Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2023 – 01:01 PM EDT

PDB ID	:	4QZ0
Title	:	yCP beta5-M45V mutant in complex with the epoxyketone inhibitor ONX 0914
Authors	:	Huber, E.M.; Heinemeyer, W.; Groll, M.
Deposited on	:	2014-07-27
Resolution	:	3.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
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:

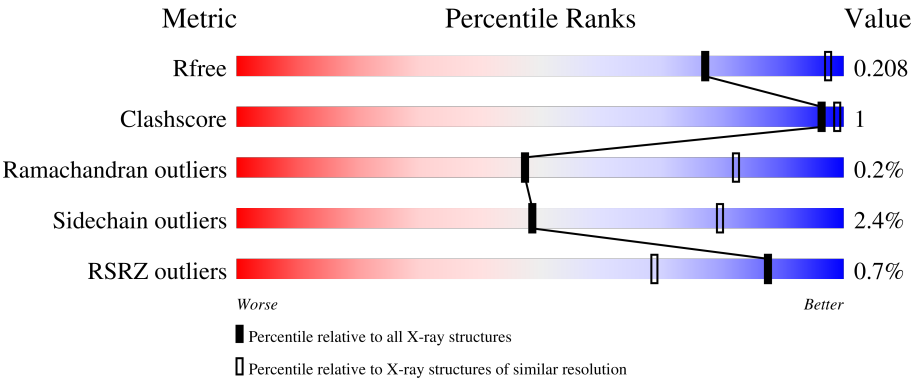
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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	98% ·
1	O	250	% 98% ·
2	B	258	2% 91% · · 5%
2	P	258	2% 90% · · 5%
3	C	254	2% 91% · · 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	4% 91% 6%
4	D	260	86% 10%
4	R	260	86% 5% 10%
5	E	234	94%
5	S	234	% 94% 5%
6	F	288	81% 16%
6	T	288	81% 16%
7	G	252	90% 6%
7	U	252	90% 5%
8	H	232	93%
8	V	232	94%
9	I	205	93% 6%
9	W	205	95%
10	J	198	% 93%
10	X	198	% 94%
11	K	212	94% 6%
11	Y	212	96%
12	L	222	96%
12	Z	222	95% 5%
13	M	246	91% 5%
13	a	246	93% 5%
14	N	196	96%
14	b	196	99%

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 49743 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	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			
8	V	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	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
			1643	1045	280	312	6			
11	Y	212	Total	C	N	O	S	0	0	0
			1643	1045	280	312	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	45	VAL	MET	engineered mutation	UNP P30656
Y	45	VAL	MET	engineered mutation	UNP P30656

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	a	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

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

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

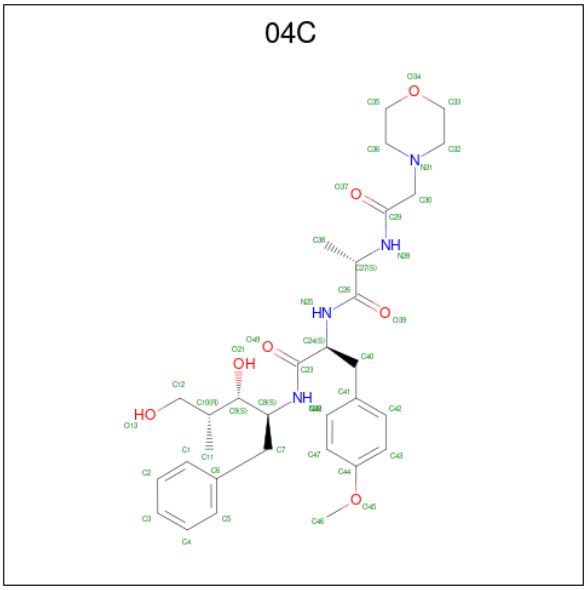
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	G	1	Total Mg 1 1	0	0
15	K	1	Total Mg 1 1	0	0
15	N	1	Total Mg 1 1	0	0
15	V	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 1,2,4-trideoxy-4-methyl-2-{[N-(morpholin-4-ylacetyl)-L-alanyl-O-methyl-L-tyrosyl]amino}-1-phenyl-D-xylitol (three-letter code: 04C) (formula: $C_{31}H_{44}N_4O_7$).



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

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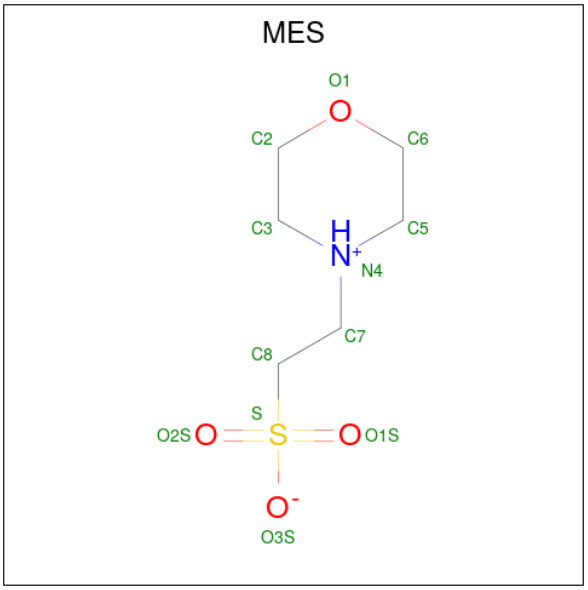
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	K	1	Total C N O 42 31 4 7	0	0
17	N	1	Total C N O 42 31 4 7	0	0
17	V	1	Total C N O 42 31 4 7	0	0
17	Y	1	Total C N O 42 31 4 7	0	0
17	b	1	Total C N O 42 31 4 7	0	0

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



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

- Molecule 19 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	4	Total O 4 4	0	0
19	B	8	Total O 8 8	0	0
19	C	4	Total O 4 4	0	0
19	D	2	Total O 2 2	0	0
19	E	3	Total O 3 3	0	0
19	F	2	Total O 2 2	0	0
19	G	5	Total O 5 5	0	0
19	H	5	Total O 5 5	0	0
19	I	5	Total O 5 5	0	0
19	J	10	Total O 10 10	0	0
19	K	5	Total O 5 5	0	0
19	L	6	Total O 6 6	0	0
19	M	7	Total O 7 7	0	0
19	N	2	Total O 2 2	0	0
19	O	2	Total O 2 2	0	0
19	P	5	Total O 5 5	0	0
19	Q	3	Total O 3 3	0	0
19	R	3	Total O 3 3	0	0
19	S	3	Total O 3 3	0	0
19	T	3	Total O 3 3	0	0
19	U	5	Total O 5 5	0	0
19	V	7	Total O 7 7	0	0

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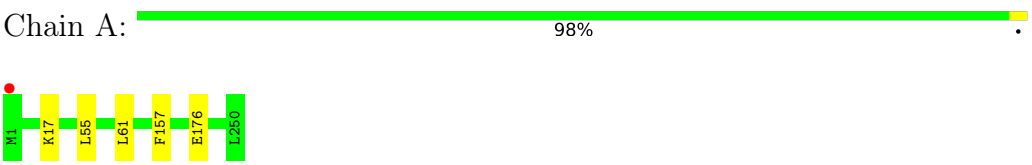
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	W	5	Total O 5 5	0	0
19	X	14	Total O 14 14	0	0
19	Y	4	Total O 4 4	0	0
19	Z	7	Total O 7 7	0	0
19	a	9	Total O 9 9	0	0
19	b	3	Total O 3 3	0	0

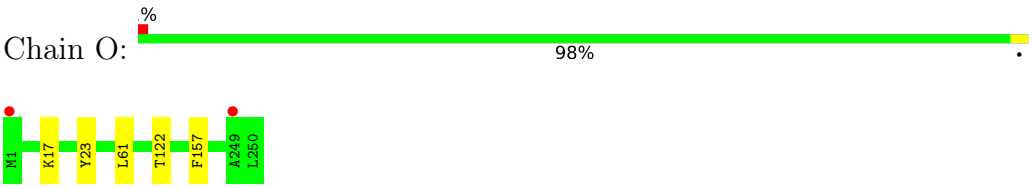
3 Residue-property plots (i)

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.

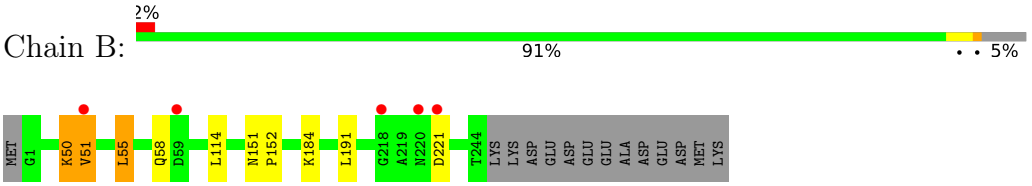
• Molecule 1: Proteasome subunit alpha type-2



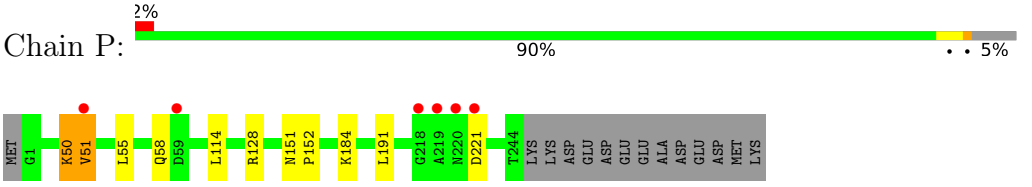
• Molecule 1: Proteasome subunit alpha type-2



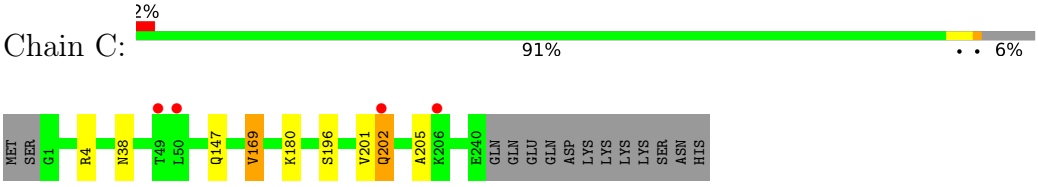
• Molecule 2: Proteasome subunit alpha type-3



• Molecule 2: Proteasome subunit alpha type-3

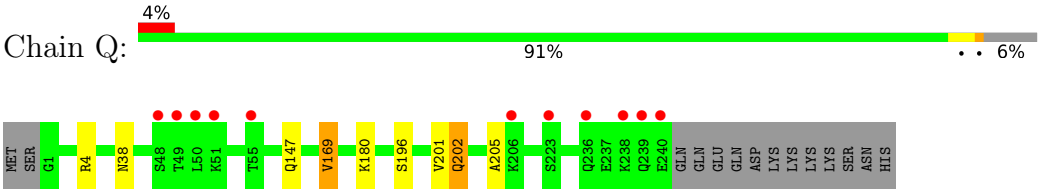


• Molecule 3: Proteasome subunit alpha type-4



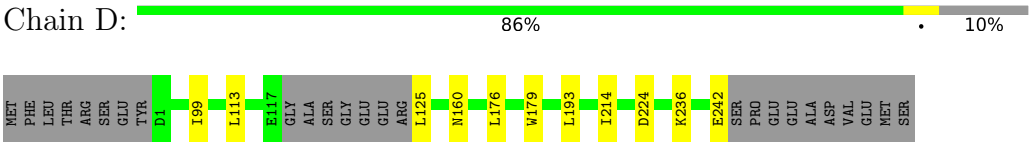
• Molecule 3: Proteasome subunit alpha type-4

Chain Q:



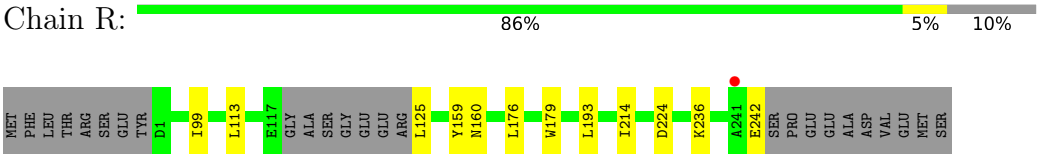
• Molecule 4: Proteasome subunit alpha type-5

Chain D:



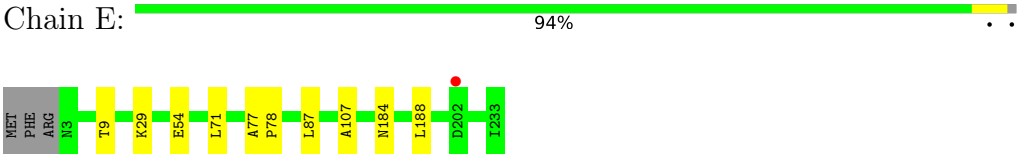
• Molecule 4: Proteasome subunit alpha type-5

Chain R:



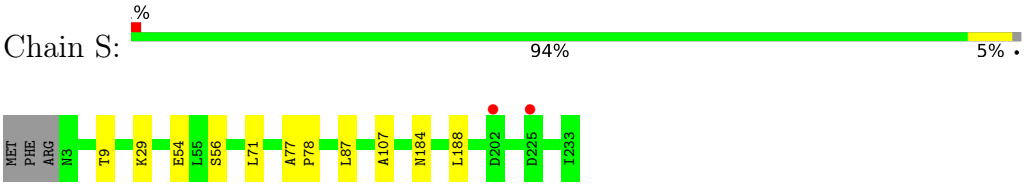
• Molecule 5: Proteasome subunit alpha type-6

Chain E:



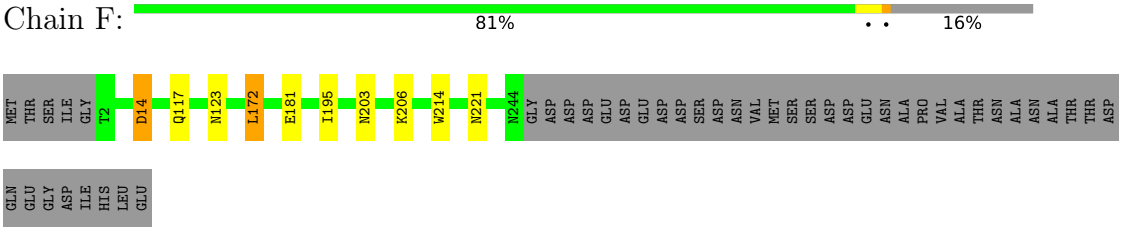
• Molecule 5: Proteasome subunit alpha type-6

Chain S:



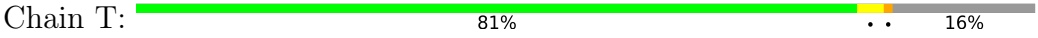
• Molecule 6: Probable proteasome subunit alpha type-7

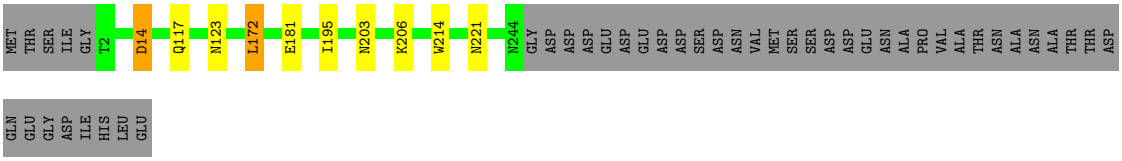
Chain F:



• Molecule 6: Probable proteasome subunit alpha type-7

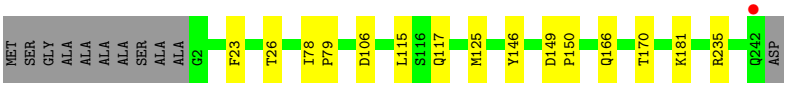
Chain T:





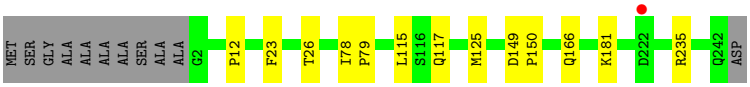
• Molecule 7: Proteasome subunit alpha type-1

Chain G:



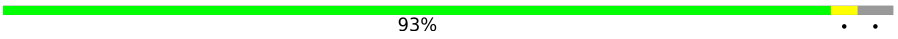
• Molecule 7: Proteasome subunit alpha type-1

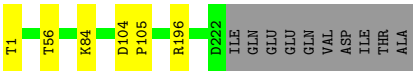
Chain U:



• Molecule 8: Proteasome subunit beta type-2

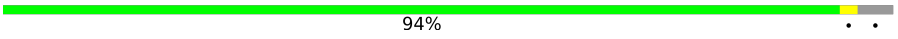
Chain H:

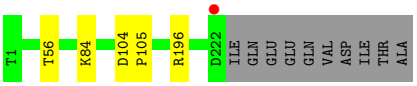




• Molecule 8: Proteasome subunit beta type-2

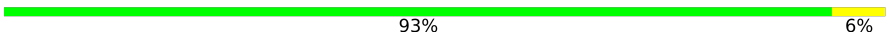
Chain V:

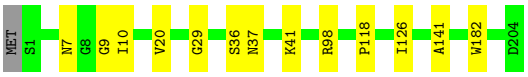




• Molecule 9: Proteasome subunit beta type-3

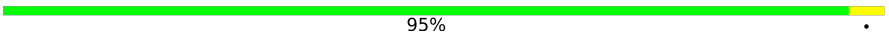
Chain I:

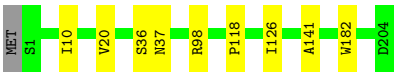




• Molecule 9: Proteasome subunit beta type-3

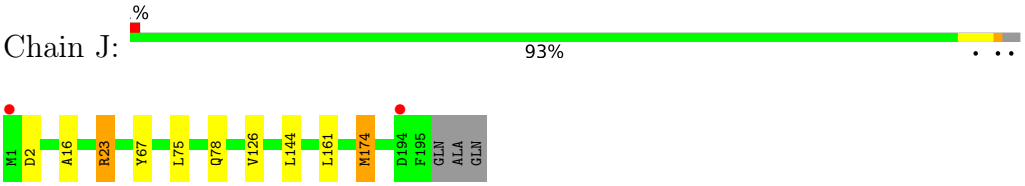
Chain W:





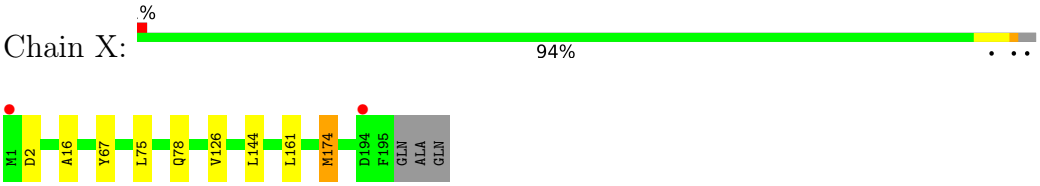
• Molecule 10: Proteasome subunit beta type-4

Chain J:



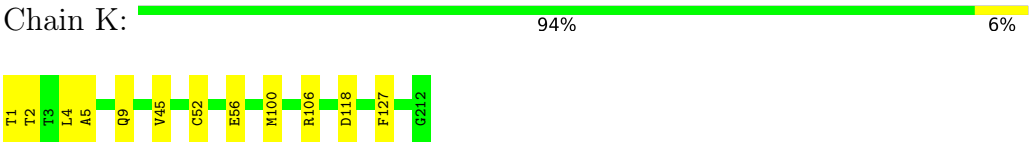
• Molecule 10: Proteasome subunit beta type-4

Chain X:



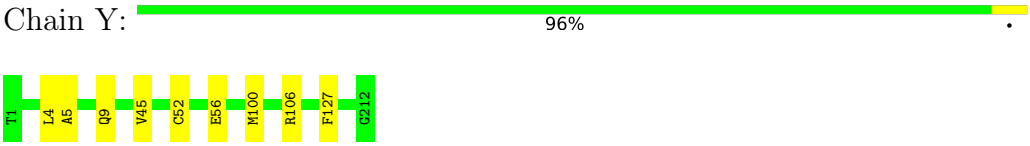
• Molecule 11: Proteasome subunit beta type-5

Chain K:



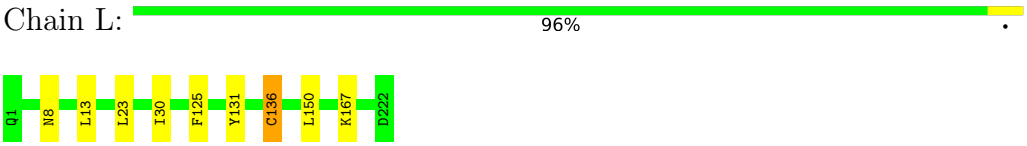
• Molecule 11: Proteasome subunit beta type-5

Chain Y:



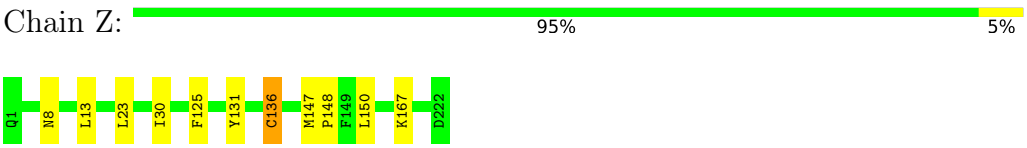
• Molecule 12: Proteasome subunit beta type-6

Chain L:



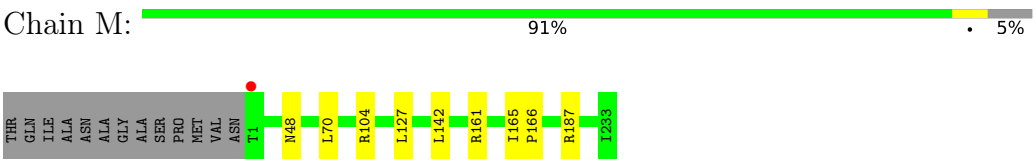
• Molecule 12: Proteasome subunit beta type-6

Chain Z:



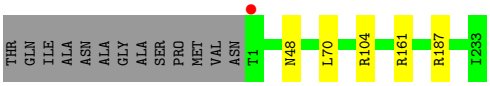
• Molecule 13: Proteasome subunit beta type-7

Chain M:



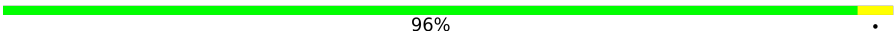
• Molecule 13: Proteasome subunit beta type-7

Chain a:



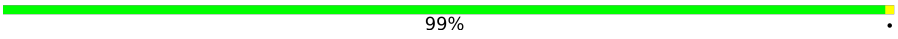
• Molecule 14: Proteasome subunit beta type-1

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	136.05Å 299.92Å 145.01Å 90.00° 112.94° 90.00°	Depositor
Resolution (Å)	15.00 – 3.00 15.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.8 (15.00-3.00) 98.0 (15.00-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.00 (at 3.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.169 , 0.201 0.175 , 0.208	Depositor DCC
R_{free} test set	10345 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	67.4	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 51.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	49743	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% 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: MES, MG, 04C, CL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.27	0/1952	0.46	0/2642
1	O	0.27	0/1952	0.46	0/2642
2	B	0.27	0/1934	0.48	0/2618
2	P	0.27	0/1934	0.48	0/2618
3	C	0.27	0/1910	0.50	0/2586
3	Q	0.27	0/1910	0.50	0/2586
4	D	0.26	0/1837	0.46	0/2475
4	R	0.26	0/1837	0.46	0/2475
5	E	0.27	0/1800	0.46	0/2433
5	S	0.26	0/1800	0.46	0/2433
6	F	0.27	0/1932	0.44	0/2609
6	T	0.26	0/1932	0.44	0/2609
7	G	0.27	0/1945	0.46	0/2634
7	U	0.27	0/1945	0.46	0/2634
8	H	0.25	0/1715	0.47	1/2326 (0.0%)
8	V	0.25	0/1715	0.47	0/2326
9	I	0.27	0/1611	0.47	0/2174
9	W	0.27	0/1611	0.47	0/2174
10	J	0.27	0/1589	0.48	0/2142
10	X	0.27	0/1589	0.48	0/2142
11	K	0.26	0/1680	0.50	0/2274
11	Y	0.26	0/1680	0.49	0/2274
12	L	0.27	0/1795	0.46	0/2420
12	Z	0.27	0/1795	0.46	0/2420
13	M	0.27	0/1855	0.51	0/2514
13	a	0.27	0/1855	0.51	0/2514
14	N	0.25	0/1541	0.47	0/2087
14	b	0.25	0/1541	0.47	0/2087
All	All	0.27	0/50192	0.47	1/67868 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	1	THR	N-CA-C	5.09	124.74	111.00

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	2	0
1	O	1915	0	1929	2	0
2	B	1904	0	1904	3	0
2	P	1904	0	1904	3	0
3	C	1881	0	1895	3	0
3	Q	1881	0	1895	3	0
4	D	1813	0	1797	2	0
4	R	1813	0	1797	3	0
5	E	1773	0	1775	3	0
5	S	1773	0	1775	3	0
6	F	1892	0	1883	2	0
6	T	1892	0	1883	2	0
7	G	1907	0	1901	5	0
7	U	1907	0	1901	4	0
8	H	1684	0	1685	1	0
8	V	1684	0	1685	1	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	1643	0	1592	7	0
11	Y	1643	0	1592	6	0
12	L	1757	0	1711	5	0
12	Z	1757	0	1711	6	0
13	M	1824	0	1832	2	0
13	a	1824	0	1832	0	0
14	N	1512	0	1478	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	b	1512	0	1478	0	0
15	G	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	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	42	0	42	2	0
17	K	42	0	42	0	0
17	N	42	0	42	5	0
17	V	42	0	42	1	0
17	Y	42	0	42	0	0
17	b	42	0	42	0	0
18	H	12	0	13	1	0
18	K	12	0	13	0	0
18	V	12	0	13	0	0
18	Y	12	0	13	0	0
19	A	4	0	0	0	0
19	B	8	0	0	0	0
19	C	4	0	0	0	0
19	D	2	0	0	0	0
19	E	3	0	0	0	0
19	F	2	0	0	0	0
19	G	5	0	0	0	0
19	H	5	0	0	0	0
19	I	5	0	0	0	0
19	J	10	0	0	0	0
19	K	5	0	0	0	0
19	L	6	0	0	0	0
19	M	7	0	0	0	0
19	N	2	0	0	0	0
19	O	2	0	0	0	0
19	P	5	0	0	0	0
19	Q	3	0	0	0	0
19	R	3	0	0	1	0
19	S	3	0	0	0	0
19	T	3	0	0	0	0
19	U	5	0	0	0	0
19	V	7	0	0	0	0
19	W	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	X	14	0	0	0	0
19	Y	4	0	0	0	0
19	Z	7	0	0	0	0
19	a	9	0	0	0	0
19	b	3	0	0	0	0
All	All	49743	0	49354	87	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (87) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:301:04C:H24	17:V:301:04C:H6	1.42	1.02
17:H:301:04C:H6	17:H:301:04C:H24	1.42	1.01
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.80	0.64
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.80	0.62
11:K:5:ALA:HB3	11:K:100:MET:HE2	1.84	0.60
11:Y:5:ALA:HB3	11:Y:100:MET:HE2	1.84	0.60
14:N:45:ARG:CZ	17:N:201:04C:H44	2.36	0.56
14:N:48:SER:HB2	17:N:201:04C:H25	1.88	0.56
17:N:201:04C:O21	17:N:201:04C:O13	2.23	0.53
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.44	0.52
3:C:201:VAL:O	3:C:202:GLN:CB	2.58	0.52
10:X:67:TYR:CE1	10:X:75:LEU:HD13	2.44	0.52
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.58	0.52
14:N:152:VAL:HA	14:N:175:MET:HE1	1.92	0.52
7:G:23:PHE:O	7:G:26:THR:HB	2.11	0.51
17:N:201:04C:H8	17:N:201:04C:H24	1.94	0.50
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.94	0.50
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.94	0.50
7:U:23:PHE:O	7:U:26:THR:HB	2.12	0.49
4:R:113:LEU:HB2	19:R:301:HOH:O	2.13	0.48
9:I:98:ARG:O	9:I:126:ILE:HD11	2.13	0.47
9:W:98:ARG:O	9:W:126:ILE:HD11	2.15	0.47
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.45	0.46
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.98	0.46
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.98	0.46
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.98	0.46
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.98	0.45
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:45:VAL:HG11	11:K:56:GLU:HG3	1.98	0.45
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.99	0.45
12:L:136:CYS:SG	12:L:150:LEU:HB3	2.57	0.45
1:A:176:GLU:HG2	2:B:55:LEU:HD13	1.99	0.44
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.99	0.44
11:Y:45:VAL:HG11	11:Y:56:GLU:HG3	2.00	0.44
9:I:10:ILE:HG21	9:I:141:ALA:HB3	2.00	0.44
10:J:23:ARG:NH2	11:K:118:ASP:OD2	2.51	0.44
12:Z:136:CYS:SG	12:Z:150:LEU:HB3	2.57	0.44
9:W:36:SER:HB2	10:X:126:VAL:HG11	2.00	0.43
7:G:78:ILE:N	7:G:79:PRO:CD	2.81	0.43
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.54	0.43
9:W:10:ILE:HG21	9:W:141:ALA:HB3	2.00	0.43
10:J:174:MET:HA	10:X:174:MET:HA	2.00	0.43
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.19	0.43
17:H:301:04C:O21	18:H:302:MES:O1S	2.36	0.43
11:Y:100:MET:HE3	11:Y:127:PHE:HB2	2.00	0.42
6:F:172:LEU:CD1	6:F:195:ILE:HD13	2.49	0.42
12:L:8:ASN:HA	12:L:30:ILE:O	2.18	0.42
5:S:77:ALA:N	5:S:78:PRO:CD	2.83	0.42
6:T:14:ASP:OD2	6:T:14:ASP:N	2.51	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.42
11:Y:45:VAL:CG1	11:Y:56:GLU:HG3	2.49	0.42
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.50	0.42
11:K:100:MET:HE3	11:K:127:PHE:HB2	2.01	0.42
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.49	0.42
6:T:172:LEU:CD1	6:T:195:ILE:HD13	2.48	0.42
11:K:45:VAL:CG1	11:K:56:GLU:HG3	2.48	0.42
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.54	0.42
11:K:45:VAL:HB	11:K:52:CYS:HB3	2.02	0.42
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.49	0.42
5:E:77:ALA:N	5:E:78:PRO:CD	2.83	0.42
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.50	0.42
3:C:201:VAL:HG13	3:C:202:GLN:N	2.34	0.42
10:X:16:ALA:HB2	10:X:161:LEU:HD21	2.02	0.42
6:F:14:ASP:OD2	6:F:14:ASP:N	2.52	0.41
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.85	0.41
4:D:113:LEU:HD12	5:E:78:PRO:HB2	2.01	0.41
10:J:16:ALA:HB2	10:J:161:LEU:HD21	2.01	0.41
11:Y:45:VAL:HB	11:Y:52:CYS:HB3	2.02	0.41
9:I:9:GLY:HA3	9:I:41:LYS:HE2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:1:THR:CG2	14:N:3:ILE:HG23	2.49	0.41
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.56	0.41
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.35	0.41
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.56	0.41
9:I:36:SER:HB2	10:J:126:VAL:HG11	2.03	0.41
2:P:50:LYS:O	2:P:51:VAL:C	2.59	0.41
1:A:55:LEU:HD12	7:G:170:THR:HG23	2.03	0.41
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.56	0.41
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.03	0.41
11:K:1:THR:HG22	11:K:2:THR:N	2.36	0.40
13:M:127:LEU:HG	13:M:142:LEU:HD12	2.03	0.40
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.56	0.40
12:Z:147:MET:N	12:Z:148:PRO:HD2	2.36	0.40
9:I:7:ASN:HA	9:I:29:GLY:O	2.21	0.40
11:Y:100:MET:CE	11:Y:127:PHE:HB2	2.52	0.40
14:N:45:ARG:NH2	17:N:201:04C:H44	2.37	0.40
2:B:50:LYS:O	2:B:51:VAL:C	2.60	0.40
7:G:106:ASP:HB3	7:G:146:TYR:CZ	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	242 (98%)	6 (2%)	0	100	100
1	O	248/250 (99%)	242 (98%)	6 (2%)	0	100	100
2	B	242/258 (94%)	232 (96%)	8 (3%)	2 (1%)	19	57
2	P	242/258 (94%)	232 (96%)	8 (3%)	2 (1%)	19	57
3	C	238/254 (94%)	230 (97%)	6 (2%)	2 (1%)	19	57
3	Q	238/254 (94%)	230 (97%)	6 (2%)	2 (1%)	19	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	231/260 (89%)	225 (97%)	6 (3%)	0	100	100
4	R	231/260 (89%)	225 (97%)	6 (3%)	0	100	100
5	E	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
5	S	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
6	F	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
6	T	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
7	G	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
7	U	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
8	H	220/232 (95%)	216 (98%)	4 (2%)	0	100	100
8	V	220/232 (95%)	216 (98%)	4 (2%)	0	100	100
9	I	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
9	W	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
10	J	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	29	68
10	X	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	29	68
11	K	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
11	Y	210/212 (99%)	204 (97%)	6 (3%)	0	100	100
12	L	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
12	Z	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
13	M	231/246 (94%)	219 (95%)	12 (5%)	0	100	100
13	a	231/246 (94%)	219 (95%)	12 (5%)	0	100	100
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	b	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
All	All	6276/6614 (95%)	6093 (97%)	173 (3%)	10 (0%)	47	82

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN
2	P	51	VAL
3	Q	202	GLN
10	J	2	ASP
10	X	2	ASP
3	C	205	ALA

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Mol	Chain	Res	Type
3	Q	205	ALA
2	B	221	ASP
2	P	221	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	206 (99%)	3 (1%)	67	88
1	O	209/209 (100%)	206 (99%)	3 (1%)	67	88
2	B	203/216 (94%)	197 (97%)	6 (3%)	41	75
2	P	203/216 (94%)	197 (97%)	6 (3%)	41	75
3	C	212/226 (94%)	207 (98%)	5 (2%)	49	79
3	Q	212/226 (94%)	207 (98%)	5 (2%)	49	79
4	D	194/215 (90%)	186 (96%)	8 (4%)	30	67
4	R	194/215 (90%)	186 (96%)	8 (4%)	30	67
5	E	190/193 (98%)	184 (97%)	6 (3%)	39	74
5	S	190/193 (98%)	184 (97%)	6 (3%)	39	74
6	F	201/239 (84%)	192 (96%)	9 (4%)	27	64
6	T	201/239 (84%)	192 (96%)	9 (4%)	27	64
7	G	206/210 (98%)	200 (97%)	6 (3%)	42	76
7	U	206/210 (98%)	200 (97%)	6 (3%)	42	76
8	H	181/190 (95%)	178 (98%)	3 (2%)	60	85
8	V	181/190 (95%)	178 (98%)	3 (2%)	60	85
9	I	172/173 (99%)	170 (99%)	2 (1%)	71	90
9	W	172/173 (99%)	170 (99%)	2 (1%)	71	90
10	J	173/175 (99%)	169 (98%)	4 (2%)	50	80
10	X	173/175 (99%)	170 (98%)	3 (2%)	60	85
11	K	169/169 (100%)	166 (98%)	3 (2%)	59	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	Y	169/169 (100%)	166 (98%)	3 (2%)	59 85
12	L	185/185 (100%)	182 (98%)	3 (2%)	62 86
12	Z	185/185 (100%)	182 (98%)	3 (2%)	62 86
13	M	199/208 (96%)	194 (98%)	5 (2%)	47 79
13	a	199/208 (96%)	194 (98%)	5 (2%)	47 79
14	N	162/162 (100%)	161 (99%)	1 (1%)	86 95
14	b	162/162 (100%)	161 (99%)	1 (1%)	86 95
All	All	5312/5540 (96%)	5185 (98%)	127 (2%)	49 79

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	61	LEU
1	A	157	PHE
2	B	50	LYS
2	B	55	LEU
2	B	58	GLN
2	B	114	LEU
2	B	184	LYS
2	B	191	LEU
3	C	4	ARG
3	C	38	ASN
3	C	147	GLN
3	C	169	VAL
3	C	180	LYS
4	D	99	ILE
4	D	125	LEU
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	224	ASP
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	29	LYS
5	E	54	GLU
5	E	71	LEU
5	E	184	ASN
5	E	188	LEU

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Mol	Chain	Res	Type
6	F	14	ASP
6	F	117	GLN
6	F	123	ASN
6	F	172	LEU
6	F	181	GLU
6	F	203	ASN
6	F	206	LYS
6	F	214	TRP
6	F	221	ASN
7	G	115	LEU
7	G	117	GLN
7	G	125	MET
7	G	166	GLN
7	G	181	LYS
7	G	235	ARG
8	H	56	THR
8	H	84	LYS
8	H	196	ARG
9	I	37	ASN
9	I	182	TRP
10	J	23	ARG
10	J	78	GLN
10	J	144	LEU
10	J	174	MET
11	K	4	LEU
11	K	9	GLN
11	K	106	ARG
12	L	23	LEU
12	L	136	CYS
12	L	167	LYS
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
14	N	39	ASP
1	O	17	LYS
1	O	61	LEU
1	O	157	PHE
2	P	50	LYS
2	P	55	LEU
2	P	58	GLN

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Mol	Chain	Res	Type
2	P	114	LEU
2	P	184	LYS
2	P	191	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	147	GLN
3	Q	169	VAL
3	Q	180	LYS
4	R	99	ILE
4	R	125	LEU
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	224	ASP
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	54	GLU
5	S	71	LEU
5	S	184	ASN
5	S	188	LEU
6	T	14	ASP
6	T	117	GLN
6	T	123	ASN
6	T	172	LEU
6	T	181	GLU
6	T	203	ASN
6	T	206	LYS
6	T	214	TRP
6	T	221	ASN
7	U	115	LEU
7	U	117	GLN
7	U	125	MET
7	U	166	GLN
7	U	181	LYS
7	U	235	ARG
8	V	56	THR
8	V	84	LYS
8	V	196	ARG
9	W	37	ASN
9	W	182	TRP

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Mol	Chain	Res	Type
10	X	78	GLN
10	X	144	LEU
10	X	174	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	106	ARG
12	Z	23	LEU
12	Z	136	CYS
12	Z	167	LYS
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
14	b	39	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	119	GLN
2	B	123	GLN
3	C	38	ASN
3	C	147	GLN
3	C	160	GLN
4	D	91	HIS
5	E	68	HIS
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	184	ASN
6	F	117	GLN
6	F	191	GLN
6	F	240	GLN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
10	J	55	GLN
11	K	85	ASN
11	K	143	ASN

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Mol	Chain	Res	Type
11	K	176	ASN
12	L	3	ASN
12	L	158	ASN
13	M	102	GLN
1	O	94	HIS
2	P	119	GLN
2	P	123	GLN
2	P	176	GLN
3	Q	38	ASN
3	Q	147	GLN
3	Q	160	GLN
4	R	91	HIS
5	S	68	HIS
5	S	92	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	184	ASN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
6	T	240	GLN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
10	X	55	GLN
10	X	146	HIS
10	X	147	HIS
11	Y	85	ASN
11	Y	176	ASN
12	Z	3	ASN
12	Z	70	ASN
12	Z	79	HIS
12	Z	158	ASN
13	a	102	GLN
13	a	194	ASN
13	a	213	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 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	04C	Y	301	11	44,44,44	1.33	3 (6%)	56,58,58	1.14	8 (14%)
18	MES	Y	303	-	12,12,12	2.26	1 (8%)	14,16,16	1.37	2 (14%)
17	04C	b	201	14	44,44,44	1.49	4 (9%)	56,58,58	1.31	8 (14%)
18	MES	K	303	-	12,12,12	2.25	1 (8%)	14,16,16	1.48	2 (14%)
17	04C	K	301	11	44,44,44	1.29	3 (6%)	56,58,58	1.14	7 (12%)
17	04C	V	301	8	44,44,44	1.24	3 (6%)	56,58,58	1.26	8 (14%)
17	04C	N	201	14	44,44,44	1.53	5 (11%)	56,58,58	1.29	8 (14%)
18	MES	V	303	-	12,12,12	2.22	1 (8%)	14,16,16	1.42	3 (21%)
18	MES	H	302	-	12,12,12	2.19	1 (8%)	14,16,16	1.30	2 (14%)
17	04C	H	301	8	44,44,44	1.27	3 (6%)	56,58,58	1.26	8 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	04C	Y	301	11	-	12/44/52/52	0/3/3/3
18	MES	Y	303	-	-	0/6/14/14	0/1/1/1
17	04C	b	201	14	-	14/44/52/52	0/3/3/3
18	MES	K	303	-	-	0/6/14/14	0/1/1/1
17	04C	K	301	11	-	12/44/52/52	0/3/3/3
17	04C	V	301	8	-	16/44/52/52	0/3/3/3
17	04C	N	201	14	-	15/44/52/52	0/3/3/3
18	MES	V	303	-	-	2/6/14/14	0/1/1/1
18	MES	H	302	-	-	2/6/14/14	0/1/1/1
17	04C	H	301	8	-	16/44/52/52	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Y	303	MES	C8-S	-7.49	1.66	1.77
18	K	303	MES	C8-S	-7.46	1.66	1.77
18	V	303	MES	C8-S	-7.39	1.67	1.77
18	H	302	MES	C8-S	-7.28	1.67	1.77
17	N	201	04C	C10-C9	6.01	1.64	1.53
17	b	201	04C	C10-C9	5.54	1.63	1.53
17	Y	301	04C	C10-C9	5.10	1.62	1.53
17	K	301	04C	C10-C9	4.91	1.62	1.53
17	H	301	04C	C40-C41	-4.59	1.40	1.51
17	V	301	04C	C40-C41	-4.48	1.40	1.51
17	K	301	04C	C40-C41	-4.45	1.40	1.51
17	H	301	04C	C10-C9	4.34	1.61	1.53
17	Y	301	04C	C40-C41	-4.33	1.40	1.51
17	V	301	04C	C10-C9	4.30	1.61	1.53
17	b	201	04C	C40-C41	-4.26	1.41	1.51
17	N	201	04C	C40-C41	-4.21	1.41	1.51
17	N	201	04C	C7-C6	-3.91	1.41	1.51
17	H	301	04C	C7-C6	-3.86	1.42	1.51
17	b	201	04C	C7-C6	-3.86	1.42	1.51
17	Y	301	04C	C7-C6	-3.76	1.42	1.51
17	V	301	04C	C7-C6	-3.75	1.42	1.51
17	K	301	04C	C7-C6	-3.69	1.42	1.51
17	N	201	04C	C12-C10	3.10	1.56	1.52
17	b	201	04C	C12-C10	2.73	1.56	1.52
17	N	201	04C	C30-C29	2.01	1.55	1.52

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	N	201	04C	C11-C10-C12	-4.63	103.79	109.88
17	b	201	04C	C11-C10-C12	-4.60	103.83	109.88
17	V	301	04C	C30-N31-C32	-3.98	104.93	111.09
17	H	301	04C	C30-N31-C32	-3.93	105.00	111.09
17	b	201	04C	C29-C30-N31	-3.63	104.92	113.36
17	N	201	04C	C29-C30-N31	-3.57	105.08	113.36
18	K	303	MES	O1S-S-C8	3.50	111.13	106.92
17	H	301	04C	C33-C32-N31	3.27	115.06	110.10
17	V	301	04C	C33-C32-N31	3.25	115.04	110.10
18	V	303	MES	O1S-S-C8	3.21	110.78	106.92
17	Y	301	04C	C30-N31-C36	-2.92	106.57	111.09
18	Y	303	MES	O1S-S-C8	2.88	110.38	106.92
17	K	301	04C	C30-N31-C36	-2.83	106.71	111.09
17	H	301	04C	O34-C33-C32	-2.80	105.63	111.80
18	H	302	MES	O2S-S-C8	2.70	110.17	106.92
17	b	201	04C	C7-C8-C9	-2.67	105.61	111.11
17	Y	301	04C	O34-C33-C32	-2.65	105.97	111.80
17	V	301	04C	O34-C33-C32	-2.64	105.99	111.80
17	N	201	04C	C7-C8-C9	-2.63	105.69	111.11
18	Y	303	MES	O2S-S-C8	2.63	110.09	106.92
18	H	302	MES	O3S-S-C8	2.60	109.97	105.77
17	K	301	04C	C7-C6-C5	2.58	126.03	120.91
17	b	201	04C	C35-C36-N31	-2.57	106.21	110.10
17	b	201	04C	C7-C6-C5	2.55	125.98	120.91
17	K	301	04C	O34-C33-C32	-2.54	106.19	111.80
17	V	301	04C	C7-C6-C5	2.52	125.92	120.91
17	b	201	04C	O34-C33-C32	-2.52	106.25	111.80
17	Y	301	04C	C41-C40-C24	-2.49	106.51	113.39
17	Y	301	04C	C7-C6-C5	2.48	125.83	120.91
17	K	301	04C	C41-C40-C24	-2.48	106.55	113.39
17	N	201	04C	C7-C6-C1	-2.47	116.00	120.91
17	N	201	04C	C7-C6-C5	2.47	125.81	120.91
17	N	201	04C	C35-C36-N31	-2.47	106.36	110.10
17	b	201	04C	C7-C6-C1	-2.45	116.03	120.91
18	K	303	MES	O2S-S-C8	2.45	109.86	106.92
17	N	201	04C	O34-C33-C32	-2.43	106.45	111.80
17	H	301	04C	C7-C6-C5	2.42	125.72	120.91
18	V	303	MES	O2S-S-C8	2.41	109.81	106.92
17	V	301	04C	C7-C6-C1	-2.40	116.15	120.91
17	H	301	04C	C7-C6-C1	-2.34	116.26	120.91
17	K	301	04C	C7-C6-C1	-2.34	116.27	120.91
17	Y	301	04C	C7-C6-C1	-2.33	116.29	120.91
17	V	301	04C	C7-C8-C9	-2.32	106.33	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	Y	301	04C	C7-C8-C9	-2.31	106.35	111.11
17	H	301	04C	C7-C8-C9	-2.30	106.36	111.11
17	V	301	04C	C35-C36-N31	-2.27	106.66	110.10
18	V	303	MES	O3S-S-C8	2.27	109.44	105.77
17	H	301	04C	C35-C36-N31	-2.26	106.68	110.10
17	H	301	04C	C7-C8-N22	-2.24	106.80	110.07
17	K	301	04C	C7-C8-C9	-2.22	106.54	111.11
17	V	301	04C	C7-C8-N22	-2.20	106.86	110.07
17	K	301	04C	C33-C32-N31	2.14	113.34	110.10
17	Y	301	04C	C29-C30-N31	-2.07	108.54	113.36
17	Y	301	04C	C33-C32-N31	2.05	113.21	110.10
17	N	201	04C	C7-C8-N22	-2.03	107.11	110.07
17	b	201	04C	C7-C8-N22	-2.02	107.12	110.07

There are no chirality outliers.

All (89) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	H	301	04C	C11-C10-C9-O21
17	H	301	04C	C9-C10-C12-O13
17	H	301	04C	C11-C10-C12-O13
17	K	301	04C	C11-C10-C9-C8
17	K	301	04C	C12-C10-C9-C8
17	K	301	04C	C9-C10-C12-O13
17	K	301	04C	C11-C10-C12-O13
17	N	201	04C	C11-C10-C9-C8
17	N	201	04C	C12-C10-C9-C8
17	V	301	04C	C11-C10-C9-O21
17	V	301	04C	C9-C10-C12-O13
17	V	301	04C	C11-C10-C12-O13
17	Y	301	04C	C11-C10-C9-C8
17	Y	301	04C	C12-C10-C9-C8
17	Y	301	04C	C9-C10-C12-O13
17	Y	301	04C	C11-C10-C12-O13
17	b	201	04C	C11-C10-C9-C8
17	b	201	04C	C12-C10-C9-C8
17	H	301	04C	C47-C44-O45-C46
17	H	301	04C	C43-C44-O45-C46
17	V	301	04C	C47-C44-O45-C46
17	V	301	04C	C43-C44-O45-C46
17	N	201	04C	C43-C44-O45-C46
17	b	201	04C	C43-C44-O45-C46

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Mol	Chain	Res	Type	Atoms
17	N	201	04C	C47-C44-O45-C46
17	b	201	04C	C47-C44-O45-C46
17	Y	301	04C	C47-C44-O45-C46
17	K	301	04C	C47-C44-O45-C46
17	Y	301	04C	C43-C44-O45-C46
17	K	301	04C	C43-C44-O45-C46
17	N	201	04C	N25-C24-C40-C41
17	b	201	04C	N25-C24-C40-C41
17	Y	301	04C	C5-C6-C7-C8
17	K	301	04C	C5-C6-C7-C8
17	V	301	04C	C5-C6-C7-C8
17	H	301	04C	C5-C6-C7-C8
17	K	301	04C	C11-C10-C9-O21
17	K	301	04C	C12-C10-C9-O21
17	Y	301	04C	C11-C10-C9-O21
17	Y	301	04C	C12-C10-C9-O21
17	H	301	04C	C1-C6-C7-C8
17	V	301	04C	C1-C6-C7-C8
17	K	301	04C	C1-C6-C7-C8
17	Y	301	04C	C1-C6-C7-C8
17	b	201	04C	C5-C6-C7-C8
17	N	201	04C	C5-C6-C7-C8
17	H	301	04C	C11-C10-C9-C8
17	V	301	04C	C11-C10-C9-C8
17	b	201	04C	C1-C6-C7-C8
17	N	201	04C	C1-C6-C7-C8
17	b	201	04C	N28-C29-C30-N31
17	H	301	04C	C6-C7-C8-N22
17	V	301	04C	C6-C7-C8-N22
17	N	201	04C	N28-C29-C30-N31
17	N	201	04C	C23-C24-C40-C41
17	b	201	04C	C23-C24-C40-C41
17	N	201	04C	O37-C29-C30-N31
17	b	201	04C	O37-C29-C30-N31
17	N	201	04C	C11-C10-C9-O21
17	N	201	04C	C12-C10-C9-O21
17	b	201	04C	C11-C10-C9-O21
17	b	201	04C	C12-C10-C9-O21
17	H	301	04C	O37-C29-C30-N31
17	V	301	04C	O37-C29-C30-N31
17	H	301	04C	N28-C29-C30-N31
17	V	301	04C	N28-C29-C30-N31

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Mol	Chain	Res	Type	Atoms
17	N	201	04C	C29-C30-N31-C32
17	b	201	04C	C29-C30-N31-C32
17	N	201	04C	C9-C10-C12-O13
17	H	301	04C	C6-C7-C8-C9
17	H	301	04C	C12-C10-C9-C8
17	V	301	04C	C6-C7-C8-C9
17	V	301	04C	C12-C10-C9-C8
17	N	201	04C	C29-C30-N31-C36
17	b	201	04C	C29-C30-N31-C36
18	V	303	MES	C8-C7-N4-C5
17	Y	301	04C	O49-C23-C24-N25
17	K	301	04C	O49-C23-C24-N25
17	V	301	04C	O49-C23-C24-N25
17	H	301	04C	O49-C23-C24-N25
17	V	301	04C	N22-C23-C24-N25
17	H	301	04C	N22-C23-C24-N25
17	Y	301	04C	N22-C23-C24-N25
17	K	301	04C	N22-C23-C24-N25
17	H	301	04C	N25-C24-C40-C41
18	H	302	MES	C7-C8-S-O3S
17	V	301	04C	N25-C24-C40-C41
18	H	302	MES	C7-C8-S-O1S
18	V	303	MES	C8-C7-N4-C3

There are no ring outliers.

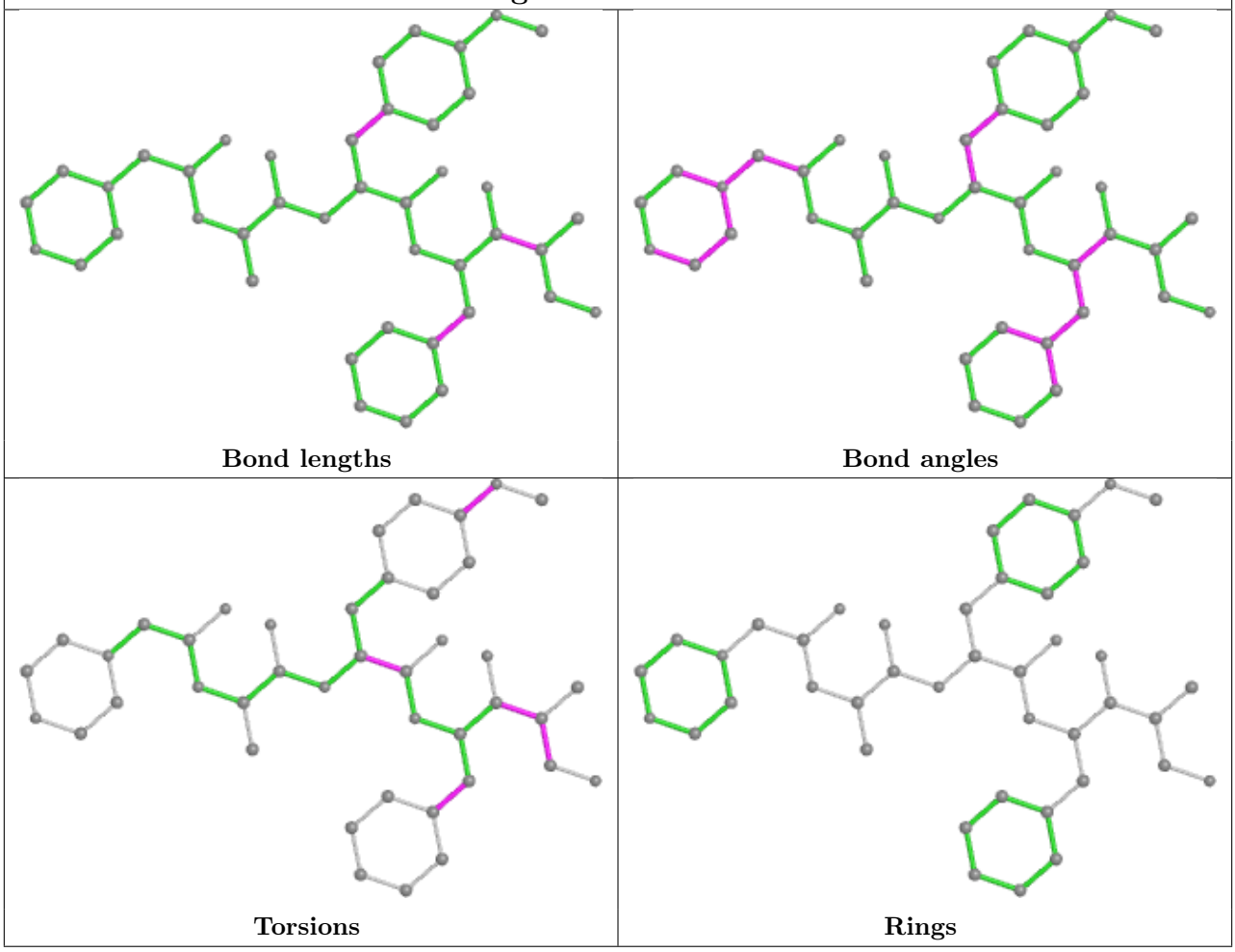
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	V	301	04C	1	0
17	N	201	04C	5	0
18	H	302	MES	1	0
17	H	301	04C	2	0

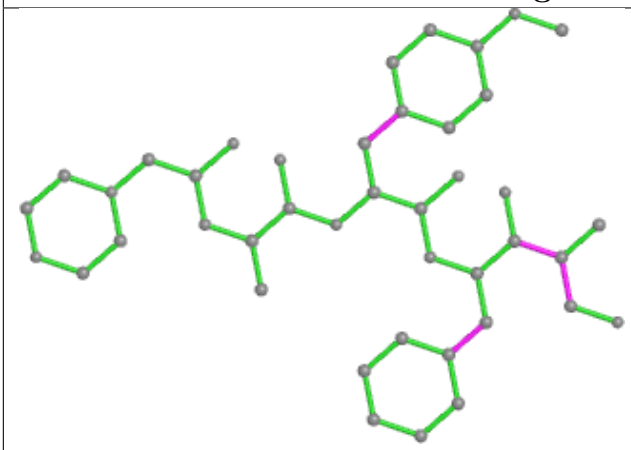
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

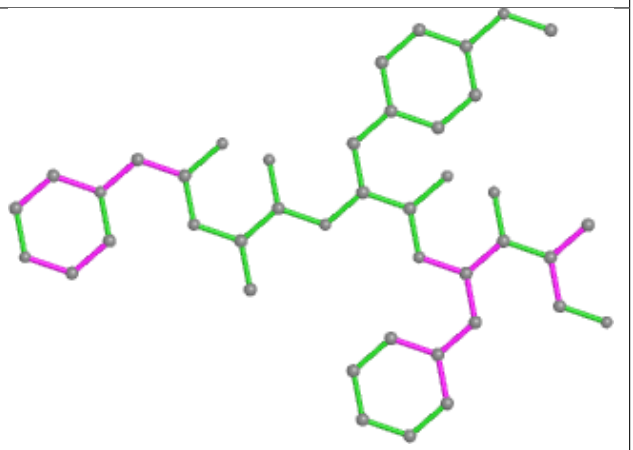
Ligand 04C Y 301



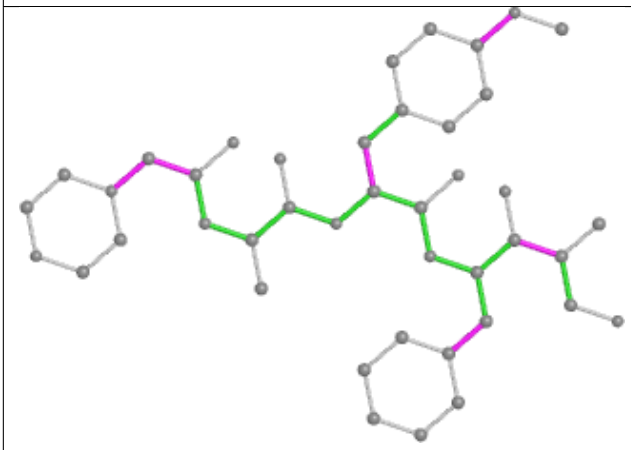
Ligand 04C b 201



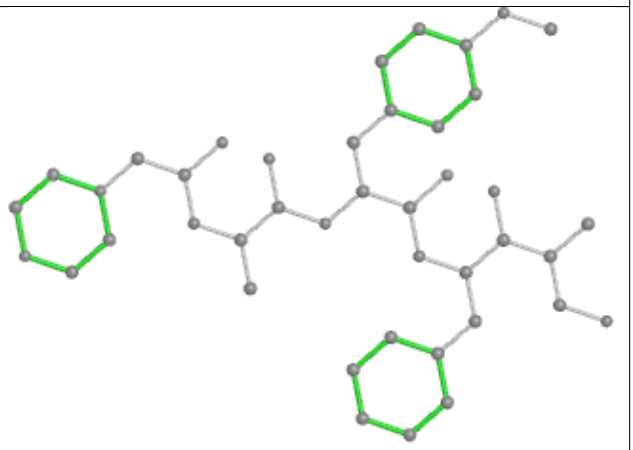
Bond lengths



Bond angles

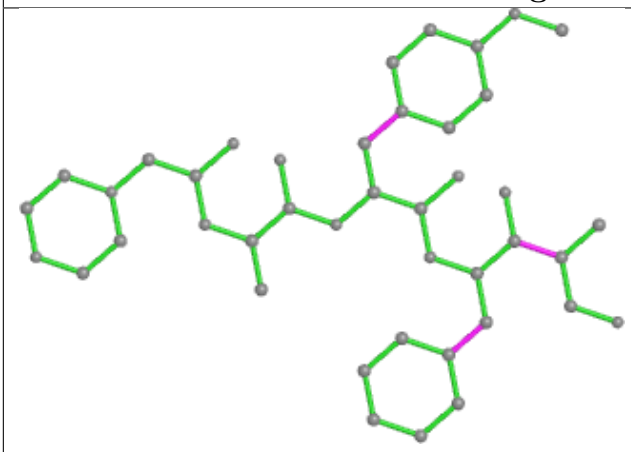


Torsions

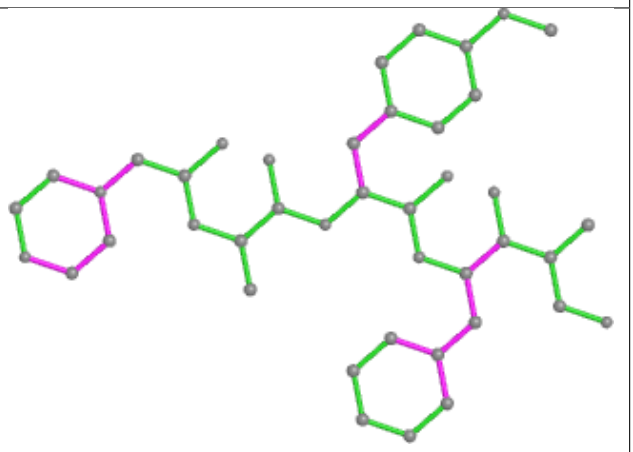


Rings

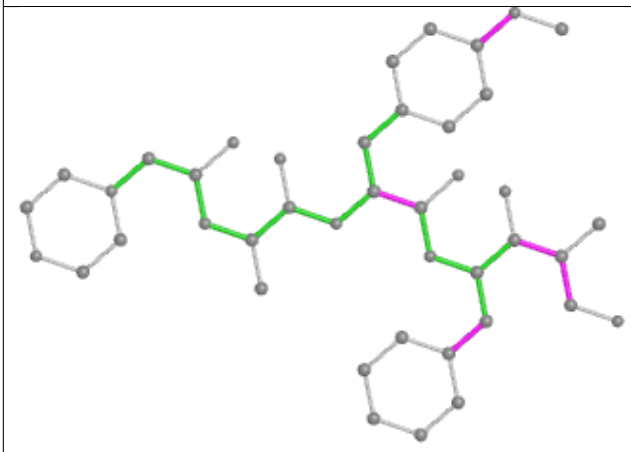
Ligand 04C K 301



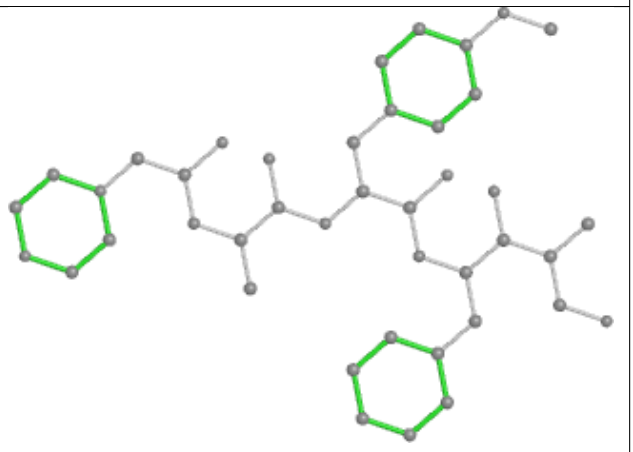
Bond lengths



Bond angles

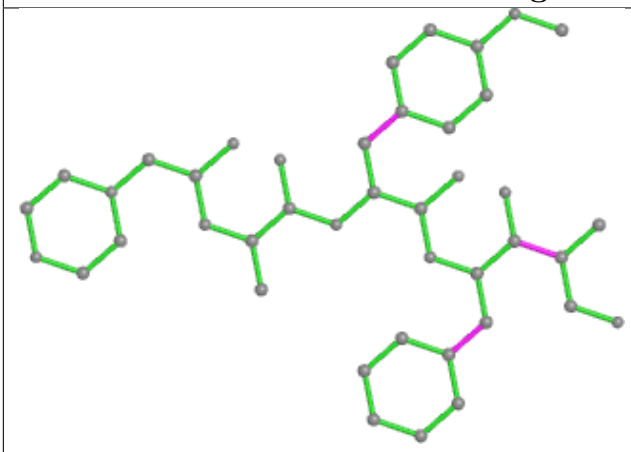


Torsions

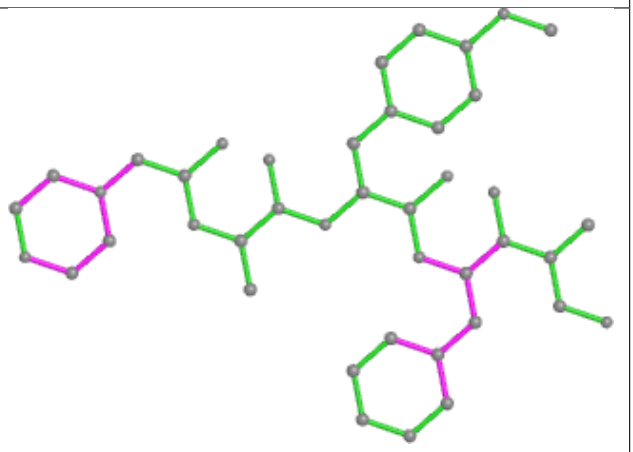


Rings

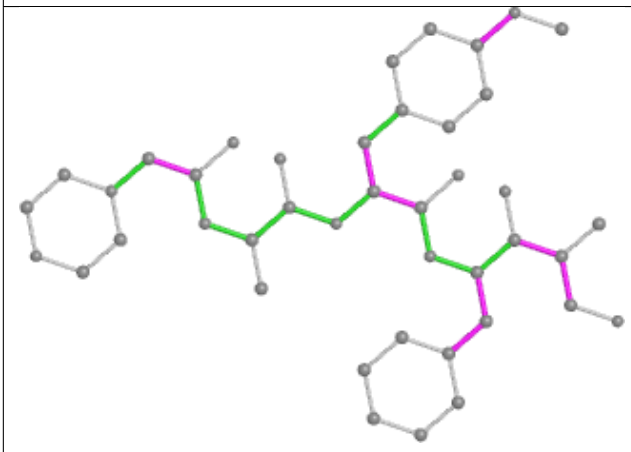
Ligand 04C V 301



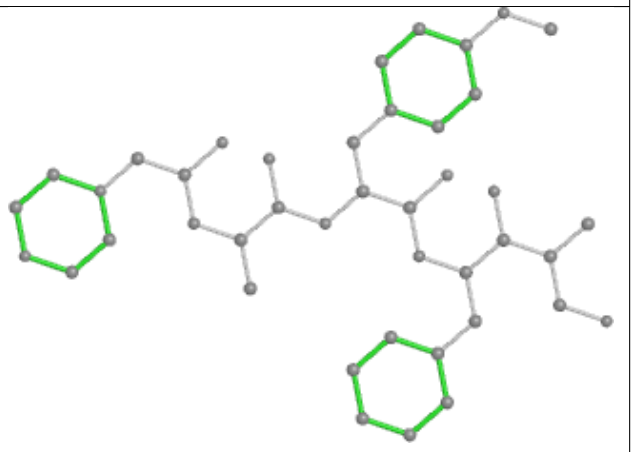
Bond lengths



Bond angles

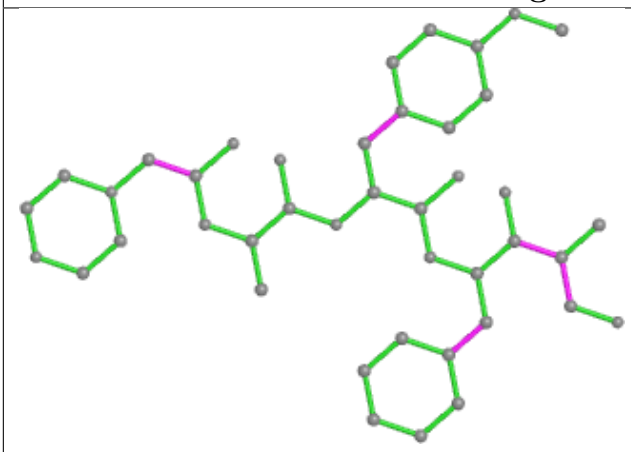


Torsions

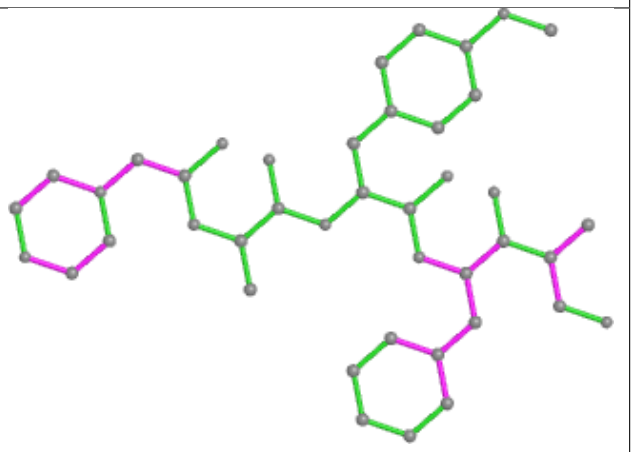


Rings

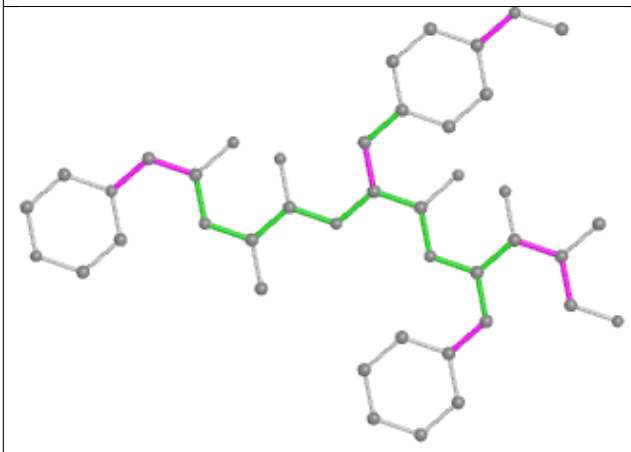
Ligand 04C N 201



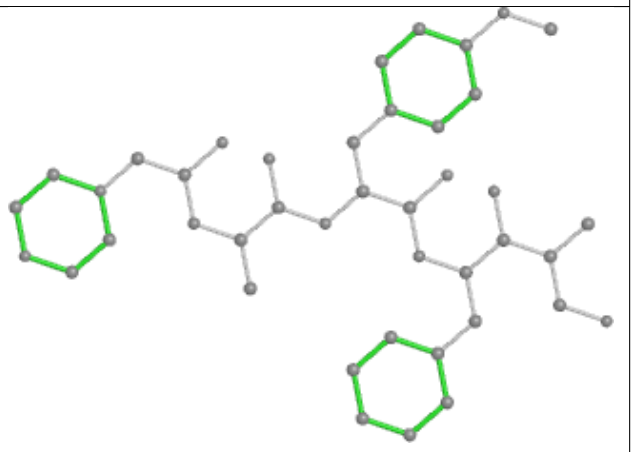
Bond lengths



Bond angles

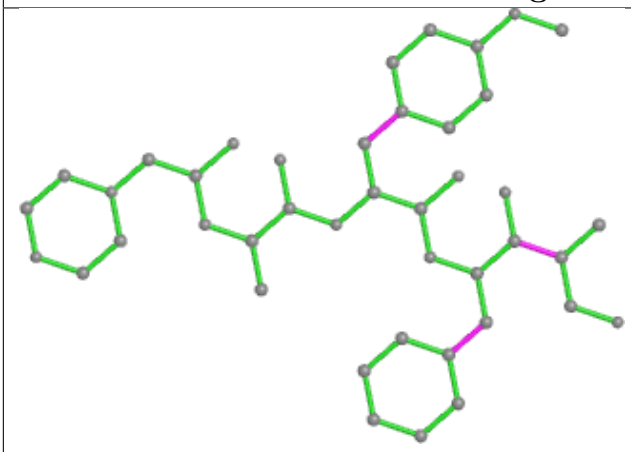


Torsions

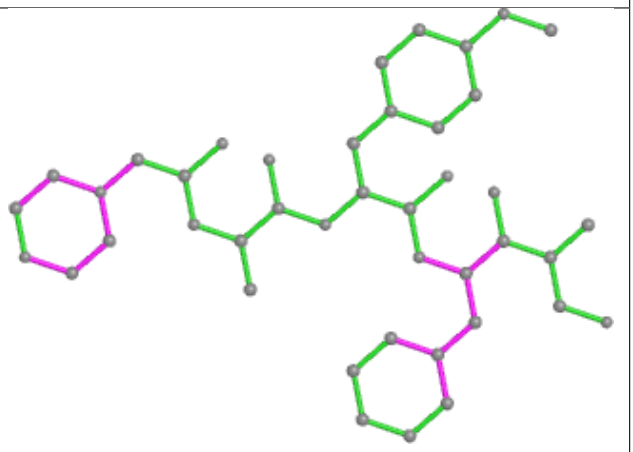


Rings

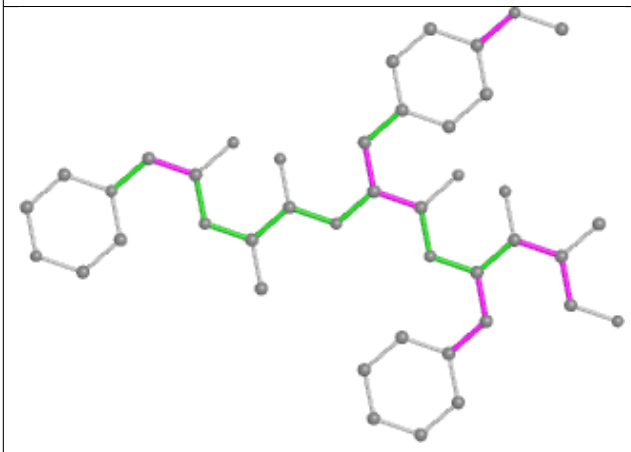
Ligand 04C H 301



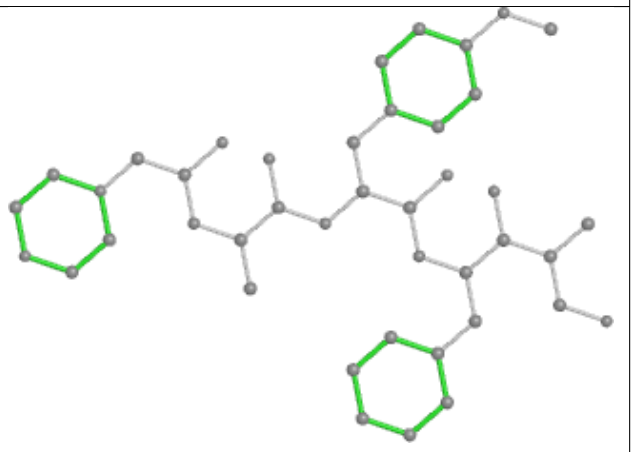
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.64	1 (0%) 92 79	45, 64, 106, 155	0
1	O	250/250 (100%)	-0.61	2 (0%) 86 65	46, 69, 113, 160	0
2	B	244/258 (94%)	-0.60	5 (2%) 65 36	44, 67, 116, 165	0
2	P	244/258 (94%)	-0.57	6 (2%) 57 29	47, 70, 116, 160	0
3	C	240/254 (94%)	-0.46	4 (1%) 70 41	44, 72, 142, 174	0
3	Q	240/254 (94%)	-0.28	11 (4%) 32 12	52, 86, 172, 199	0
4	D	235/260 (90%)	-0.61	0 100 100	52, 77, 109, 144	0
4	R	235/260 (90%)	-0.57	1 (0%) 92 79	55, 79, 123, 171	0
5	E	231/234 (98%)	-0.53	1 (0%) 92 79	54, 82, 120, 171	0
5	S	231/234 (98%)	-0.43	2 (0%) 84 63	56, 89, 149, 186	0
6	F	243/288 (84%)	-0.64	0 100 100	50, 75, 125, 156	0
6	T	243/288 (84%)	-0.57	0 100 100	51, 83, 147, 186	0
7	G	241/252 (95%)	-0.63	1 (0%) 92 79	45, 69, 115, 157	0
7	U	241/252 (95%)	-0.67	1 (0%) 92 79	46, 66, 107, 138	0
8	H	222/232 (95%)	-0.70	0 100 100	46, 66, 98, 117	0
8	V	222/232 (95%)	-0.70	1 (0%) 91 75	47, 66, 97, 119	0
9	I	204/205 (99%)	-0.86	0 100 100	39, 58, 90, 115	0
9	W	204/205 (99%)	-0.85	0 100 100	40, 57, 88, 112	0
10	J	195/198 (98%)	-0.77	2 (1%) 82 59	38, 56, 89, 126	0
10	X	195/198 (98%)	-0.79	2 (1%) 82 59	41, 58, 90, 142	0
11	K	212/212 (100%)	-0.79	0 100 100	40, 58, 91, 112	0
11	Y	212/212 (100%)	-0.77	0 100 100	34, 61, 92, 122	0
12	L	222/222 (100%)	-0.77	0 100 100	40, 64, 95, 117	0
12	Z	222/222 (100%)	-0.79	0 100 100	38, 64, 97, 117	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	233/246 (94%)	-0.70	1 (0%) 92 79	40, 66, 97, 121	0
13	a	233/246 (94%)	-0.70	1 (0%) 92 79	40, 65, 96, 133	0
14	N	196/196 (100%)	-0.79	0 100 100	44, 61, 93, 119	0
14	b	196/196 (100%)	-0.75	0 100 100	45, 61, 99, 121	0
All	All	6336/6614 (95%)	-0.65	42 (0%) 87 69	34, 68, 119, 199	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	49	THR	7.4
3	Q	50	LEU	5.0
3	C	206	LYS	5.0
1	O	1	MET	4.3
3	Q	206	LYS	4.1
2	B	220	ASN	3.9
5	E	202	ASP	3.9
3	C	49	THR	3.5
1	A	1	MET	3.4
2	P	218	GLY	3.4
4	R	241	ALA	3.3
2	P	220	ASN	3.2
5	S	202	ASP	3.1
3	Q	55	THR	3.0
2	B	218	GLY	3.0
3	Q	48	SER	3.0
3	Q	239	GLN	3.0
8	V	222	ASP	2.9
2	B	221	ASP	2.8
3	Q	236	GLN	2.7
2	P	51	VAL	2.6
7	U	222	ASP	2.6
10	J	194	ASP	2.6
13	a	1	THR	2.6
3	Q	238	LYS	2.5
10	X	194	ASP	2.5
3	Q	240	GLU	2.5
1	O	249	ALA	2.4
10	J	1	MET	2.4
2	P	219	ALA	2.4
10	X	1	MET	2.4
2	P	59	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	202	GLN	2.3
13	M	1	THR	2.3
2	B	59	ASP	2.3
2	B	51	VAL	2.2
2	P	221	ASP	2.2
3	C	50	LEU	2.2
7	G	242	GLN	2.2
5	S	225	ASP	2.2
3	Q	223	SER	2.0
3	Q	51	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no 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
15	MG	G	301	1/1	0.87	0.19	64,64,64,64	0
17	04C	N	201	42/42	0.88	0.36	48,76,87,91	0
17	04C	b	201	42/42	0.88	0.35	50,77,90,91	0
17	04C	H	301	42/42	0.93	0.20	50,55,73,76	0
18	MES	V	303	12/12	0.93	0.33	57,60,88,95	0
17	04C	V	301	42/42	0.94	0.19	48,56,78,81	0
18	MES	H	302	12/12	0.95	0.30	58,62,77,81	0
17	04C	K	301	42/42	0.95	0.15	37,49,63,65	0
17	04C	Y	301	42/42	0.96	0.16	33,50,64,65	0
15	MG	N	202	1/1	0.96	0.16	42,42,42,42	0
15	MG	Z	301	1/1	0.97	0.17	70,70,70,70	0
16	CL	G	302	1/1	0.98	0.19	55,55,55,55	0
15	MG	Y	302	1/1	0.98	0.09	58,58,58,58	0

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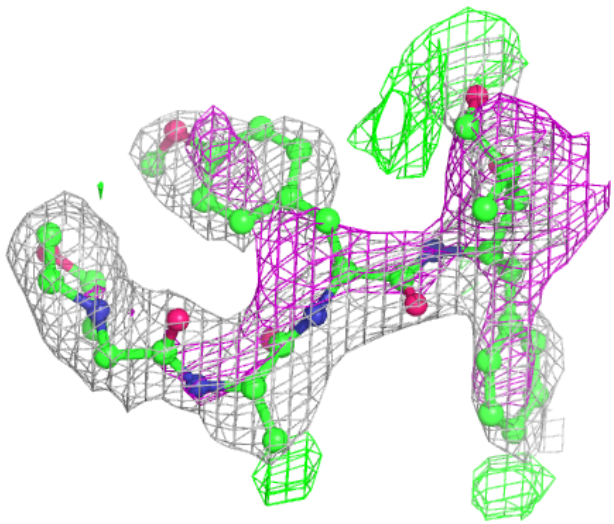
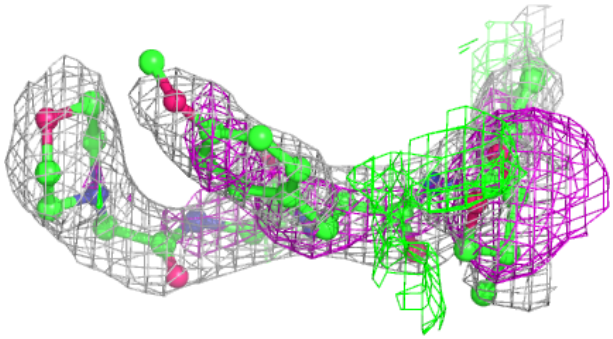
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
18	MES	K	303	12/12	0.98	0.20	34,36,48,54	0
15	MG	K	302	1/1	0.98	0.07	60,60,60,60	0
18	MES	Y	303	12/12	0.98	0.19	37,39,48,49	0
15	MG	V	302	1/1	0.99	0.07	73,73,73,73	0
16	CL	U	301	1/1	0.99	0.17	51,51,51,51	0

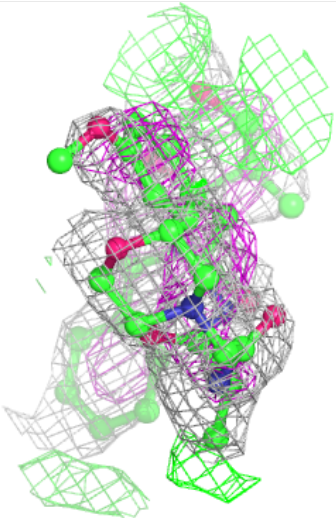
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 04C 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)

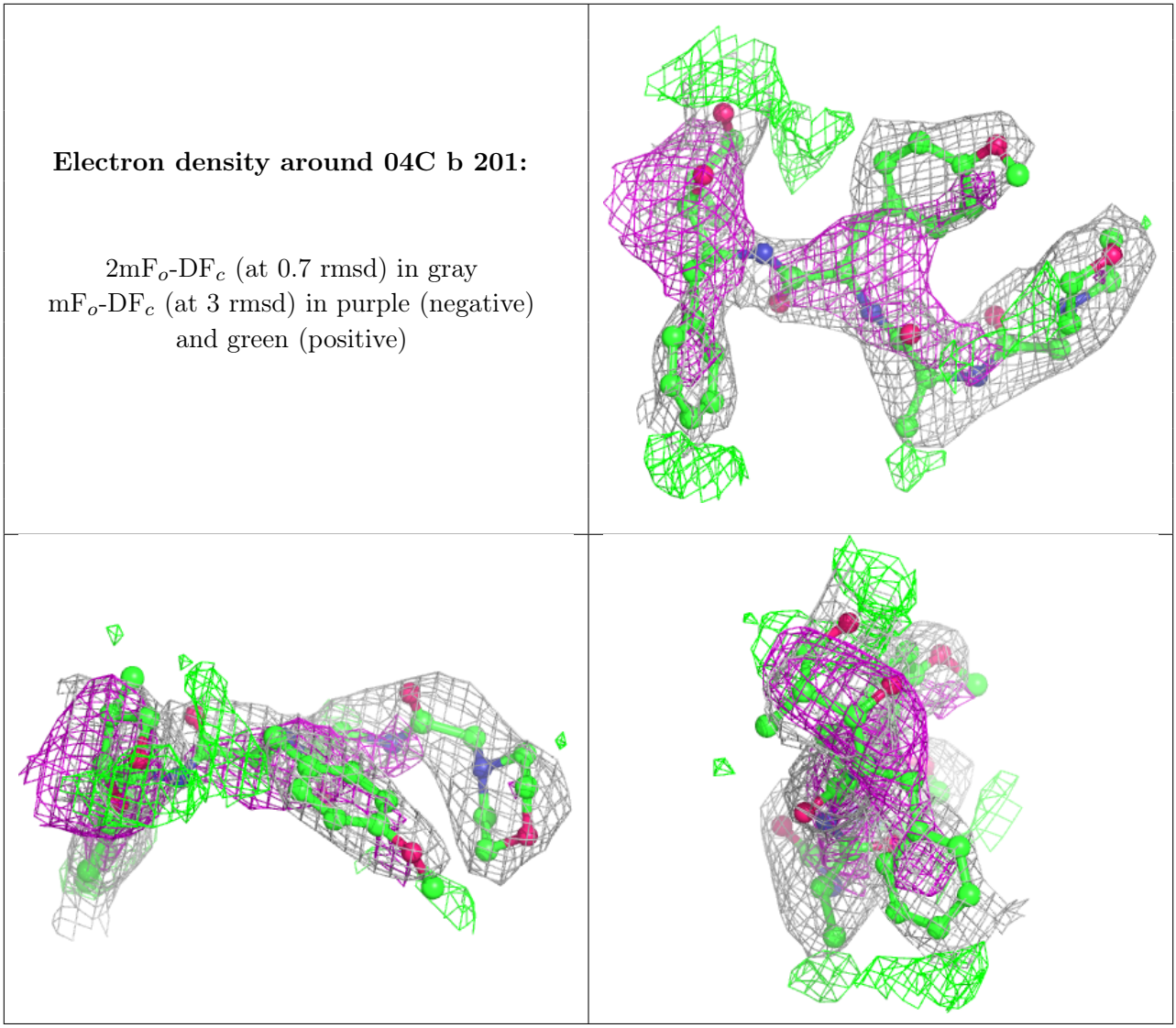






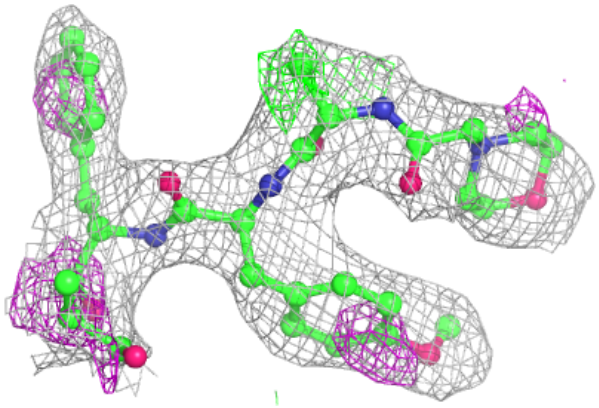
Electron density around 04C b 201:

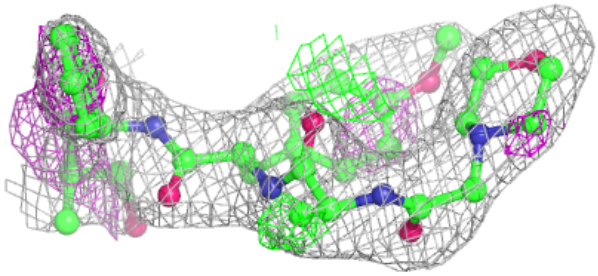
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

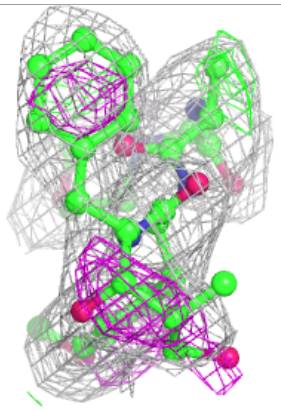


Electron density around 04C H 301:

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

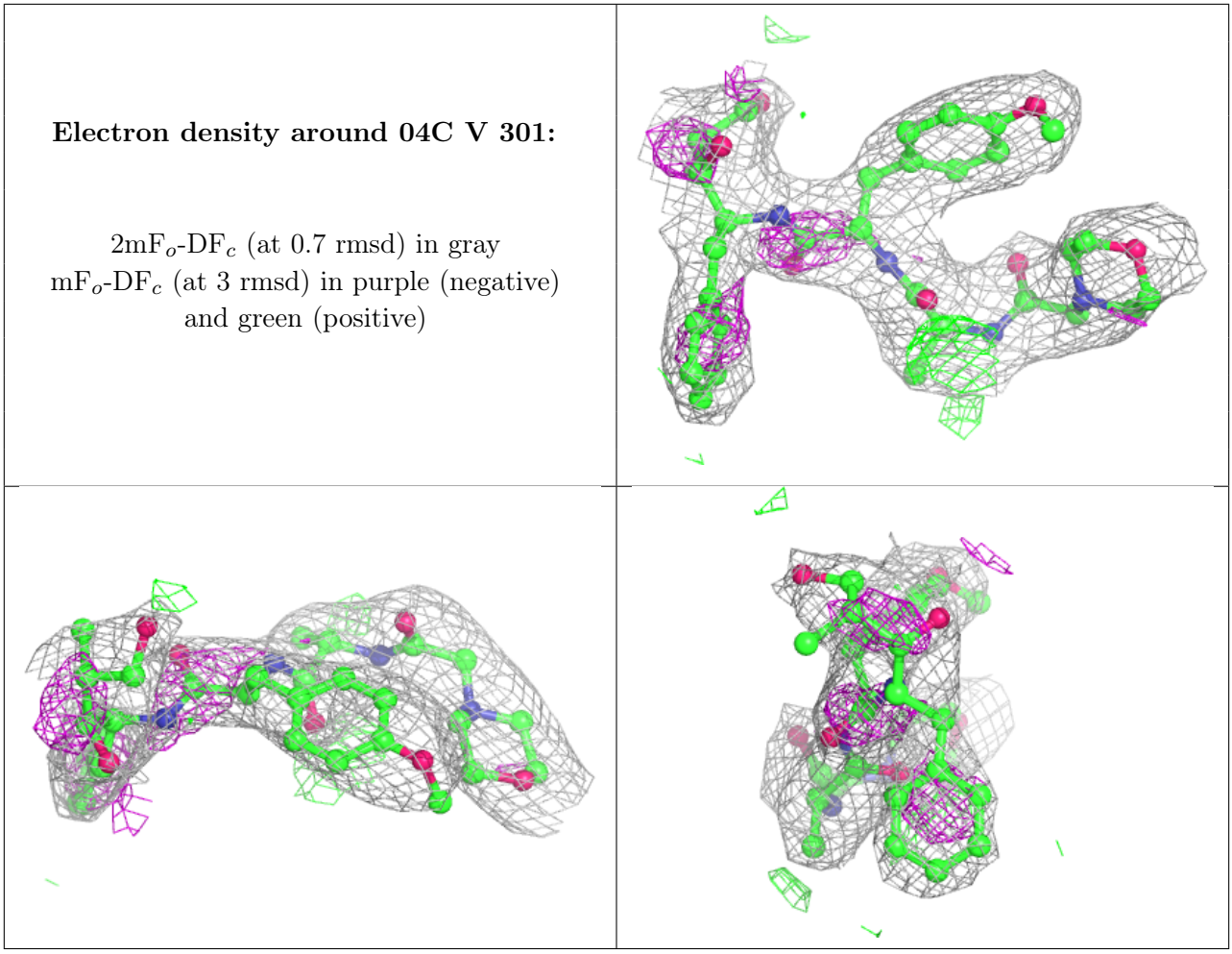






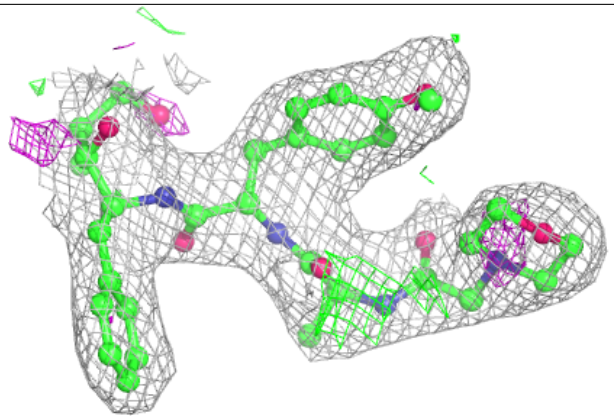
Electron density around 04C V 301:

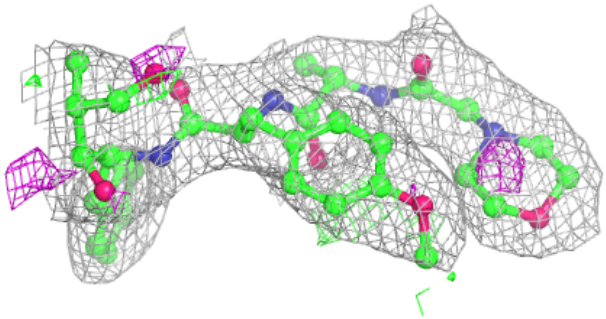
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

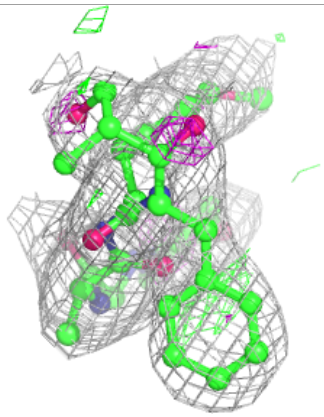


Electron density around 04C K 301:

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

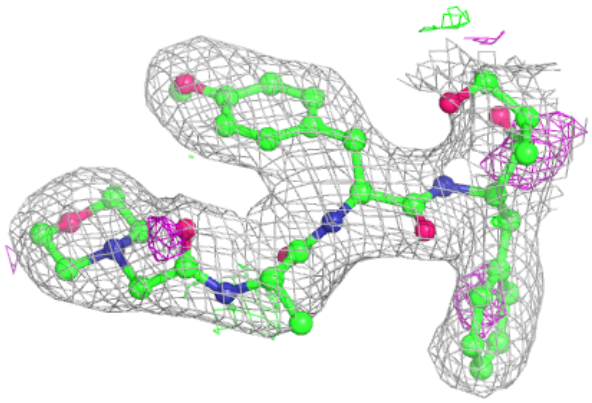


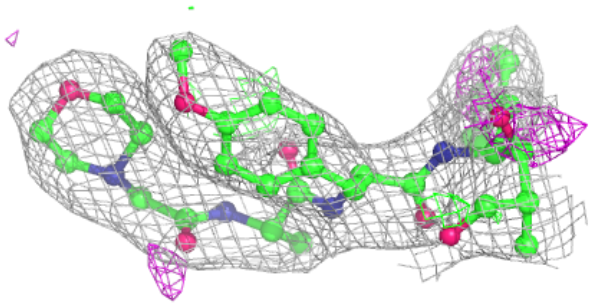


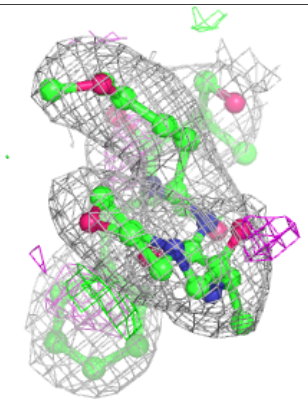


Electron density around 04C Y 301:

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







6.5 Other polymers (i)

There are no such residues in this entry.