3:ILE:HD11	8:V:127:LEU:HB3	1.99	0.44
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.98	0.44
9:I:10:ILE:HG21	9:I:141:ALA:HB3	2.00	0.44
14:N:35:THR:HG21	14:N:45:ARG:HE	1.82	0.44
6:F:123:ASN:HD22	6:F:124:SER:N	2.15	0.44
7:G:73:VAL:HG12	7:G:133:THR:HB	1.99	0.44
4:D:88:ALA:HA	4:D:99:ILE:HG21	2.00	0.43
8:V:80:LEU:CD2	8:V:111:PHE:CG	3.01	0.43
7:G:122:ARG:HD2	18:G:409:HOH:O	2.18	0.43
4:R:91:HIS:CD2	4:R:99:ILE:HG22	2.53	0.43
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.54	0.43
7:G:64:PHE:CE2	7:G:85:ALA:HB2	2.54	0.43
6:F:123:ASN:HD22	6:F:123:ASN:C	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:141:ALA:HB2	9:I:177:ASP:HB2	2.00	0.43
7:U:64:PHE:CD2	7:U:85:ALA:CB	3.01	0.43
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.66	0.43
7:G:167:GLN:HE21	7:G:171:THR:HG23	1.84	0.42
8:H:80:LEU:CD2	8:H:111:PHE:CG	3.02	0.42
9:W:141:ALA:HB2	9:W:177:ASP:HB2	2.01	0.42
10:J:3:ILE:HG23	10:J:18:SER:HB3	2.02	0.42
7:U:64:PHE:CE2	7:U:85:ALA:HB2	2.54	0.42
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.84	0.42
9:I:9:GLY:HA3	9:I:41:LYS:HE2	2.01	0.42
4:D:91:HIS:CD2	4:D:99:ILE:HG22	2.55	0.42
11:Y:116:ASP:OD1	11:Y:116:ASP:C	2.58	0.42
11:Y:116:ASP:OD1	11:Y:117:SER:N	2.53	0.42
10:J:21:VAL:HG11	11:K:122:LEU:HD11	2.02	0.41
17:Y:301:QOH:C9	12:Z:106:TYR:CD1	3.03	0.41
3:C:35:LYS:HG2	3:C:158:SER:O	2.20	0.41
13:M:156:ARG:HH11	8:V:165:ASN:HD22	1.68	0.41
12:Z:31:THR:CG2	12:Z:36:ASN:HD21	2.33	0.41
12:Z:146:ILE:HG22	12:Z:150:LEU:HD22	2.03	0.41
3:C:201:VAL:O	3:C:202:GLN:CB	2.68	0.41
8:H:196:ARG:NH2	9:I:150:GLU:O	2.54	0.41
10:J:25:ILE:O	10:X:139:TYR:OH	2.38	0.41
7:G:165:LYS:HD2	7:G:205:LEU:HD22	2.03	0.41
7:U:165:LYS:HD2	7:U:205:LEU:HD22	2.02	0.41
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.56	0.41
11:K:116:ASP:OD1	11:K:117:SER:N	2.53	0.41
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.55	0.41
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.21	0.41
10:X:3:ILE:HG23	10:X:18:SER:HB3	2.03	0.41
12:L:146:ILE:HG22	12:L:150:LEU:HD22	2.03	0.41
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.56	0.41
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.21	0.41
12:L:5:TYR:CE1	12:L:106:TYR:HB2	2.56	0.41
12:L:8:ASN:HA	12:L:30:ILE:O	2.20	0.41
9:W:9:GLY:HA3	9:W:41:LYS:HE2	2.02	0.41
4:D:64:ARG:HD2	18:D:304:HOH:O	2.21	0.40
8:H:84:LYS:HE2	8:H:119:THR:HG23	2.03	0.40
12:Z:5:TYR:CE1	12:Z:106:TYR:HB2	2.56	0.40
11:K:128:CYS:HB2	11:K:137:TYR:CE2	2.56	0.40
11:K:209:ASN:O	9:W:38:LYS:NZ	2.54	0.40
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:123:ASN:HD22	6:T:124:SER:N	2.18	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%)	239 (96%)	8 (3%)	1 (0%)	34	66
1	O	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	34	66
2	B	242/258 (94%)	235 (97%)	3 (1%)	4 (2%)	9	31
2	P	242/258 (94%)	236 (98%)	2 (1%)	4 (2%)	9	31
3	C	238/254 (94%)	233 (98%)	2 (1%)	3 (1%)	12	37
3	Q	238/254 (94%)	233 (98%)	2 (1%)	3 (1%)	12	37
4	D	231/260 (89%)	228 (99%)	3 (1%)	0	100	100
4	R	231/260 (89%)	228 (99%)	3 (1%)	0	100	100
5	E	229/234 (98%)	224 (98%)	5 (2%)	0	100	100
5	S	229/234 (98%)	224 (98%)	5 (2%)	0	100	100
6	F	241/288 (84%)	239 (99%)	2 (1%)	0	100	100
6	T	241/288 (84%)	239 (99%)	2 (1%)	0	100	100
7	G	239/252 (95%)	238 (100%)	1 (0%)	0	100	100
7	U	239/252 (95%)	238 (100%)	1 (0%)	0	100	100
8	H	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
8	V	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
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%)	187 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	X	193/198 (98%)	187 (97%)	6 (3%)	0	100	100
11	K	210/212 (99%)	207 (99%)	3 (1%)	0	100	100
11	Y	210/212 (99%)	206 (98%)	4 (2%)	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%)	222 (96%)	7 (3%)	1 (0%)	34	66
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%)	6141 (98%)	121 (2%)	17 (0%)	41	71

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	89
1	O	209/209 (100%)	206 (99%)	3 (1%)	67	89
2	B	203/216 (94%)	198 (98%)	5 (2%)	47	78
2	P	203/216 (94%)	198 (98%)	5 (2%)	47	78
3	C	212/226 (94%)	202 (95%)	10 (5%)	26	59
3	Q	212/226 (94%)	202 (95%)	10 (5%)	26	59
4	D	194/215 (90%)	186 (96%)	8 (4%)	30	64
4	R	194/215 (90%)	186 (96%)	8 (4%)	30	64
5	E	190/193 (98%)	178 (94%)	12 (6%)	18	46
5	S	190/193 (98%)	179 (94%)	11 (6%)	20	50
6	F	201/239 (84%)	191 (95%)	10 (5%)	24	57
6	T	201/239 (84%)	191 (95%)	10 (5%)	24	57
7	G	206/210 (98%)	197 (96%)	9 (4%)	28	61
7	U	206/210 (98%)	196 (95%)	10 (5%)	25	57
8	H	185/190 (97%)	177 (96%)	8 (4%)	29	62
8	V	185/190 (97%)	179 (97%)	6 (3%)	39	73
9	I	172/173 (99%)	169 (98%)	3 (2%)	60	86
9	W	172/173 (99%)	169 (98%)	3 (2%)	60	86
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%)	162 (96%)	7 (4%)	30	64
11	Y	169/169 (100%)	163 (96%)	6 (4%)	35	69
12	L	185/185 (100%)	179 (97%)	6 (3%)	39	73
12	Z	185/185 (100%)	179 (97%)	6 (3%)	39	73
13	M	195/208 (94%)	189 (97%)	6 (3%)	40	74
13	a	198/208 (95%)	192 (97%)	6 (3%)	41	75
14	N	162/162 (100%)	157 (97%)	5 (3%)	40	74
14	b	162/162 (100%)	157 (97%)	5 (3%)	40	74
All	All	5315/5540 (96%)	5124 (96%)	191 (4%)	35	69

All (191) 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	113	ARG
2	B	119	GLN
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	51	LYS
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	206	LYS
3	C	240	GLU
4	D	99	ILE
4	D	125	LEU
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	8	ASP
5	E	9	THR
5	E	29	LYS
5	E	55	LEU
5	E	71	LEU
5	E	99	ASN
5	E	116	GLN
5	E	184	ASN
5	E	188	LEU
5	E	202	ASP
5	E	208	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

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Mol	Chain	Res	Type
6	F	201	GLU
6	F	202	ASP
6	F	207	ASP
6	F	214	TRP
6	F	240	GLN
7	G	13	GLU
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	3	ILE
8	H	4	VAL
8	H	14	ILE
8	H	30	ASN
8	H	43	CYS
8	H	68	LEU
8	H	113	ILE
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	9	GLN
11	K	100	MET
11	K	104	TYR
11	K	107	LYS
11	K	116	ASP
11	K	140	LEU
11	K	148	LEU
12	L	23	LEU
12	L	49	ASN
12	L	130	SER
12	L	136	CYS
12	L	150	LEU

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Mol	Chain	Res	Type
12	L	161	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
14	N	9	LYS
14	N	39	ASP
14	N	83	LYS
14	N	104	ASP
14	N	107	LYS
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	50	LYS
2	P	113	ARG
2	P	119	GLN
2	P	191	LEU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	51	LYS
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	206	LYS
3	Q	240	GLU
4	R	99	ILE
4	R	125	LEU
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	8	ASP
5	S	9	THR
5	S	29	LYS
5	S	55	LEU

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Mol	Chain	Res	Type
5	S	71	LEU
5	S	99	ASN
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
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	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	4	VAL
8	V	30	ASN
8	V	43	CYS
8	V	68	LEU
8	V	113	ILE
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	9	GLN

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Mol	Chain	Res	Type
11	Y	104	TYR
11	Y	107	LYS
11	Y	116	ASP
11	Y	140	LEU
11	Y	148	LEU
12	Z	23	LEU
12	Z	49	ASN
12	Z	130	SER
12	Z	136	CYS
12	Z	150	LEU
12	Z	161	GLU
13	a	2	GLN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
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 (110) 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

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Mol	Chain	Res	Type
4	D	91	HIS
4	D	100	ASN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	151	ASN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
6	F	240	GLN
7	G	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	167	GLN
7	G	175	ASN
8	H	22	GLN
8	H	165	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	48	ASN
13	M	102	GLN
13	M	179	ASN
1	O	94	HIS
2	P	20	GLN
2	P	58	GLN

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Mol	Chain	Res	Type
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	176	GLN
3	Q	17	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
4	R	225	ASN
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	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
7	U	167	GLN
7	U	175	ASN
8	V	22	GLN
8	V	165	ASN
9	W	37	ASN
10	X	55	GLN
10	X	86	GLN

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Mol	Chain	Res	Type
11	Y	85	ASN
11	Y	176	ASN
11	Y	208	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	158	ASN
13	a	48	ASN
13	a	102	GLN
13	a	179	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	QOH	V	301	8	38,38,38	1.99	3 (7%)	46,48,48	1.45	6 (13%)
17	QOH	Y	301	11	38,38,38	1.95	5 (13%)	46,48,48	1.23	3 (6%)
17	QOH	K	301	11	38,38,38	2.15	7 (18%)	46,48,48	1.70	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	QOH	H	301	8	38,38,38	2.08	4 (10%)	46,48,48	1.34	6 (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	QOH	V	301	8	-	13/51/51/51	0/0/1/1
17	QOH	Y	301	11	-	14/51/51/51	0/0/1/1
17	QOH	K	301	11	-	16/51/51/51	0/0/1/1
17	QOH	H	301	8	-	11/51/51/51	0/0/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	H	301	QOH	C26-C24	-8.58	1.35	1.51
17	K	301	QOH	C26-C24	-8.58	1.35	1.51
17	V	301	QOH	C26-C24	-8.37	1.35	1.51
17	Y	301	QOH	C17-C31	-7.42	1.33	1.52
17	Y	301	QOH	C26-C24	-7.01	1.38	1.51
17	K	301	QOH	C17-C31	-7.01	1.34	1.52
17	H	301	QOH	C17-C31	-6.73	1.35	1.52
17	V	301	QOH	C17-C31	-6.31	1.36	1.52
17	K	301	QOH	C34-C14	-2.69	1.45	1.53
17	V	301	QOH	C27-C28	-2.68	1.48	1.53
17	K	301	QOH	C27-C28	-2.57	1.48	1.53
17	K	301	QOH	C24-N23	2.55	1.39	1.33
17	K	301	QOH	C27-C26	-2.40	1.45	1.52
17	K	301	QOH	C14-C15	-2.31	1.46	1.52
17	H	301	QOH	C21-C19	-2.22	1.45	1.52
17	Y	301	QOH	C18-C17	-2.17	1.46	1.53
17	Y	301	QOH	O35-C34	-2.15	1.37	1.43
17	H	301	QOH	C18-C19	-2.06	1.47	1.52
17	Y	301	QOH	C24-N23	2.03	1.38	1.33

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	K	301	QOH	O35-C34-C14	-5.30	98.49	109.13
17	K	301	QOH	C34-C14-N13	-5.22	98.35	111.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	V	301	QOH	C26-C27-C28	-4.66	106.86	114.02
17	V	301	QOH	C2-C1-C12	-3.76	102.70	113.26
17	K	301	QOH	C26-C27-C28	-3.68	108.35	114.02
17	V	301	QOH	C34-C14-N13	-3.51	102.74	111.72
17	H	301	QOH	C2-C1-C12	-3.45	103.57	113.26
17	H	301	QOH	C34-C14-N13	-3.22	103.49	111.72
17	K	301	QOH	C22-N23-C24	3.09	128.57	122.84
17	Y	301	QOH	C15-C14-N13	-2.87	102.57	110.36
17	H	301	QOH	C26-C27-C28	-2.72	109.84	114.02
17	Y	301	QOH	C26-C27-C28	-2.53	110.13	114.02
17	K	301	QOH	C36-C34-C14	-2.34	107.56	112.29
17	V	301	QOH	O32-C31-N30	-2.33	118.62	122.93
17	V	301	QOH	C7-C8-C9	-2.19	105.89	113.62
17	Y	301	QOH	C36-C34-C14	-2.14	107.96	112.29
17	H	301	QOH	C17-C31-N30	2.11	121.33	116.70
17	H	301	QOH	O35-C34-C14	-2.05	105.03	109.13
17	V	301	QOH	C29-C28-C27	-2.04	107.61	111.47
17	H	301	QOH	C7-C8-C9	-2.01	106.52	113.62

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	H	301	QOH	N16-C17-C18-C19
17	H	301	QOH	O20-C19-C21-C22
17	K	301	QOH	N16-C17-C18-C19
17	K	301	QOH	O20-C19-C21-C22
17	K	301	QOH	C18-C19-C21-C22
17	K	301	QOH	C15-C14-C34-O35
17	K	301	QOH	N13-C14-C34-O35
17	V	301	QOH	N16-C17-C18-C19
17	V	301	QOH	O20-C19-C21-C22
17	Y	301	QOH	N16-C17-C18-C19
17	Y	301	QOH	O20-C19-C21-C22
17	Y	301	QOH	C18-C19-C21-C22
17	Y	301	QOH	C17-C18-C19-C21
17	Y	301	QOH	C17-C18-C19-O20
17	H	301	QOH	C31-C17-C18-C19
17	K	301	QOH	C31-C17-C18-C19
17	V	301	QOH	C24-C26-C27-C28
17	V	301	QOH	C31-C17-C18-C19
17	Y	301	QOH	C31-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
17	K	301	QOH	C17-C18-C19-O20
17	Y	301	QOH	C7-C8-C9-C10
17	K	301	QOH	C17-C18-C19-C21
17	V	301	QOH	C3-C4-C5-C6
17	H	301	QOH	C5-C6-C7-C8
17	V	301	QOH	C5-C6-C7-C8
17	H	301	QOH	C2-C3-C4-C5
17	K	301	QOH	N13-C14-C34-C36
17	V	301	QOH	C2-C3-C4-C5
17	H	301	QOH	C4-C5-C6-C7
17	H	301	QOH	C24-C26-C27-C28
17	V	301	QOH	C12-C1-C2-C3
17	V	301	QOH	C4-C5-C6-C7
17	Y	301	QOH	C6-C7-C8-C9
17	Y	301	QOH	C12-C1-C2-C3
17	Y	301	QOH	C5-C6-C7-C8
17	H	301	QOH	C18-C19-C21-C22
17	V	301	QOH	C18-C19-C21-C22
17	H	301	QOH	C12-C1-C2-C3
17	K	301	QOH	C12-C1-C2-C3
17	K	301	QOH	N16-C17-C31-O32
17	K	301	QOH	C6-C7-C8-C9
17	K	301	QOH	N16-C17-C31-N30
17	K	301	QOH	C24-C26-C27-C28
17	Y	301	QOH	C24-C26-C27-C28
17	V	301	QOH	N16-C17-C31-O32
17	K	301	QOH	C7-C8-C9-C10
17	Y	301	QOH	N16-C17-C31-O32
17	V	301	QOH	C11-C10-C9-C8
17	H	301	QOH	N16-C17-C31-O32
17	V	301	QOH	N16-C17-C31-N30
17	Y	301	QOH	N16-C17-C31-N30
17	Y	301	QOH	C4-C5-C6-C7
17	K	301	QOH	C1-C2-C3-C4
17	H	301	QOH	N16-C17-C31-N30

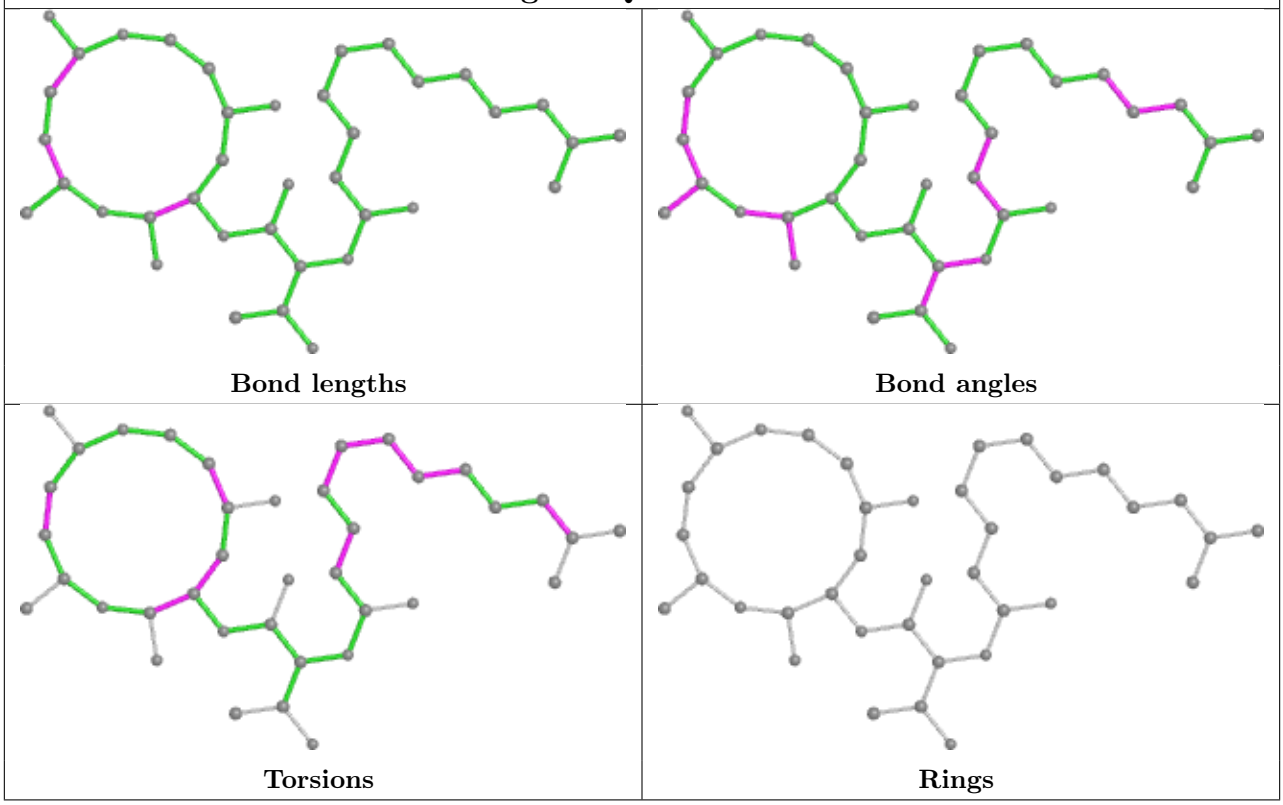
There are no ring outliers.

2 monomers are involved in 4 short contacts:

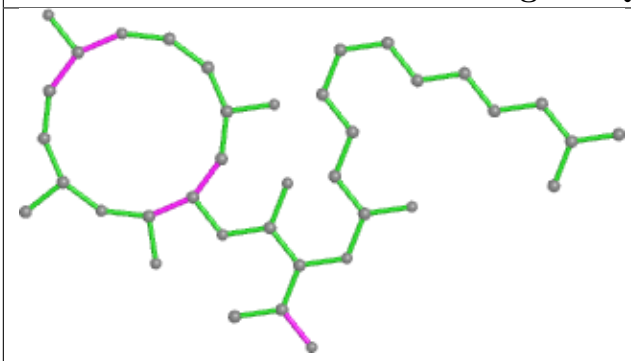
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	Y	301	QOH	3	0
17	K	301	QOH	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

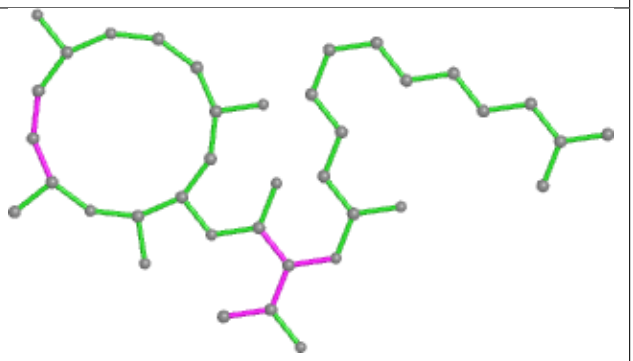
Ligand QOH V 301



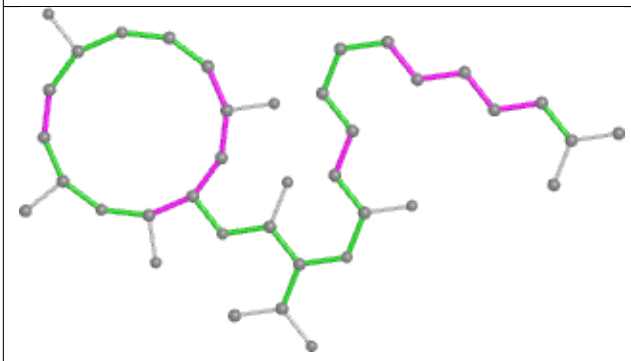
Ligand QOH Y 301



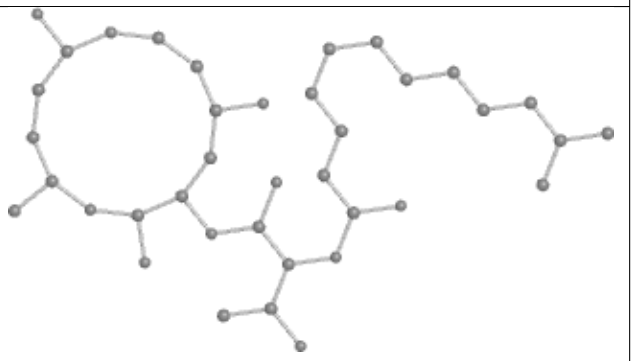
Bond lengths



Bond angles

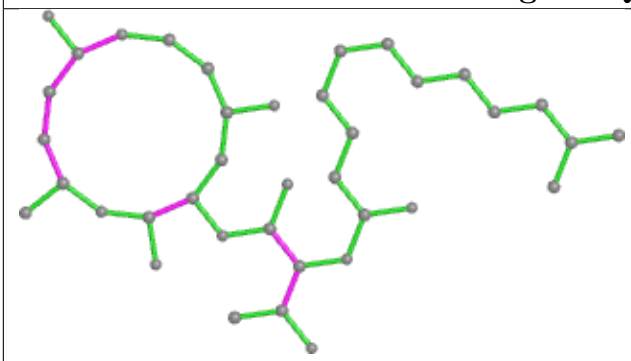


Torsions

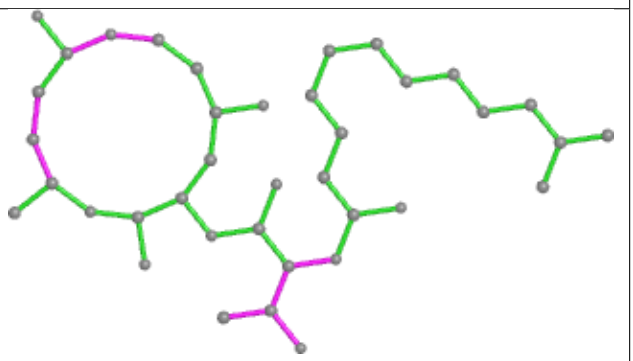


Rings

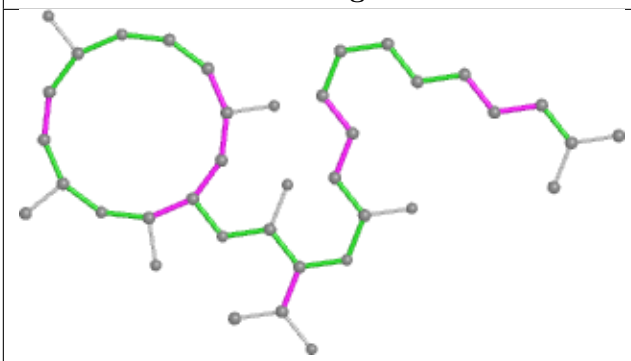
Ligand QOH K 301



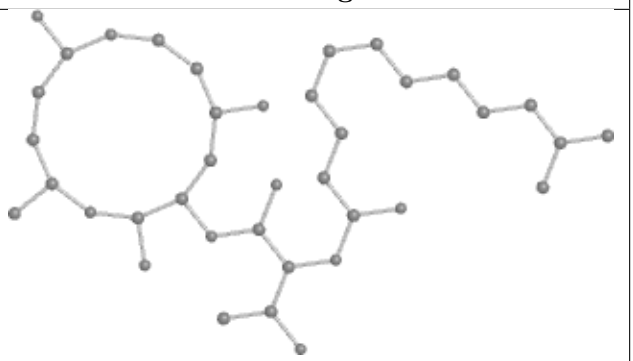
Bond lengths



Bond angles

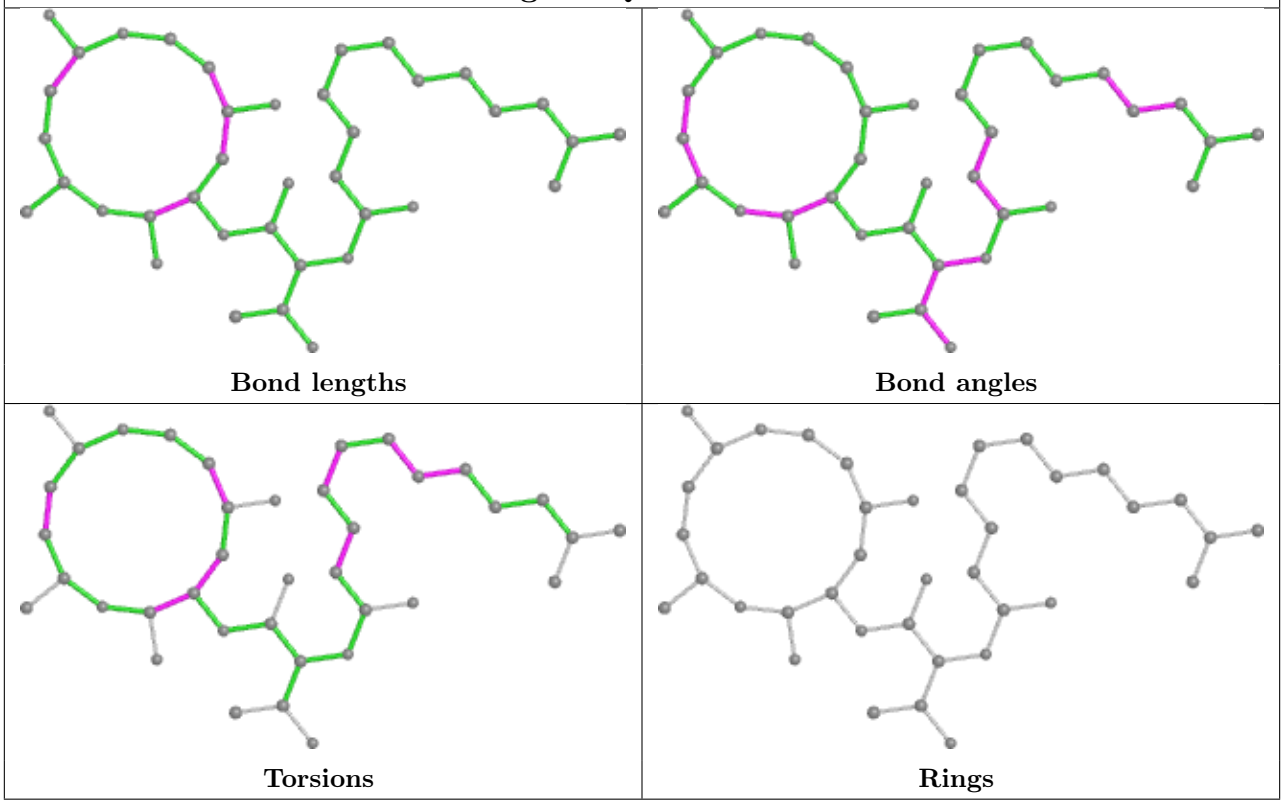


Torsions



Rings

Ligand QOH H 301



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	250/250 (100%)	-0.43	5 (2%)	65	63	50, 65, 100, 142	0
1	O	250/250 (100%)	-0.38	3 (1%)	79	79	54, 72, 117, 150	0
2	B	244/258 (94%)	-0.28	10 (4%)	37	32	52, 73, 122, 173	0
2	P	244/258 (94%)	-0.20	14 (5%)	23	19	56, 76, 123, 168	0
3	C	240/254 (94%)	-0.22	14 (5%)	23	19	52, 76, 139, 164	0
3	Q	240/254 (94%)	-0.04	15 (6%)	20	16	58, 86, 167, 192	0
4	D	235/260 (90%)	-0.42	2 (0%)	84	84	57, 78, 113, 150	0
4	R	235/260 (90%)	-0.36	5 (2%)	63	61	57, 80, 121, 154	0
5	E	231/234 (98%)	-0.27	3 (1%)	77	77	61, 83, 121, 161	0
5	S	231/234 (98%)	-0.18	6 (2%)	56	52	58, 87, 134, 176	0
6	F	243/288 (84%)	-0.43	5 (2%)	63	61	52, 73, 124, 152	0
6	T	243/288 (84%)	-0.41	4 (1%)	72	71	50, 78, 136, 169	0
7	G	241/252 (95%)	-0.50	8 (3%)	46	41	46, 66, 102, 148	0
7	U	241/252 (95%)	-0.46	3 (1%)	79	79	52, 68, 101, 147	0
8	H	226/232 (97%)	-0.48	6 (2%)	54	50	44, 61, 100, 163	0
8	V	226/232 (97%)	-0.40	7 (3%)	49	44	50, 66, 103, 176	0
9	I	204/205 (99%)	-0.67	1 (0%)	91	91	46, 63, 95, 121	0
9	W	204/205 (99%)	-0.69	1 (0%)	91	91	49, 64, 97, 124	0
10	J	195/198 (98%)	-0.52	2 (1%)	82	82	48, 66, 92, 144	0
10	X	195/198 (98%)	-0.50	3 (1%)	73	73	49, 68, 92, 158	0
11	K	212/212 (100%)	-0.52	1 (0%)	91	91	49, 68, 98, 117	0
11	Y	212/212 (100%)	-0.54	2 (0%)	84	84	52, 67, 99, 119	0
12	L	222/222 (100%)	-0.50	6 (2%)	54	50	51, 66, 105, 137	0
12	Z	222/222 (100%)	-0.54	5 (2%)	60	58	48, 64, 104, 136	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	M	229/246 (93%)	-0.57	2 (0%)	84	84	48, 66, 91, 108	0
13	a	232/246 (94%)	-0.61	1 (0%)	92	93	46, 62, 86, 99	0
14	N	196/196 (100%)	-0.68	2 (1%)	82	82	47, 59, 90, 117	0
14	b	196/196 (100%)	-0.61	2 (1%)	82	82	47, 61, 90, 125	0
All	All	6339/6614 (95%)	-0.44	138 (2%)	62	59	44, 70, 118, 192	0

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	49	THR	10.0
3	Q	206	LYS	6.5
2	P	220	ASN	6.0
8	V	224	GLN	5.8
2	P	59	ASP	5.8
3	Q	50	LEU	5.4
3	Q	236	GLN	5.3
10	X	194	ASP	5.3
8	V	222	ASP	5.3
3	C	49	THR	5.1
10	X	1	MET	5.1
3	C	206	LYS	4.9
8	V	226	GLU	4.8
1	O	249	ALA	4.5
10	J	1	MET	4.3
5	E	202	ASP	4.3
8	H	226	GLU	4.3
2	P	221	ASP	4.2
8	V	223	ILE	4.2
3	Q	239	GLN	4.2
1	A	2	THR	4.1
12	L	174	TYR	4.0
2	B	220	ASN	3.9
2	P	219	ALA	3.8
8	V	225	GLU	3.8
2	P	51	VAL	3.7
2	B	221	ASP	3.7
1	A	249	ALA	3.6
2	B	60	THR	3.5
2	B	59	ASP	3.5
5	S	202	ASP	3.4
14	b	195	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	218	GLY	3.4
7	U	242	GLN	3.4
12	Z	174	TYR	3.4
3	C	236	GLN	3.3
1	A	1	MET	3.3
2	B	51	VAL	3.2
2	P	222	GLY	3.2
8	H	224	GLN	3.2
4	D	241	ALA	3.2
8	H	222	ASP	3.2
13	M	47	ASP	3.1
3	C	50	LEU	3.0
3	Q	240	GLU	3.0
8	V	221	CYS	3.0
1	O	231	LYS	3.0
2	P	60	THR	3.0
11	Y	212	GLY	2.9
3	C	205	ALA	2.9
12	Z	163	GLY	2.9
3	C	238	LYS	2.9
6	F	244	ASN	2.8
4	R	241	ALA	2.8
6	T	230	ASP	2.8
11	K	212	GLY	2.8
3	Q	48	SER	2.8
3	Q	180	LYS	2.8
6	F	178	HIS	2.8
3	C	240	GLU	2.7
8	H	225	GLU	2.7
1	A	201	GLU	2.7
2	P	218	GLY	2.7
3	C	225	GLU	2.7
3	C	239	GLN	2.7
14	N	195	GLN	2.7
3	C	1	GLY	2.6
4	R	125	LEU	2.6
5	E	54	GLU	2.6
4	D	242	GLU	2.6
7	G	2	GLY	2.6
5	S	54	GLU	2.6
2	B	219	ALA	2.6
6	T	244	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
3	Q	229	GLN	2.6
3	C	202	GLN	2.5
2	P	232	GLN	2.5
8	H	221	CYS	2.5
7	G	179	LYS	2.5
6	T	241	LYS	2.5
12	Z	165	ASN	2.5
5	S	180	LYS	2.5
7	G	242	GLN	2.5
12	Z	173	LYS	2.5
3	C	216	ASP	2.5
13	a	1	THR	2.5
6	F	181	GLU	2.4
7	G	188	GLU	2.4
1	O	2	THR	2.4
2	P	203	SER	2.4
3	C	60	SER	2.4
2	B	203	SER	2.4
14	b	105	LYS	2.4
7	U	222	ASP	2.3
3	Q	238	LYS	2.3
10	X	193	ASP	2.3
7	G	3	TYR	2.3
7	U	2	GLY	2.3
3	Q	55	THR	2.3
12	L	171	PRO	2.3
12	L	163	GLY	2.3
2	P	50	LYS	2.3
4	R	217	GLN	2.3
7	G	240	ALA	2.2
3	Q	202	GLN	2.2
9	W	192	ASP	2.2
12	L	1	GLN	2.2
3	Q	233	GLN	2.2
2	P	182	ASP	2.2
6	T	181	GLU	2.2
7	G	241	GLU	2.2
2	B	182	ASP	2.2
11	Y	183	ASP	2.2
3	C	48	SER	2.2
4	R	242	GLU	2.2
6	F	241	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
12	Z	116	GLU	2.2
3	Q	205	ALA	2.2
2	P	61	SER	2.2
8	V	145	ASP	2.1
1	A	228	PRO	2.1
14	N	105	LYS	2.1
13	M	1	THR	2.1
5	S	225	ASP	2.1
8	H	223	ILE	2.1
2	B	61	SER	2.1
12	L	173	LYS	2.1
9	I	1	SER	2.1
7	G	222	ASP	2.1
5	S	52	ALA	2.1
10	J	194	ASP	2.0
3	Q	203	THR	2.0
4	R	226	GLU	2.0
12	L	165	ASN	2.0
5	S	173	ARG	2.0
2	P	52	THR	2.0
5	E	203	GLU	2.0
6	F	205	GLU	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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
17	QOH	K	301	38/38	0.94	0.18	56,62,75,77	0

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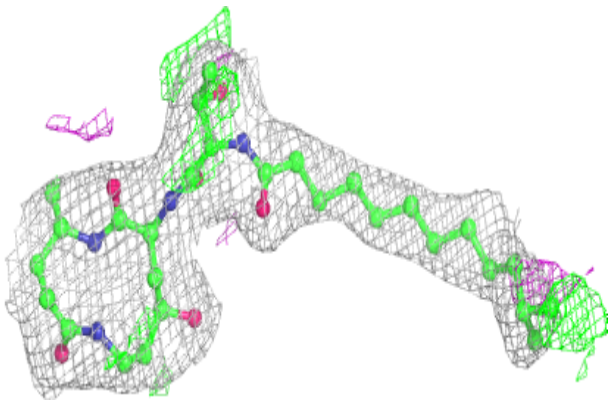
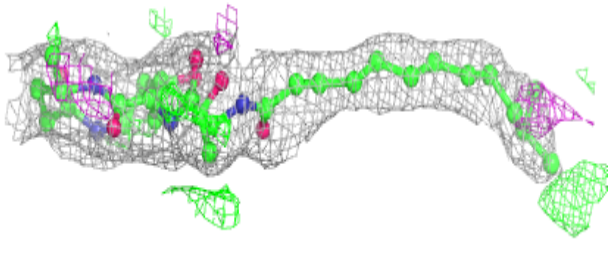
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
17	QOH	Y	301	38/38	0.94	0.20	57,61,74,78	0
17	QOH	H	301	38/38	0.95	0.18	45,52,57,58	0
17	QOH	V	301	38/38	0.96	0.17	48,54,60,66	0
15	MG	K	302	1/1	0.97	0.10	92,92,92,92	0
15	MG	I	301	1/1	0.98	0.34	78,78,78,78	0
15	MG	G	301	1/1	0.98	0.06	63,63,63,63	0
15	MG	V	302	1/1	0.98	0.08	99,99,99,99	0
15	MG	Z	301	1/1	0.98	0.23	62,62,62,62	0
15	MG	W	301	1/1	0.99	0.38	87,87,87,87	0
16	CL	G	302	1/1	0.99	0.12	54,54,54,54	0
15	MG	Y	302	1/1	0.99	0.16	83,83,83,83	0
15	MG	N	201	1/1	1.00	0.06	46,46,46,46	0
16	CL	U	301	1/1	1.00	0.20	59,59,59,59	0

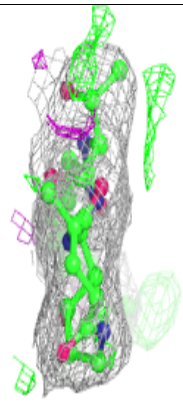
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around QOH K 301:

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

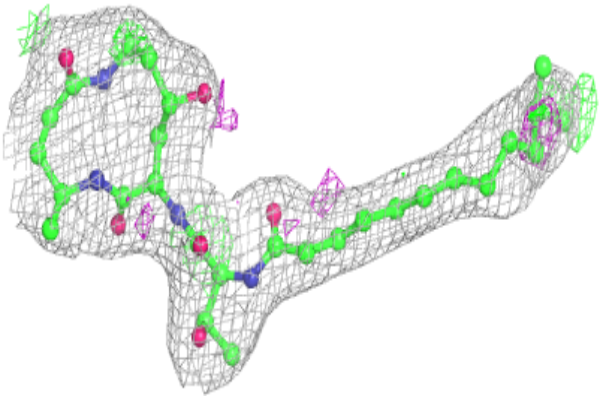


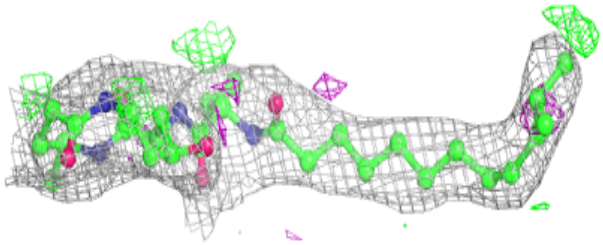


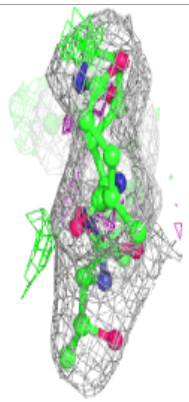


Electron density around QOH Y 301:

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

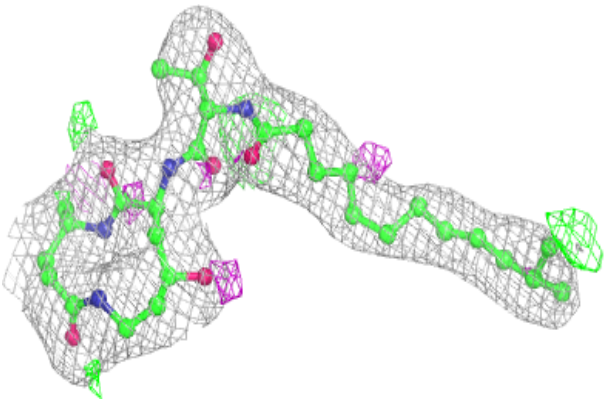


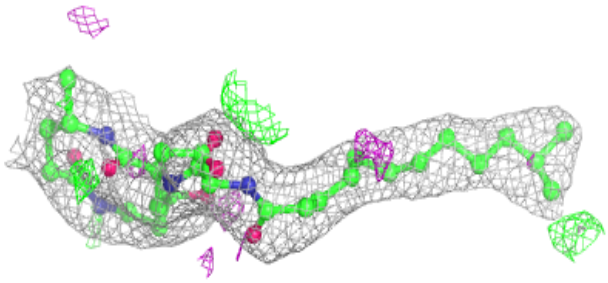


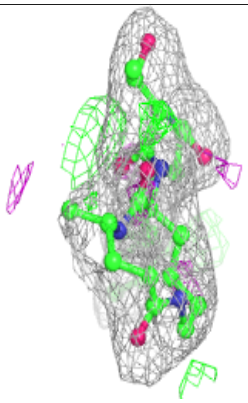


Electron density around QOH H 301:

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

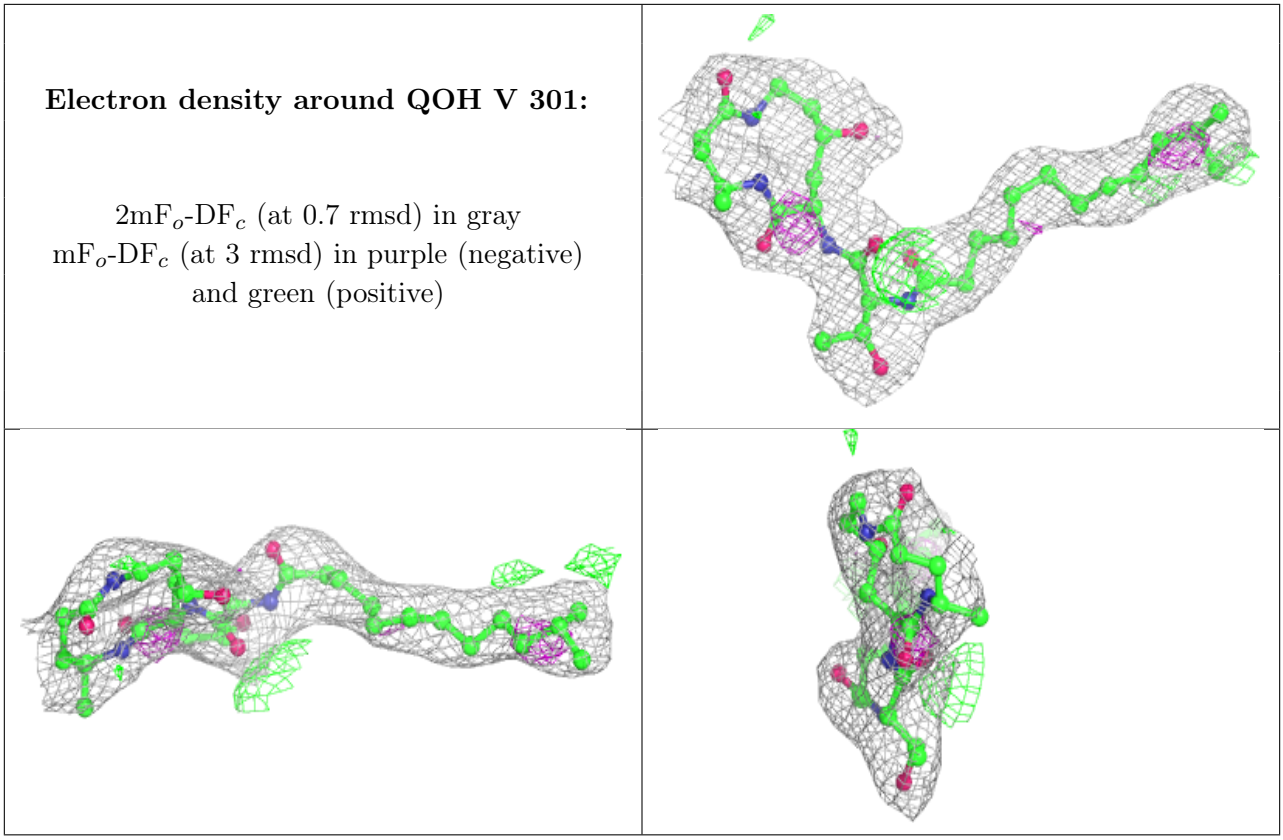






Electron density around QOH V 301:

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



6.5 Other polymers (i)

There are no such residues in this entry.