



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 01:49 PM BST

PDB ID : 4HNP
Title : Crystal structure of yeast 20S proteasome in complex with vinylketone carmaphyycin analogue VNK1
Authors : Trivella, D.B.B.; Stein, M.; Groll, M.
Deposited on : 2012-10-20
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

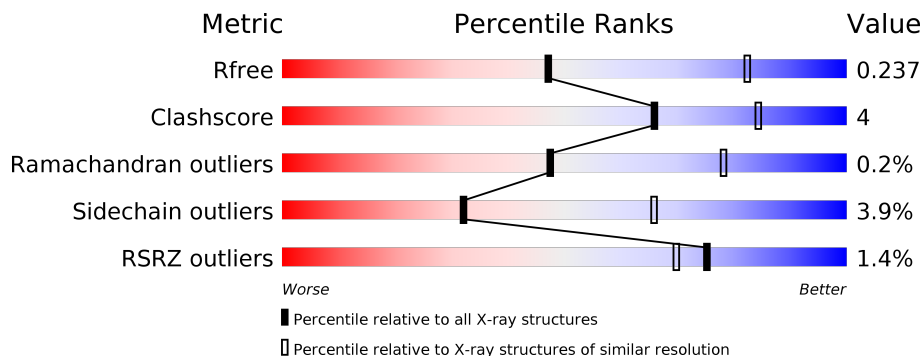
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	250	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 89%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: red;"></div> </div> <p style="text-align: center; margin-top: 5px;">89% 10% •</p>
1	O	250	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 90%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: red;"></div> </div> <p style="text-align: center; margin-top: 5px;">90% 10% •</p>
2	B	244	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 84%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: red;"></div> </div> <p style="text-align: center; margin-top: 5px;">84% 13% •</p>
2	P	244	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 88%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: red;"></div> </div> <p style="text-align: center; margin-top: 5px;">88% 11% •</p>
3	C	241	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 85%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: red;"></div> </div> <p style="text-align: center; margin-top: 5px;">85% 13% •</p>
3	Q	241	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 89%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: red;"></div> </div> <p style="text-align: center; margin-top: 5px;">89% 11%</p>

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Mol	Chain	Length	Quality of chain
4	D	242	<p>2% 90% 9%</p>
4	R	242	<p>3% 91% 9%</p>
5	E	233	<p>2% 89% 10%</p>
5	S	233	<p>2% 86% 13%</p>
6	F	244	<p>0% 84% 14%</p>
6	T	244	<p>2% 86% 13%</p>
7	G	243	<p>0% 88% 11%</p>
7	U	243	<p>0% 89% 11%</p>
8	H	222	<p>0% 91% 9%</p>
8	V	222	<p>0% 90% 10%</p>
9	I	204	<p>0% 91% 9%</p>
9	W	204	<p>0% 88% 12%</p>
10	J	198	<p>2% 89% 10%</p>
10	X	198	<p>2% 88% 12%</p>
11	K	212	<p>0% 87% 11%</p>
11	Y	212	<p>0% 92% 7%</p>
12	L	222	<p>0% 89% 9%</p>
12	Z	222	<p>0% 89% 9%</p>
13	M	233	<p>0% 80% 20%</p>
13	a	233	<p>0% 95% 5%</p>
14	N	196	<p>0% 92% 8%</p>
14	b	196	<p>0% 97% 0%</p>

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 50504 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 component Y7.

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

- Molecule 2 is a protein called Proteasome component Y13.

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

- Molecule 3 is a protein called Proteasome component PRE6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	241	Total	C	N	O	S	0	0	0
			1890	1181	331	374	4			
3	Q	241	Total	C	N	O	S	0	0	0
			1890	1181	331	374	4			

- Molecule 4 is a protein called Proteasome component PUP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	242	Total	C	N	O	S	0	0	0
			1861	1162	314	378	7			
4	R	242	Total	C	N	O	S	0	0	0
			1861	1162	314	378	7			

- Molecule 5 is a protein called Proteasome component PRE5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	233	Total 1795	C 1129	N 312	O 350	S 4	0	0	0
5	S	233	Total 1795	C 1129	N 312	O 350	S 4	0	0	0

- Molecule 6 is a protein called Proteasome component C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	244	Total 1896	C 1205	N 330	O 357	S 4	0	0	0
6	T	244	Total 1896	C 1205	N 330	O 357	S 4	0	0	0

- Molecule 7 is a protein called Proteasome component C7-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	243	Total 1921	C 1221	N 322	O 370	S 8	0	0	0
7	U	243	Total 1921	C 1221	N 322	O 370	S 8	0	0	0

- Molecule 8 is a protein called Proteasome component PUP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	222	Total 1684	C 1061	N 293	O 323	S 7	0	0	0
8	V	222	Total 1684	C 1061	N 293	O 323	S 7	0	0	0

- Molecule 9 is a protein called Proteasome component PUP3.

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

- Molecule 10 is a protein called Proteasome component C11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	J	198	Total 1585	C 1005	N 269	O 305	S 6	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	X	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

- Molecule 11 is a protein called Proteasome component PRE2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
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 component C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
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			

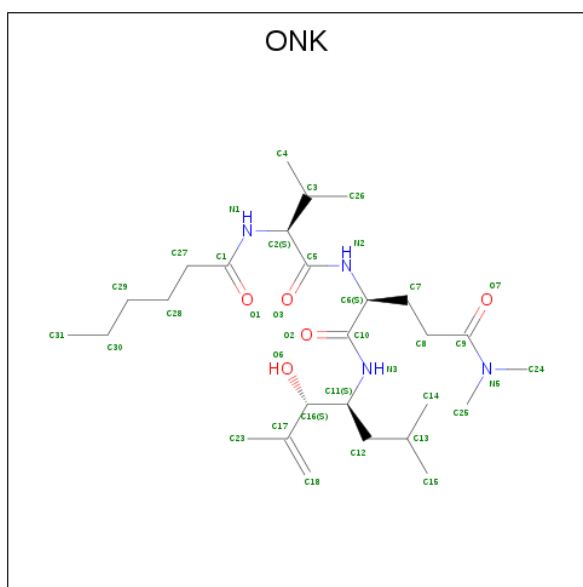
- Molecule 13 is a protein called Proteasome component PRE4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
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 component PRE3.

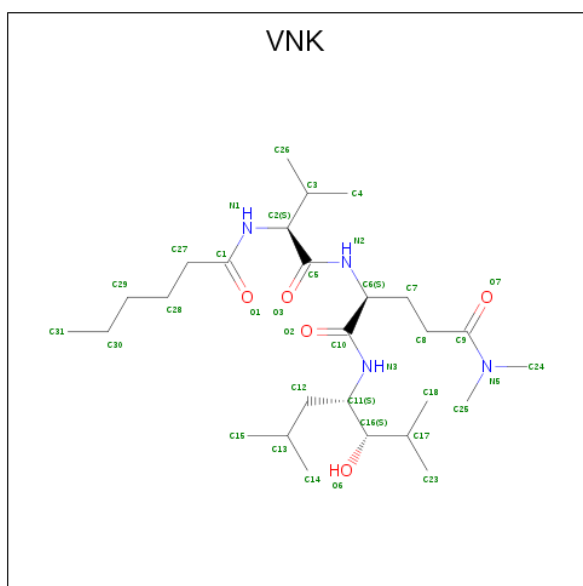
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	N	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
14	b	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

- Molecule 15 is N-hexanoyl-L-valyl-N 1 -[(3S,4S)-3-hydroxy-2,6-dimethylhept-1-en-4-yl]-N 5 ,N 5 -dimethyl-L-glutamamide (three-letter code: ONK) (formula: C₂₇H₅₀N₄O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	H	1	Total	C	N	O	0	0
			36	27	4	5		
15	V	1	Total	C	N	O	0	0
			36	27	4	5		

- Molecule 16 is N-hexanoyl-L-valyl-N 1 -[(3S,4S)-3-hydroxy-2,6-dimethylheptan-4-yl]-N 5 ,N 5 -dimethyl-L-glutamamide (three-letter code: VNK) (formula: C₂₇H₅₂N₄O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	K	1	Total	C	N	O	0	0
			36	27	4	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
16	N	1	36	27	4	5	0	0
16	Y	1	36	27	4	5	0	0
16	b	1	36	27	4	5	0	0

- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	29	Total	O	0	0
			29	29		
17	B	21	Total	O	0	0
			21	21		
17	C	30	Total	O	0	0
			30	30		
17	D	29	Total	O	0	0
			29	29		
17	E	38	Total	O	0	0
			38	38		
17	F	22	Total	O	0	0
			22	22		
17	G	30	Total	O	0	0
			30	30		
17	H	27	Total	O	0	0
			27	27		
17	I	40	Total	O	0	0
			40	40		
17	J	22	Total	O	0	0
			22	22		
17	K	23	Total	O	0	0
			23	23		
17	L	32	Total	O	0	0
			32	32		
17	M	27	Total	O	0	0
			27	27		
17	N	31	Total	O	0	0
			31	31		
17	O	22	Total	O	0	0
			22	22		
17	P	23	Total	O	0	0
			23	23		

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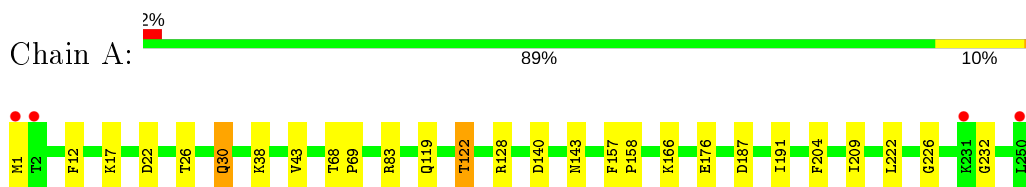
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	Q	29	Total O 29 29	0	0
17	R	28	Total O 28 28	0	0
17	S	26	Total O 26 26	0	0
17	T	30	Total O 30 30	0	0
17	U	21	Total O 21 21	0	0
17	V	37	Total O 37 37	0	0
17	W	19	Total O 19 19	0	0
17	X	18	Total O 18 18	0	0
17	Y	27	Total O 27 27	0	0
17	Z	16	Total O 16 16	0	0
17	a	29	Total O 29 29	0	0
17	b	24	Total O 24 24	0	0

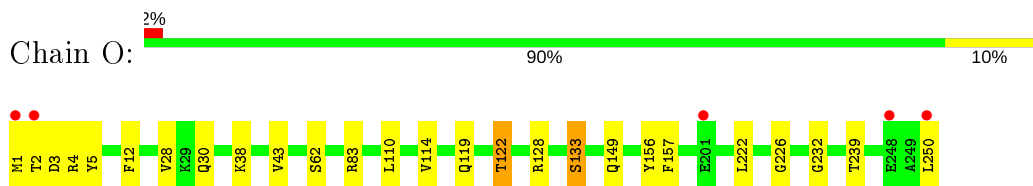
3 Residue-property plots [i](#)

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.

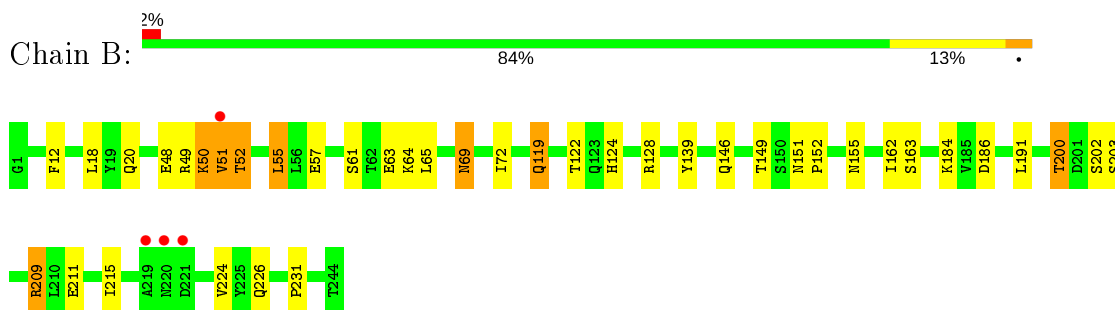
- Molecule 1: Proteasome component Y7



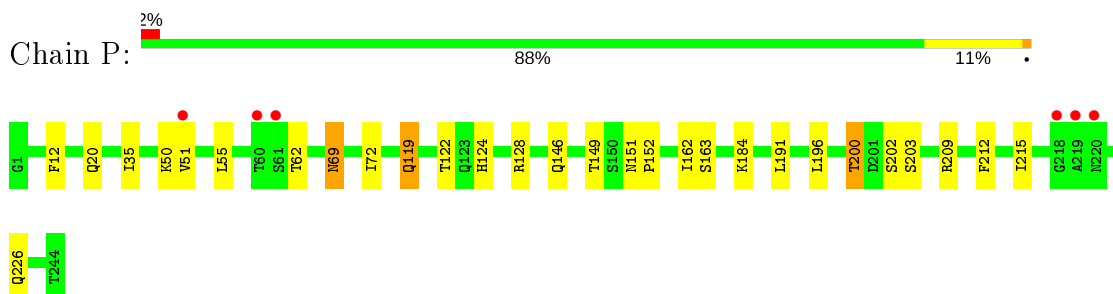
- Molecule 1: Proteasome component Y7



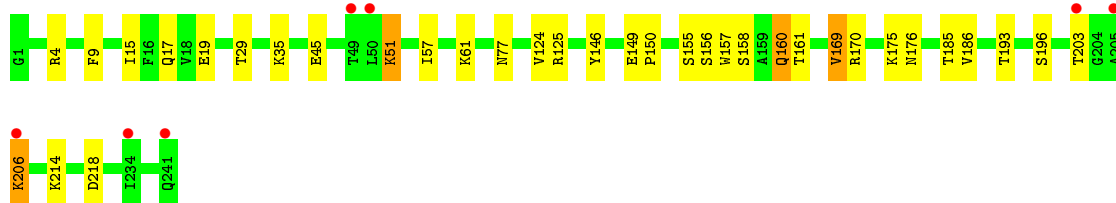
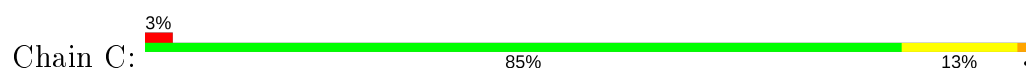
- Molecule 2: Proteasome component Y13



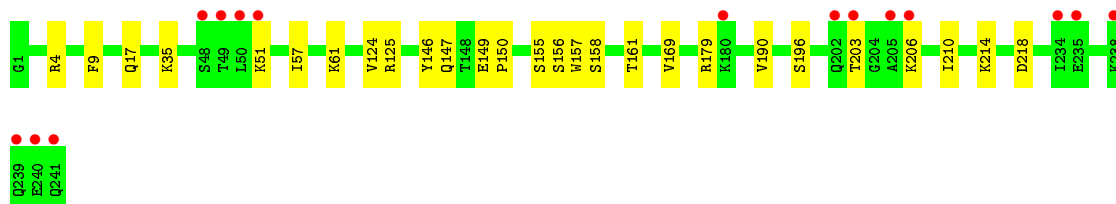
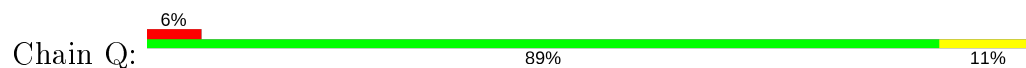
- Molecule 2: Proteasome component Y13



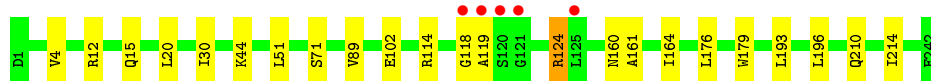
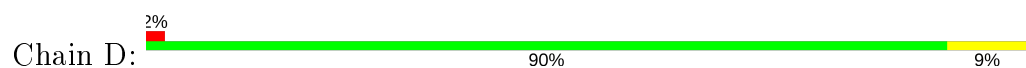
- Molecule 3: Proteasome component PRE6



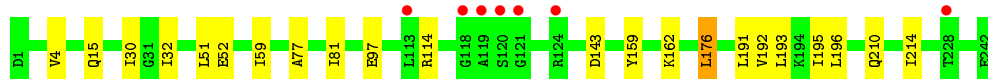
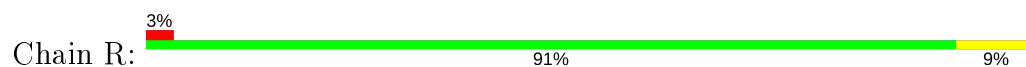
- Molecule 3: Proteasome component PRE6



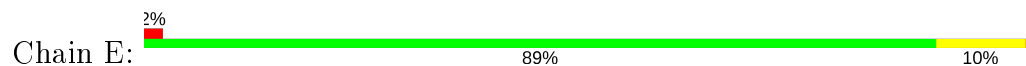
- Molecule 4: Proteasome component PUP2



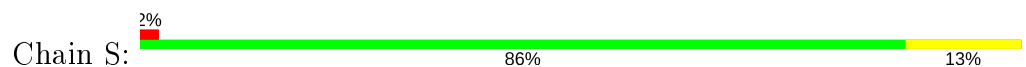
- Molecule 4: Proteasome component PUP2



- Molecule 5: Proteasome component PRE5

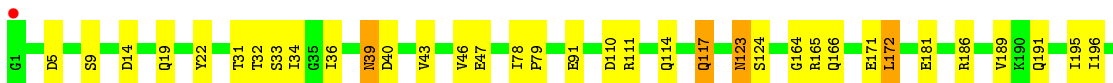
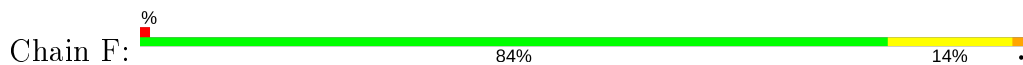


- Molecule 5: Proteasome component PRE5

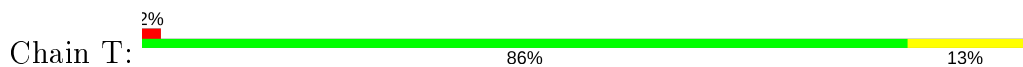




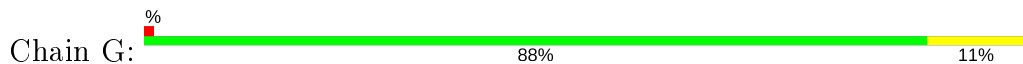
- Molecule 6: Proteasome component C1



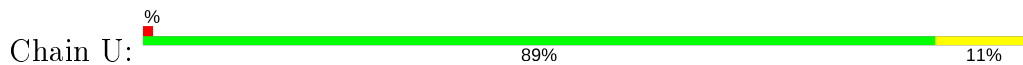
- Molecule 6: Proteasome component C1



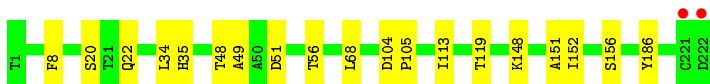
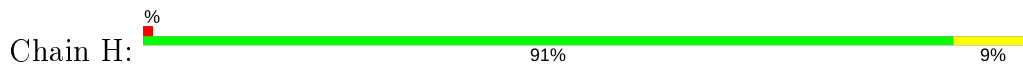
- Molecule 7: Proteasome component C7-alpha



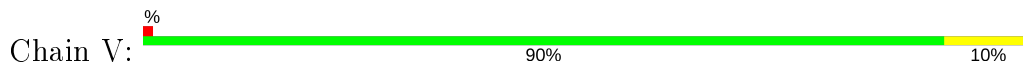
- Molecule 7: Proteasome component C7-alpha



- Molecule 8: Proteasome component PUP1



- Molecule 8: Proteasome component PUP1

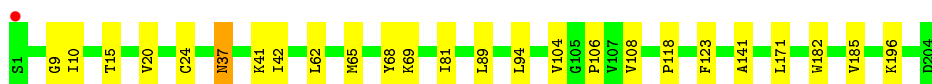




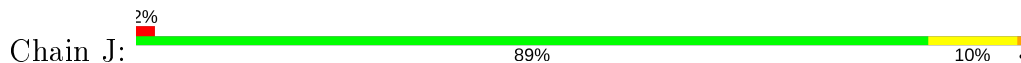
- Molecule 9: Proteasome component PUP3



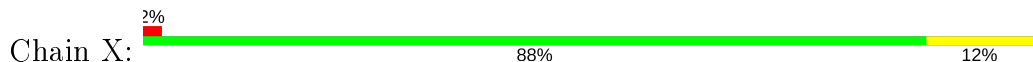
- Molecule 9: Proteasome component PUP3



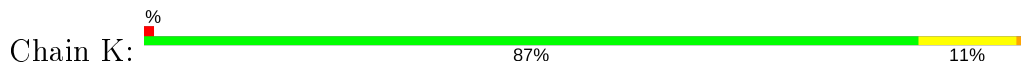
- Molecule 10: Proteasome component C11



- Molecule 10: Proteasome component C11




- Molecule 11: Proteasome component PRE2



- Molecule 11: Proteasome component PRE2




- Molecule 12: Proteasome component C5

Chain L:  89% 9%




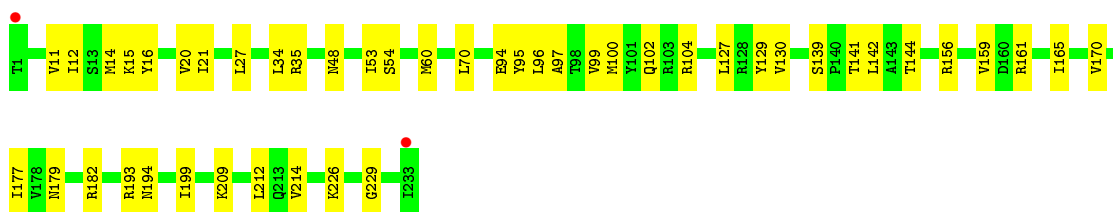
- Molecule 12: Proteasome component C5

Chain Z:  89% 9%



- Molecule 13: Proteasome component PRE4

Chain M:  80% 20%

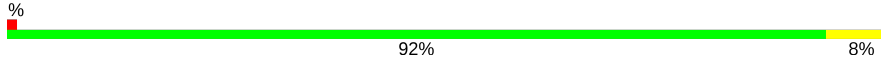


- Molecule 13: Proteasome component PRE4

Chain a:  95% 5%



- Molecule 14: Proteasome component PRE3

Chain N:  92% 8%



- Molecule 14: Proteasome component PRE3

Chain b:  97%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.85Å 301.36Å 144.46Å 90.00° 112.82° 90.00°	Depositor
Resolution (Å)	48.42 – 2.80 48.42 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.3 (48.42-2.80) 98.3 (48.42-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 2.81Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.203 , 0.239 0.203 , 0.237	Depositor DCC
R_{free} test set	12815 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	59.7	Xtrriage
Anisotropy	0.030	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	50504	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ONK, VNK

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	0.33	0/1952	0.50	0/2642
1	O	0.36	0/1952	0.48	0/2642
2	B	0.35	0/1934	0.51	0/2618
2	P	0.33	0/1934	0.50	0/2618
3	C	0.33	0/1919	0.50	0/2598
3	Q	0.33	0/1919	0.50	0/2598
4	D	0.32	0/1886	0.52	0/2541
4	R	0.32	0/1886	0.50	0/2541
5	E	0.33	0/1823	0.48	0/2463
5	S	0.33	0/1823	0.48	0/2463
6	F	0.34	0/1936	0.46	0/2614
6	T	0.33	0/1936	0.48	0/2614
7	G	0.34	0/1959	0.49	0/2652
7	U	0.33	0/1959	0.48	0/2652
8	H	0.30	0/1715	0.49	0/2326
8	V	0.32	0/1715	0.48	0/2326
9	I	0.33	0/1611	0.50	0/2174
9	W	0.33	0/1611	0.50	0/2174
10	J	0.33	0/1613	0.50	0/2173
10	X	0.32	0/1613	0.49	0/2173
11	K	0.33	0/1681	0.52	1/2274 (0.0%)
11	Y	0.32	0/1681	0.51	1/2274 (0.0%)
12	L	0.34	0/1795	0.50	0/2420
12	Z	0.40	0/1795	0.52	0/2420
13	M	0.34	0/1855	0.53	0/2514
13	a	0.33	0/1855	0.51	0/2514
14	N	0.31	0/1541	0.47	0/2087
14	b	0.31	0/1541	0.47	0/2087
All	All	0.33	0/50440	0.50	2/68192 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
11	K	0	1
11	Y	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Y	4	LEU	CA-CB-CG	5.96	129.00	115.30
11	K	4	LEU	CA-CB-CG	5.71	128.44	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	K	1	THR	Peptide
11	Y	1	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	21	0
1	O	1915	0	1929	21	0
2	B	1904	0	1904	55	0
2	P	1904	0	1904	16	0
3	C	1890	0	1903	24	0
3	Q	1890	0	1903	15	0
4	D	1861	0	1839	12	0
4	R	1861	0	1839	12	0
5	E	1795	0	1800	15	0
5	S	1795	0	1800	15	0
6	F	1896	0	1889	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	T	1896	0	1889	15	0
7	G	1921	0	1913	15	0
7	U	1921	0	1913	15	0
8	H	1684	0	1687	10	0
8	V	1684	0	1687	12	0
9	I	1581	0	1574	9	0
9	W	1581	0	1574	15	0
10	J	1585	0	1590	11	0
10	X	1585	0	1590	11	0
11	K	1644	0	1592	15	0
11	Y	1644	0	1592	10	0
12	L	1757	0	1711	14	0
12	Z	1757	0	1711	11	0
13	M	1824	0	1832	23	0
13	a	1824	0	1832	0	0
14	N	1512	0	1478	7	0
14	b	1512	0	1478	0	0
15	H	36	0	49	2	0
15	V	36	0	49	0	0
16	K	36	0	50	1	0
16	N	36	0	50	2	0
16	Y	36	0	50	0	0
16	b	36	0	50	0	0
17	A	29	0	0	0	0
17	B	21	0	0	0	0
17	C	30	0	0	1	0
17	D	29	0	0	0	0
17	E	38	0	0	0	0
17	F	22	0	0	0	0
17	G	30	0	0	0	0
17	H	27	0	0	0	0
17	I	40	0	0	0	0
17	J	22	0	0	0	0
17	K	23	0	0	0	0
17	L	32	0	0	0	0
17	M	27	0	0	1	0
17	N	31	0	0	0	0
17	O	22	0	0	0	0
17	P	23	0	0	0	0
17	Q	29	0	0	0	0
17	R	28	0	0	0	0
17	S	26	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	T	30	0	0	0	0
17	U	21	0	0	0	0
17	V	37	0	0	0	0
17	W	19	0	0	0	0
17	X	18	0	0	0	0
17	Y	27	0	0	0	0
17	Z	16	0	0	0	0
17	a	29	0	0	0	0
17	b	24	0	0	0	0
All	All	50504	0	49580	363	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 4.

All (363) 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)
2:B:209:ARG:HH21	2:B:209:ARG:CG	1.61	1.12
2:B:52:THR:CG2	2:B:209:ARG:HD3	1.82	1.08
7:G:92:ALA:HA	7:G:103:MET:HE2	1.48	0.96
2:B:209:ARG:HG3	2:B:209:ARG:NH2	1.51	0.94
2:B:52:THR:HG22	2:B:209:ARG:HD3	1.55	0.89
2:B:52:THR:HG21	2:B:209:ARG:HG2	1.56	0.88
2:B:52:THR:HG21	2:B:209:ARG:CG	2.06	0.85
2:B:51:VAL:C	2:B:52:THR:HG23	1.96	0.84
2:B:51:VAL:O	2:B:52:THR:HG23	1.78	0.83
6:T:91:GLU:HG2	6:T:111:ARG:HB3	1.61	0.82
2:B:52:THR:CG2	2:B:209:ARG:CD	2.61	0.79
2:B:202:SER:HB2	2:B:209:ARG:HH12	1.47	0.79
2:B:209:ARG:HG3	2:B:209:ARG:HH21	0.69	0.79
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.65	0.79
2:B:202:SER:CB	2:B:209:ARG:NH1	2.47	0.78
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.64	0.78
2:B:51:VAL:CG1	2:B:52:THR:N	2.46	0.77
2:B:202:SER:CB	2:B:209:ARG:HH12	1.97	0.77
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.53	0.73
3:C:9:PHE:H	4:D:15:GLN:HE22	1.36	0.73
1:O:12:PHE:H	2:P:20:GLN:HE22	1.37	0.73
1:A:83:ARG:HE	7:G:114:ASN:HD21	1.39	0.71
2:B:202:SER:OG	2:B:209:ARG:NH1	2.23	0.71
2:B:51:VAL:HG12	2:B:52:THR:H	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:3:ASP:C	1:O:3:ASP:OD1	2.30	0.70
14:N:20:THR:HG22	16:N:301:VNK:H35	1.74	0.69
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.58	0.69
2:B:202:SER:HB2	2:B:209:ARG:NH1	2.08	0.69
1:A:128:ARG:HH21	7:G:120:THR:HG22	1.59	0.68
6:F:91:GLU:HG2	6:F:111:ARG:HB3	1.75	0.68
12:Z:195:HIS:HD2	12:Z:197:GLN:H	1.42	0.68
1:O:83:ARG:HE	7:U:114:ASN:HD21	1.42	0.67
1:O:128:ARG:HH21	7:U:120:THR:HG22	1.58	0.67
2:B:12:PHE:H	3:C:17:GLN:HE22	1.42	0.67
2:B:51:VAL:HG12	2:B:52:THR:N	2.09	0.67
7:U:187:GLU:HG2	7:U:192:LYS:HB2	1.77	0.66
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.78	0.66
11:K:38:ASN:HB2	11:K:39:PRO:HD2	1.77	0.65
1:A:122:THR:CG2	2:B:128:ARG:HH21	2.09	0.65
2:B:209:ARG:NH2	2:B:209:ARG:CG	2.32	0.64
1:O:122:THR:CG2	2:P:128:ARG:HH21	2.11	0.64
10:X:92:ILE:HG21	10:X:122:LEU:HA	1.80	0.63
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.28	0.63
1:A:176:GLU:HG3	2:B:55:LEU:HD21	1.81	0.62
2:B:124:HIS:HB3	3:C:124:VAL:HG12	1.81	0.62
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.46	0.62
1:A:12:PHE:H	2:B:20:GLN:HE22	1.47	0.61
12:L:177:VAL:O	12:L:181:ILE:HG12	1.99	0.61
2:B:119:GLN:O	2:B:122:THR:HB	2.00	0.61
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.30	0.61
10:J:174:MET:HA	10:X:174:MET:HA	1.83	0.61
5:E:178:PHE:HA	5:E:181:ILE:HG12	1.83	0.60
2:P:122:THR:HG22	3:Q:125:ARG:HH21	1.65	0.60
2:B:51:VAL:C	2:B:52:THR:CG2	2.68	0.60
1:A:83:ARG:HE	7:G:114:ASN:ND2	1.99	0.60
6:T:31:THR:HG21	6:T:47:GLU:O	2.01	0.60
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.65	0.60
6:F:31:THR:HG21	6:F:47:GLU:O	2.02	0.60
9:W:185:VAL:HG21	9:W:196:LYS:HE3	1.84	0.60
13:M:179:ASN:HD22	13:M:182:ARG:NH1	2.00	0.59
2:B:52:THR:CG2	2:B:209:ARG:CG	2.79	0.59
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	1.84	0.59
11:Y:209:ASN:HD22	11:Y:209:ASN:H	1.50	0.59
3:C:157:TRP:CE2	4:D:51:LEU:HD23	2.36	0.59
3:C:160:GLN:HE22	3:C:170:ARG:HE	1.48	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:127:TYR:O	5:S:148:PRO:HB3	2.03	0.59
8:H:35:HIS:CB	8:H:56:THR:HG21	2.33	0.59
5:S:206:THR:H	5:S:209:ASN:HB3	1.66	0.58
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.52	0.58
12:L:109:THR:HG23	12:L:125:PHE:HB2	1.85	0.57
5:E:92:ASN:HD21	12:L:70:ASN:HD21	1.50	0.57
1:O:83:ARG:HE	7:U:114:ASN:ND2	2.02	0.57
1:A:140:ASP:OD1	1:A:143:ASN:HB2	2.04	0.57
6:F:32:THR:HB	6:F:164:GLY:H	1.69	0.57
2:B:52:THR:HG22	2:B:209:ARG:CD	2.32	0.57
12:L:195:HIS:HD2	12:L:197:GLN:H	1.53	0.56
8:V:35:HIS:CB	8:V:56:THR:HG21	2.35	0.56
9:W:62:LEU:HD11	9:W:104:VAL:HG21	1.87	0.56
2:B:52:THR:CG2	2:B:209:ARG:HG2	2.31	0.56
3:C:29:THR:HB	3:C:45:GLU:HG3	1.86	0.56
2:B:122:THR:HG22	3:C:125:ARG:HH21	1.71	0.56
2:P:35:ILE:HD12	2:P:196:LEU:HG	1.87	0.55
3:C:77:ASN:H	3:C:77:ASN:HD22	1.54	0.55
1:O:2:THR:CG2	1:O:3:ASP:N	2.69	0.55
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.36	0.55
9:W:106:PRO:HD2	9:W:123:PHE:HB2	1.88	0.55
6:T:31:THR:HG23	6:T:47:GLU:HB3	1.88	0.55
2:P:146:GLN:HG2	3:Q:57:ILE:HG21	1.87	0.55
13:M:209:LYS:HB3	13:M:212:LEU:HD11	1.89	0.54
6:F:191:GLN:O	6:F:195:ILE:HG12	2.07	0.54
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	1.90	0.54
3:C:51:LYS:HE3	3:C:206:LYS:HE3	1.89	0.54
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.37	0.54
3:C:186:VAL:HG21	3:C:214:LYS:HE2	1.90	0.54
8:V:148:LYS:O	8:V:152:ILE:HG12	2.08	0.54
6:F:91:GLU:HG3	6:F:111:ARG:HH11	1.72	0.54
2:P:151:ASN:HB2	2:P:152:PRO:HD2	1.90	0.54
2:B:51:VAL:HG13	2:B:52:THR:N	2.23	0.54
2:B:51:VAL:O	2:B:52:THR:CG2	2.53	0.54
1:O:226:GLY:HA3	8:V:186:TYR:HB3	1.88	0.54
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.90	0.54
11:K:12:ILE:HB	11:K:180:VAL:HB	1.91	0.53
11:K:158:LYS:HB2	11:K:177:LEU:HD11	1.90	0.53
13:M:15:LYS:HG3	13:M:165:ILE:HD12	1.91	0.53
3:Q:157:TRP:CE2	4:R:51:LEU:HD23	2.43	0.53
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:3:ILE:HB	10:J:18:SER:HB3	1.89	0.53
1:A:128:ARG:HH21	7:G:120:THR:CG2	2.22	0.53
3:Q:214:LYS:HB2	3:Q:218:ASP:HB3	1.90	0.53
8:V:78:SER:O	8:V:82:MET:HG3	2.09	0.53
6:T:91:GLU:HG3	6:T:111:ARG:HH11	1.73	0.53
11:K:176:ASN:HD21	11:K:190:ASN:HD22	1.57	0.53
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.91	0.53
9:I:120:ILE:HD12	9:I:136:ILE:HG12	1.89	0.53
4:R:176:LEU:HD22	5:S:55:LEU:HD13	1.90	0.53
10:J:22:THR:HG21	10:X:173:PRO:HB3	1.90	0.52
2:B:215:ILE:HG12	2:B:226:GLN:HG2	1.90	0.52
9:W:15:THR:HG22	9:W:20:VAL:HG12	1.91	0.52
13:M:179:ASN:HD22	13:M:182:ARG:HH11	1.57	0.52
6:T:191:GLN:O	6:T:195:ILE:HG12	2.10	0.52
1:O:2:THR:HG22	1:O:3:ASP:N	2.23	0.52
1:A:119:GLN:O	1:A:122:THR:HB	2.09	0.52
11:K:37:ILE:HB	11:K:41:LEU:HB3	1.91	0.52
12:L:18:GLU:O	12:L:119:LYS:HA	2.09	0.52
6:T:50:ILE:HD11	6:T:209:GLU:HB2	1.92	0.52
1:A:187:ASP:O	1:A:191:ILE:HD12	2.09	0.52
12:L:3:ASN:ND2	12:L:5:TYR:H	2.08	0.52
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.39	0.52
5:E:206:THR:H	5:E:209:ASN:HB3	1.75	0.52
11:Y:38:ASN:HB2	11:Y:39:PRO:HD2	1.91	0.52
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.92	0.51
1:O:5:TYR:HD2	7:U:124:TYR:HB3	1.76	0.51
4:D:114:ARG:HA	4:D:124:ARG:HE	1.75	0.51
13:M:14:MET:HG2	13:M:177:ILE:HD11	1.91	0.51
5:E:99:ASN:HB2	13:M:94:GLU:HG2	1.91	0.51
9:I:22:ILE:HG12	9:I:42:ILE:HD12	1.93	0.51
3:C:149:GLU:HB2	3:C:150:PRO:HD2	1.93	0.51
6:F:31:THR:HG23	6:F:47:GLU:HB3	1.91	0.51
12:L:49:ASN:HD21	12:L:211:GLY:HA2	1.75	0.51
2:B:52:THR:HG23	2:B:209:ARG:HD3	1.85	0.51
2:B:49:ARG:HH12	2:B:61:SER:CB	2.24	0.51
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.93	0.51
3:Q:161:THR:HG21	3:Q:169:VAL:HG13	1.93	0.51
2:B:122:THR:CG2	3:C:125:ARG:HH21	2.25	0.50
1:O:38:LYS:HG3	1:O:43:VAL:HG22	1.93	0.50
12:Z:109:THR:HG23	12:Z:125:PHE:HB2	1.92	0.50
2:B:50:LYS:O	2:B:51:VAL:HG12	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:126:ASP:HB2	12:Z:130:SER:HB3	1.93	0.50
5:S:178:PHE:HA	5:S:181:ILE:HG12	1.93	0.50
5:S:12:PHE:H	6:T:19:GLN:HE22	1.60	0.50
11:Y:78:ALA:O	11:Y:82:ILE:HG12	2.12	0.50
4:D:119:ALA:HB3	4:D:124:ARG:HD3	1.93	0.50
5:E:9:THR:HG21	5:E:119:THR:HA	1.94	0.50
10:J:184:VAL:HG22	10:J:189:ILE:HG12	1.94	0.50
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.92	0.50
2:B:200:THR:HG22	2:B:202:SER:H	1.77	0.50
2:P:69:ASN:HB3	2:P:72:ILE:H	1.77	0.50
5:S:87:LEU:HD11	5:S:107:ALA:HB1	1.93	0.50
3:Q:155:SER:HB2	4:R:51:LEU:HD21	1.94	0.50
2:B:18:LEU:HD13	2:B:122:THR:HG23	1.94	0.49
5:E:12:PHE:H	6:F:19:GLN:HE22	1.59	0.49
1:O:3:ASP:OD1	1:O:5:TYR:N	2.35	0.49
4:R:59:ILE:HG13	4:R:210:GLN:HE21	1.77	0.49
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.94	0.49
6:F:123:ASN:C	6:F:123:ASN:HD22	2.15	0.49
7:U:195:GLU:HG3	7:U:235:ARG:HG3	1.95	0.49
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.42	0.49
4:D:89:VAL:HG21	11:K:65:LEU:HD13	1.95	0.49
4:D:30:ILE:HD12	4:D:196:LEU:HG	1.95	0.49
1:O:83:ARG:HH21	7:U:114:ASN:HD22	1.58	0.49
5:S:44:VAL:HG21	5:S:188:LEU:HB3	1.93	0.49
12:Z:207:VAL:HG22	12:Z:212:VAL:HG22	1.95	0.49
9:W:94:LEU:HD11	9:W:106:PRO:HG2	1.93	0.48
13:M:96:LEU:O	13:M:100:MET:HG2	2.13	0.48
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.95	0.48
10:X:104:ILE:HB	10:X:117:TYR:HB2	1.96	0.48
8:V:20:SER:HB3	8:V:28:ASP:HB3	1.95	0.48
11:K:209:ASN:O	9:W:37:ASN:ND2	2.46	0.48
3:C:160:GLN:HE21	3:C:160:GLN:CA	2.23	0.48
5:E:92:ASN:ND2	12:L:70:ASN:HD21	2.11	0.48
6:T:32:THR:HB	6:T:164:GLY:H	1.79	0.48
3:C:175:LYS:HG3	3:C:176:ASN:HD22	1.79	0.48
13:M:129:TYR:HE2	13:M:144:THR:HG22	1.79	0.48
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.96	0.48
13:M:139:SER:HB3	13:M:141:THR:O	2.14	0.47
2:B:51:VAL:HG13	2:B:52:THR:O	2.14	0.47
11:K:99:THR:HG22	11:K:115:VAL:O	2.14	0.47
1:A:26:THR:O	1:A:30:GLN:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:39:ASN:HD22	6:F:40:ASP:N	2.12	0.47
14:N:36:ARG:HH21	14:N:60:GLN:HE21	1.61	0.47
4:R:191:LEU:O	4:R:195:ILE:HD12	2.14	0.47
6:F:171:GLU:HB3	6:F:195:ILE:HD12	1.97	0.47
8:H:148:LYS:O	8:H:152:ILE:HG12	2.13	0.47
3:Q:179:ARG:HH22	4:R:52:GLU:HA	1.79	0.47
3:C:214:LYS:HB2	3:C:218:ASP:HB3	1.96	0.47
2:B:151:ASN:HB2	2:B:152:PRO:HD2	1.97	0.47
2:B:63:GLU:HG3	2:B:64:LYS:HG3	1.96	0.47
14:N:20:THR:HG22	16:N:301:VNK:C12	2.44	0.47
7:U:92:ALA:HA	7:U:103:MET:HE1	1.96	0.47
7:U:117:GLN:O	7:U:120:THR:HB	2.14	0.47
12:Z:18:GLU:O	12:Z:119:LYS:HA	2.14	0.47
10:X:119:ILE:HG12	10:X:125:LYS:HG3	1.97	0.46
7:G:195:GLU:HG3	7:G:235:ARG:HG3	1.97	0.46
2:P:119:GLN:O	2:P:122:THR:HB	2.15	0.46
12:L:126:ASP:HB2	12:L:130:SER:HB3	1.97	0.46
1:A:17:LYS:HD2	1:A:22:ASP:OD2	2.15	0.46
5:E:131:LEU:HB2	5:E:146:PHE:HB3	1.97	0.46
10:X:147:HIS:HB3	10:X:160:LEU:HD11	1.97	0.46
12:Z:169:LYS:O	12:Z:170:LYS:C	2.53	0.46
11:K:145:LYS:HB2	11:K:148:LEU:HD13	1.98	0.46
10:X:184:VAL:HG22	10:X:189:ILE:HG12	1.98	0.46
12:L:27:THR:HB	12:L:39:TYR:HA	1.98	0.46
1:O:222:LEU:HD13	1:O:232:GLY:HA2	1.98	0.46
7:G:167:GLN:HE21	7:G:171:THR:HG23	1.81	0.45
13:M:21:ILE:HG12	13:M:199:ILE:HG12	1.97	0.45
13:M:11:VAL:HG23	13:M:54:SER:HB3	1.98	0.45
5:S:92:ASN:HD21	12:Z:70:ASN:HD21	1.64	0.45
13:M:97:ALA:HA	13:M:130:VAL:HG21	1.98	0.45
6:F:216:SER:HB3	6:F:219:GLU:HB2	1.98	0.45
9:I:20:VAL:HG23	9:I:189:ILE:HB	1.99	0.45
1:O:149:GLN:O	1:O:156:TYR:HA	2.16	0.45
14:N:175:MET:HB2	14:N:186:LEU:HB2	1.98	0.45
2:B:146:GLN:HG2	3:C:57:ILE:HG21	1.99	0.45
11:K:107:LYS:H	11:K:107:LYS:HD2	1.82	0.45
11:K:49:ALA:HB2	16:K:301:VNK:H39	1.99	0.45
5:E:92:ASN:HD21	12:L:70:ASN:ND2	2.14	0.45
7:G:106:ASP:HB3	7:G:146:TYR:CZ	2.51	0.45
1:A:83:ARG:HH21	7:G:114:ASN:HD22	1.65	0.45
2:P:162:ILE:HG13	2:P:163:SER:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:GLY:HA3	8:H:186:TYR:HB3	1.98	0.45
3:C:156:SER:HB2	17:C:307:HOH:O	2.17	0.45
2:P:215:ILE:HG12	2:P:226:GLN:HG2	1.97	0.45
6:F:36:ILE:HG12	6:F:172:LEU:HD11	1.99	0.45
6:F:33:SER:HB3	6:F:46:VAL:HG23	1.99	0.45
13:M:193:ARG:HG3	13:M:214:VAL:HB	1.99	0.45
1:O:5:TYR:HE2	7:U:124:TYR:HA	1.82	0.45
14:N:8:PHE:CE2	14:N:10:ASP:HB2	2.51	0.44
4:R:97:GLU:OE1	12:Z:75:TYR:OH	2.31	0.44
6:T:63:ILE:HB	6:T:226:PHE:HE2	1.81	0.44
12:Z:172:LEU:HA	12:Z:172:LEU:HD13	1.68	0.44
6:T:33:SER:HB3	6:T:46:VAL:HG23	2.00	0.44
8:V:48:THR:HB	8:V:51:ASP:HB2	1.99	0.44
9:W:65:MET:O	9:W:68:TYR:HB3	2.17	0.44
1:A:158:PRO:HB2	2:B:57:GLU:HB3	2.00	0.44
1:O:28:VAL:HG11	1:O:133:SER:HB2	2.00	0.44
3:C:160:GLN:NE2	3:C:161:THR:H	2.16	0.44
9:W:20:VAL:HG13	9:W:118:PRO:HB3	2.00	0.44
10:J:173:PRO:HB3	10:X:22:THR:HG21	2.00	0.44
3:Q:146:TYR:CE1	3:Q:156:SER:HB3	2.53	0.44
9:W:62:LEU:CD1	9:W:104:VAL:HG21	2.47	0.44
3:C:146:TYR:CE1	3:C:156:SER:HB3	2.52	0.44
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	1.98	0.44
6:F:123:ASN:HD22	6:F:124:SER:N	2.16	0.44
4:D:12:ARG:HH12	5:E:30:GLN:HE22	1.65	0.43
9:I:185:VAL:HG21	9:I:196:LYS:HE3	1.99	0.43
10:J:92:ILE:HA	10:J:97:PRO:HB3	1.99	0.43
10:X:101:ASN:HB3	10:X:133:HIS:CE1	2.53	0.43
14:N:177:VAL:HB	14:N:184:GLU:HB3	1.99	0.43
5:S:80:ALA:HB2	5:S:129:VAL:HG21	2.00	0.43
5:S:174:THR:O	5:S:174:THR:HG22	2.19	0.43
1:A:222:LEU:HD13	1:A:232:GLY:HA2	1.99	0.43
10:J:92:ILE:HG21	10:J:122:LEU:HA	1.99	0.43
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.19	0.43
4:R:30:ILE:HD12	4:R:196:LEU:HG	2.00	0.43
10:X:39:SER:HB2	10:X:40:PRO:HD2	2.00	0.43
11:Y:209:ASN:HD22	11:Y:209:ASN:N	2.15	0.43
6:F:78:ILE:HB	6:F:79:PRO:HD3	2.00	0.43
13:M:156:ARG:HH11	8:V:165:ASN:HD22	1.66	0.43
7:G:180:SER:O	7:G:181:LYS:HB2	2.19	0.43
7:G:182:ILE:HG13	7:G:182:ILE:H	1.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:1:MET:HE3	10:J:2:ASP:H	1.84	0.43
11:Y:12:ILE:HB	11:Y:180:VAL:HB	2.00	0.43
9:I:14:MET:HG3	9:I:135:PHE:HB3	2.00	0.43
2:B:162:ILE:HG13	2:B:163:SER:N	2.34	0.43
10:J:101:ASN:HB3	10:J:133:HIS:CE1	2.54	0.43
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.98	0.43
12:L:8:ASN:HA	12:L:30:ILE:O	2.18	0.43
2:B:48:GLU:OE2	2:B:200:THR:HG23	2.19	0.43
4:D:44:LYS:HE3	4:D:210:GLN:HB2	2.01	0.43
6:F:9:SER:HB2	7:G:126:ARG:HB3	1.99	0.43
9:W:108:VAL:HG23	9:W:123:PHE:HE1	1.84	0.43
2:B:65:LEU:HD22	2:B:211:GLU:HB3	2.01	0.42
1:A:68:THR:HB	1:A:69:PRO:HD2	2.01	0.42
5:E:106:ARG:O	5:E:110:LEU:HG	2.19	0.42
1:O:3:ASP:OD1	1:O:4:ARG:N	2.51	0.42
3:Q:190:VAL:HG13	3:Q:210:ILE:HG21	2.00	0.42
13:M:27:LEU:HD21	13:M:34:LEU:HD22	2.01	0.42
11:Y:37:ILE:HB	11:Y:41:LEU:HB3	2.02	0.42
3:C:160:GLN:HE21	3:C:161:THR:H	1.67	0.42
5:S:179:ILE:HG23	5:S:180:LYS:HG3	2.00	0.42
7:G:149:ASP:HB2	7:G:150:PRO:HD2	2.01	0.42
8:H:48:THR:HB	8:H:51:ASP:HB2	1.99	0.42
13:M:15:LYS:HB3	13:M:20:VAL:HG12	2.01	0.42
9:W:69:LYS:HD3	9:W:89:LEU:HD11	2.02	0.42
5:E:95:SER:O	5:E:99:ASN:HA	2.19	0.42
10:J:1:MET:HG2	10:J:2:ASP:H	1.85	0.42
11:K:37:ILE:HG23	11:K:60:GLY:HA2	2.01	0.42
13:M:53:ILE:HB	13:M:60:MET:HG3	2.02	0.42
2:P:50:LYS:HA	2:P:209:ARG:HH12	1.83	0.42
6:T:36:ILE:HG12	6:T:172:LEU:HD11	2.01	0.42
2:B:69:ASN:HB3	2:B:72:ILE:H	1.84	0.42
4:D:161:ALA:HB3	5:E:55:LEU:HD23	2.01	0.42
4:R:77:ALA:O	4:R:81:ILE:HG12	2.20	0.42
5:S:205:LEU:HD12	5:S:210:LEU:HD13	2.02	0.42
1:O:110:LEU:O	1:O:114:VAL:HG23	2.20	0.42
7:G:103:MET:CE	7:G:108:LEU:HD13	2.49	0.42
9:I:204:ASP:HB3	11:Y:193:VAL:HG11	2.02	0.42
5:S:68:HIS:HE1	5:S:102:LEU:O	2.03	0.42
6:F:14:ASP:OD1	6:F:14:ASP:N	2.49	0.42
9:I:141:ALA:HB2	9:I:177:ASP:HB2	2.02	0.42
5:E:205:LEU:HA	5:E:209:ASN:HD22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:8:PHE:HB3	8:H:151:ALA:HB2	2.02	0.41
8:H:49:ALA:HA	15:H:301:ONK:H29	2.03	0.41
11:K:114:TYR:O	11:K:121:ARG:HA	2.21	0.41
10:X:33:ASP:OD1	10:X:35:THR:HG22	2.20	0.41
1:A:38:LYS:HG3	1:A:43:VAL:HG22	2.02	0.41
2:B:51:VAL:O	2:B:52:THR:CB	2.68	0.41
1:A:176:GLU:HA	2:B:55:LEU:HD11	2.03	0.41
11:K:128:CYS:HB2	11:K:137:TYR:CE2	2.55	0.41
13:M:95:TYR:O	13:M:99:VAL:HG23	2.20	0.41
2:B:139:TYR:CD2	2:B:224:VAL:HG21	2.56	0.41
14:N:84:GLU:O	14:N:88:GLU:HB2	2.21	0.41
2:P:200:THR:HG22	2:P:202:SER:H	1.85	0.41
6:T:83:HIS:HD2	6:T:128:PHE:HE1	1.68	0.41
6:T:116:VAL:HG21	6:T:147:LEU:HD21	2.03	0.41
6:T:14:ASP:N	6:T:14:ASP:OD1	2.53	0.41
7:U:70:ILE:HD11	7:U:103:MET:O	2.21	0.41
1:A:204:PHE:CD1	1:A:209:ILE:HD11	2.55	0.41
5:S:38:ARG:NH1	5:S:39:SER:O	2.51	0.41
7:U:31:ILE:HG23	7:U:47:GLN:HB2	2.01	0.41
2:B:49:ARG:NH1	2:B:61:SER:OG	2.51	0.41
4:R:32:ILE:HD12	4:R:192:VAL:HG23	2.02	0.41
6:F:110:ASP:O	6:F:114:GLN:HG2	2.21	0.41
13:M:127:LEU:HG	13:M:142:LEU:HD12	2.03	0.41
1:O:119:GLN:O	1:O:122:THR:HB	2.20	0.41
9:W:37:ASN:ND2	9:W:37:ASN:H	2.19	0.41
4:D:71:SER:HB3	4:D:164:ILE:HD12	2.03	0.41
10:J:21:VAL:HG11	11:K:122:LEU:HD11	2.03	0.41
3:C:155:SER:HB2	4:D:51:LEU:HD21	2.02	0.41
3:C:35:LYS:HG2	3:C:158:SER:O	2.21	0.41
6:F:5:ASP:HB2	6:F:22:TYR:CE2	2.55	0.41
6:F:43:VAL:HG11	6:F:189:VAL:HA	2.03	0.41
8:H:113:ILE:HG12	8:H:119:THR:HG22	2.02	0.41
4:R:159:TYR:CE1	4:R:162:LYS:HD3	2.56	0.41
2:B:52:THR:HG21	2:B:209:ARG:CD	2.34	0.40
13:M:129:TYR:CE2	13:M:144:THR:HG22	2.56	0.40
9:W:24:CYS:SG	9:W:42:ILE:HG12	2.61	0.40
6:F:34:ILE:HG12	6:F:196:ILE:HD11	2.04	0.40
7:U:103:MET:HE3	7:U:108:LEU:HD13	2.03	0.40
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.56	0.40
8:H:49:ALA:HB2	15:H:301:ONK:H25	2.02	0.40
9:I:20:VAL:HG13	9:I:118:PRO:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:102:GLN:HB3	17:M:316:HOH:O	2.21	0.40
7:U:219:ALA:HB2	7:U:224:PHE:HD1	1.86	0.40
5:E:106:ARG:HE	5:E:106:ARG:HB3	1.73	0.40
6:F:117:GLN:HE21	6:F:117:GLN:HB3	1.73	0.40
13:M:16:TYR:CE2	13:M:170:VAL:HG22	2.56	0.40
5:S:70:GLY:HA3	5:S:221:PHE:CZ	2.57	0.40
6:T:83:HIS:HD2	6:T:128:PHE:CE1	2.39	0.40
8:V:162:GLY:O	8:V:166:ASP:HB3	2.22	0.40
9:W:9:GLY:HA3	9:W:41:LYS:HE2	2.03	0.40
13:M:194:ASN:HA	13:M:212:LEU:O	2.22	0.40
11:Y:37:ILE:HG23	11:Y:60:GLY:HA2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	245 (99%)	2 (1%)	1 (0%)	34	66
1	O	248/250 (99%)	243 (98%)	5 (2%)	0	100	100
2	B	242/244 (99%)	228 (94%)	12 (5%)	2 (1%)	19	49
2	P	242/244 (99%)	230 (95%)	10 (4%)	2 (1%)	19	49
3	C	239/241 (99%)	233 (98%)	5 (2%)	1 (0%)	34	66
3	Q	239/241 (99%)	231 (97%)	8 (3%)	0	100	100
4	D	240/242 (99%)	234 (98%)	5 (2%)	1 (0%)	34	66
4	R	240/242 (99%)	231 (96%)	8 (3%)	1 (0%)	34	66
5	E	231/233 (99%)	224 (97%)	7 (3%)	0	100	100
5	S	231/233 (99%)	225 (97%)	6 (3%)	0	100	100
6	F	242/244 (99%)	232 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	T	242/244 (99%)	229 (95%)	13 (5%)	0	100	100
7	G	241/243 (99%)	233 (97%)	7 (3%)	1 (0%)	34	66
7	U	241/243 (99%)	237 (98%)	3 (1%)	1 (0%)	34	66
8	H	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
8	V	220/222 (99%)	213 (97%)	7 (3%)	0	100	100
9	I	202/204 (99%)	198 (98%)	4 (2%)	0	100	100
9	W	202/204 (99%)	197 (98%)	5 (2%)	0	100	100
10	J	196/198 (99%)	188 (96%)	7 (4%)	1 (0%)	29	61
10	X	196/198 (99%)	188 (96%)	7 (4%)	1 (0%)	29	61
11	K	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
11	Y	210/212 (99%)	204 (97%)	6 (3%)	0	100	100
12	L	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
12	Z	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
13	M	231/233 (99%)	221 (96%)	9 (4%)	1 (0%)	34	66
13	a	231/233 (99%)	221 (96%)	9 (4%)	1 (0%)	34	66
14	N	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
14	b	194/196 (99%)	187 (96%)	6 (3%)	1 (0%)	29	61
All	All	6312/6368 (99%)	6111 (97%)	186 (3%)	15 (0%)	47	78

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	118	GLY
1	A	166	LYS
2	B	203	SER
2	P	203	SER
13	a	229	GLY
7	G	2	GLY
4	R	114	ARG
7	U	2	GLY
3	C	203	THR
13	M	229	GLY
10	J	9	VAL
2	B	231	PRO
2	P	51	VAL
14	b	114	PRO

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Mol	Chain	Res	Type
10	X	9	VAL

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%)	205 (98%)	4 (2%)	57	85
1	O	209/209 (100%)	201 (96%)	8 (4%)	33	67
2	B	203/203 (100%)	190 (94%)	13 (6%)	17	45
2	P	203/203 (100%)	194 (96%)	9 (4%)	28	61
3	C	213/213 (100%)	203 (95%)	10 (5%)	26	59
3	Q	213/213 (100%)	207 (97%)	6 (3%)	43	77
4	D	198/198 (100%)	191 (96%)	7 (4%)	36	70
4	R	198/198 (100%)	193 (98%)	5 (2%)	47	80
5	E	192/192 (100%)	181 (94%)	11 (6%)	20	50
5	S	192/192 (100%)	185 (96%)	7 (4%)	35	69
6	F	201/201 (100%)	191 (95%)	10 (5%)	24	56
6	T	201/201 (100%)	189 (94%)	12 (6%)	19	48
7	G	207/207 (100%)	194 (94%)	13 (6%)	18	46
7	U	207/207 (100%)	198 (96%)	9 (4%)	29	62
8	H	181/181 (100%)	176 (97%)	5 (3%)	43	77
8	V	181/181 (100%)	178 (98%)	3 (2%)	60	87
9	I	172/172 (100%)	169 (98%)	3 (2%)	60	87
9	W	172/172 (100%)	168 (98%)	4 (2%)	50	82
10	J	175/175 (100%)	169 (97%)	6 (3%)	37	71
10	X	175/175 (100%)	170 (97%)	5 (3%)	42	76
11	K	169/169 (100%)	163 (96%)	6 (4%)	35	69
11	Y	169/169 (100%)	163 (96%)	6 (4%)	35	69
12	L	185/185 (100%)	179 (97%)	6 (3%)	39	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	Z	185/185 (100%)	173 (94%)	12 (6%)	17	44
13	M	199/199 (100%)	191 (96%)	8 (4%)	31	65
13	a	199/199 (100%)	189 (95%)	10 (5%)	24	56
14	N	162/162 (100%)	157 (97%)	5 (3%)	40	74
14	b	162/162 (100%)	157 (97%)	5 (3%)	40	74
All	All	5332/5332 (100%)	5124 (96%)	208 (4%)	32	66

All (208) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	30	GLN
1	A	122	THR
1	A	157	PHE
2	B	50	LYS
2	B	51	VAL
2	B	52	THR
2	B	55	LEU
2	B	69	ASN
2	B	119	GLN
2	B	149	THR
2	B	155	ASN
2	B	184	LYS
2	B	186	ASP
2	B	191	LEU
2	B	200	THR
2	B	209	ARG
3	C	4	ARG
3	C	15	ILE
3	C	19	GLU
3	C	51	LYS
3	C	61	LYS
3	C	160	GLN
3	C	169	VAL
3	C	185	THR
3	C	193	THR
3	C	206	LYS
4	D	4	VAL
4	D	20	LEU
4	D	102	GLU

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Mol	Chain	Res	Type
4	D	124	ARG
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
5	E	8	ASP
5	E	9	THR
5	E	10	VAL
5	E	29	LYS
5	E	71	LEU
5	E	99	ASN
5	E	116	GLN
5	E	173	ARG
5	E	174	THR
5	E	184	ASN
5	E	231	LYS
6	F	39	ASN
6	F	117	GLN
6	F	123	ASN
6	F	165	ARG
6	F	166	GLN
6	F	172	LEU
6	F	181	GLU
6	F	186	ARG
6	F	201	GLU
6	F	214	TRP
7	G	34	LEU
7	G	68	ARG
7	G	83	ASN
7	G	115	LEU
7	G	120	THR
7	G	154	TYR
7	G	166	GLN
7	G	169	ILE
7	G	201	MET
7	G	207	THR
7	G	221	LYS
7	G	235	ARG
7	G	236	LEU
8	H	20	SER
8	H	22	GLN
8	H	34	LEU
8	H	68	LEU

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Mol	Chain	Res	Type
8	H	156	SER
9	I	81	ILE
9	I	171	LEU
9	I	182	TRP
10	J	35	THR
10	J	71	GLU
10	J	78	GLN
10	J	161	LEU
10	J	174	MET
10	J	196	GLN
11	K	4	LEU
11	K	9	GLN
11	K	65	LEU
11	K	107	LYS
11	K	112	ILE
11	K	148	LEU
12	L	3	ASN
12	L	23	LEU
12	L	49	ASN
12	L	109	THR
12	L	165	ASN
12	L	176	SER
13	M	12	ILE
13	M	35	ARG
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	159	VAL
13	M	161	ARG
13	M	226	LYS
14	N	83	LYS
14	N	107	LYS
14	N	119	VAL
14	N	126	ILE
14	N	178	LEU
1	O	1	MET
1	O	30	GLN
1	O	62	SER
1	O	122	THR
1	O	133	SER
1	O	157	PHE
1	O	239	THR

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Mol	Chain	Res	Type
1	O	250	LEU
2	P	55	LEU
2	P	62	THR
2	P	69	ASN
2	P	119	GLN
2	P	149	THR
2	P	184	LYS
2	P	191	LEU
2	P	200	THR
2	P	212	PHE
3	Q	4	ARG
3	Q	51	LYS
3	Q	61	LYS
3	Q	147	GLN
3	Q	203	THR
3	Q	206	LYS
4	R	4	VAL
4	R	143	ASP
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
5	S	8	ASP
5	S	9	THR
5	S	29	LYS
5	S	71	LEU
5	S	92	ASN
5	S	184	ASN
5	S	231	LYS
6	T	31	THR
6	T	39	ASN
6	T	117	GLN
6	T	123	ASN
6	T	130	VAL
6	T	165	ARG
6	T	166	GLN
6	T	181	GLU
6	T	186	ARG
6	T	203	ASN
6	T	214	TRP
6	T	243	ILE
7	U	83	ASN
7	U	115	LEU

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Mol	Chain	Res	Type
7	U	154	TYR
7	U	166	GLN
7	U	201	MET
7	U	207	THR
7	U	221	LYS
7	U	235	ARG
7	U	243	ASP
8	V	30	ASN
8	V	68	LEU
8	V	144	GLN
9	W	37	ASN
9	W	81	ILE
9	W	171	LEU
9	W	182	TRP
10	X	71	GLU
10	X	78	GLN
10	X	127	GLU
10	X	136	SER
10	X	174	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	99	THR
11	Y	106	ARG
11	Y	148	LEU
11	Y	209	ASN
12	Z	3	ASN
12	Z	23	LEU
12	Z	49	ASN
12	Z	62	ASP
12	Z	80	ASN
12	Z	109	THR
12	Z	126	ASP
12	Z	150	LEU
12	Z	165	ASN
12	Z	169	LYS
12	Z	172	LEU
12	Z	173	LYS
13	a	10	SER
13	a	12	ILE
13	a	48	ASN
13	a	70	LEU
13	a	82	ASP

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Mol	Chain	Res	Type
13	a	104	ARG
13	a	159	VAL
13	a	161	ARG
13	a	170	VAL
13	a	226	LYS
14	b	36	ARG
14	b	83	LYS
14	b	105	LYS
14	b	126	ILE
14	b	178	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (153) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	94	HIS
1	A	190	HIS
2	B	20	GLN
2	B	69	ASN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
3	C	17	GLN
3	C	77	ASN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
3	C	176	ASN
3	C	236	GLN
4	D	15	GLN
4	D	91	HIS
4	D	100	ASN
4	D	160	ASN
4	D	198	GLN
4	D	225	ASN
5	E	30	GLN
5	E	68	HIS
5	E	99	ASN
5	E	116	GLN
5	E	120	GLN

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Mol	Chain	Res	Type
5	E	184	ASN
5	E	198	GLN
6	F	19	GLN
6	F	39	ASN
6	F	83	HIS
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	179	HIS
6	F	200	HIS
6	F	203	ASN
7	G	6	HIS
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	167	GLN
7	G	175	ASN
8	H	30	ASN
8	H	66	HIS
8	H	165	ASN
8	H	172	ASN
8	H	189	ASN
9	I	88	GLN
9	I	156	ASN
10	J	55	GLN
10	J	86	GLN
10	J	118	GLN
10	J	146	HIS
10	J	147	HIS
10	J	196	GLN
11	K	85	ASN
11	K	133	GLN
11	K	143	ASN
11	K	176	ASN
11	K	209	ASN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	79	HIS
12	L	80	ASN

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Mol	Chain	Res	Type
12	L	158	ASN
12	L	165	ASN
12	L	195	HIS
13	M	2	GLN
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	108	ASN
13	M	171	GLN
13	M	179	ASN
14	N	60	GLN
14	N	161	GLN
1	O	94	HIS
2	P	20	GLN
2	P	69	ASN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	155	ASN
3	Q	17	GLN
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
4	R	160	ASN
4	R	210	GLN
4	R	225	ASN
5	S	68	HIS
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	184	ASN
5	S	198	GLN
6	T	19	GLN
6	T	39	ASN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN

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Mol	Chain	Res	Type
6	T	191	GLN
7	U	6	HIS
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	175	ASN
7	U	186	ASN
8	V	30	ASN
8	V	144	GLN
8	V	165	ASN
8	V	172	ASN
8	V	189	ASN
9	W	37	ASN
9	W	71	ASN
10	X	55	GLN
10	X	86	GLN
10	X	118	GLN
10	X	147	HIS
10	X	191	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	143	ASN
11	Y	176	ASN
11	Y	209	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	79	HIS
12	Z	80	ASN
12	Z	195	HIS
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN
13	a	179	ASN
13	a	194	ASN
13	a	213	GLN
14	b	38	HIS
14	b	161	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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
15	ONK	H	301	8	34,35,35	0.34	0	40,46,46	0.64	0
16	VNK	Y	301	11	35,35,35	0.50	1 (2%)	42,46,46	1.28	3 (7%)
16	VNK	b	301	14	35,35,35	0.47	0	42,46,46	0.90	1 (2%)
16	VNK	N	301	14	35,35,35	0.59	1 (2%)	42,46,46	0.95	2 (4%)
16	VNK	K	301	11	35,35,35	0.46	0	42,46,46	1.19	1 (2%)
15	ONK	V	301	8	34,35,35	0.33	0	40,46,46	0.86	2 (5%)

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
15	ONK	H	301	8	-	11/50/50/50	-
16	VNK	Y	301	11	-	20/50/50/50	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	VNK	b	301	14	-	13/50/50/50	-
16	VNK	N	301	14	-	16/50/50/50	-
16	VNK	K	301	11	-	18/50/50/50	-
15	ONK	V	301	8	-	11/50/50/50	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	N	301	VNK	C17-C16	2.39	1.56	1.53
16	Y	301	VNK	C17-C16	2.03	1.56	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Y	301	VNK	C12-C11-N3	-6.34	101.98	110.18
16	K	301	VNK	C12-C11-N3	-5.63	102.91	110.18
16	b	301	VNK	C12-C11-N3	-4.18	104.78	110.18
16	N	301	VNK	C13-C12-C11	3.75	123.32	115.84
15	V	301	ONK	C8-C7-C6	-2.30	108.86	113.16
15	V	301	ONK	C12-C11-N3	-2.13	107.43	110.18
16	Y	301	VNK	C18-C17-C23	-2.06	104.83	110.59
16	N	301	VNK	C2-N1-C1	2.02	125.70	121.83
16	Y	301	VNK	C3-C2-N1	-2.01	106.46	111.43

There are no chirality outliers.

All (89) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	H	301	ONK	C8-C9-N5-C24
15	H	301	ONK	C8-C9-N5-C25
15	H	301	ONK	O7-C9-N5-C24
15	H	301	ONK	O7-C9-N5-C25
15	H	301	ONK	N3-C11-C12-C13
16	Y	301	VNK	C8-C9-N5-C24
16	Y	301	VNK	C8-C9-N5-C25
16	Y	301	VNK	O7-C9-N5-C24
16	Y	301	VNK	O7-C9-N5-C25
16	Y	301	VNK	C16-C11-C12-C13
16	Y	301	VNK	C11-C16-C17-C23
16	Y	301	VNK	C11-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
16	Y	301	VNK	O6-C16-C17-C23
16	b	301	VNK	C8-C9-N5-C24
16	b	301	VNK	C8-C9-N5-C25
16	b	301	VNK	O7-C9-N5-C24
16	b	301	VNK	O7-C9-N5-C25
16	b	301	VNK	C16-C11-C12-C13
16	b	301	VNK	C11-C16-C17-C23
16	N	301	VNK	C8-C9-N5-C24
16	N	301	VNK	C8-C9-N5-C25
16	N	301	VNK	O7-C9-N5-C24
16	N	301	VNK	O7-C9-N5-C25
16	N	301	VNK	C12-C11-C16-O6
16	N	301	VNK	C12-C11-C16-C17
16	N	301	VNK	C11-C16-C17-C23
16	N	301	VNK	C11-C16-C17-C18
16	N	301	VNK	O6-C16-C17-C23
16	N	301	VNK	O6-C16-C17-C18
16	K	301	VNK	C5-C2-C3-C26
16	K	301	VNK	C8-C9-N5-C24
16	K	301	VNK	C8-C9-N5-C25
16	K	301	VNK	O7-C9-N5-C24
16	K	301	VNK	O7-C9-N5-C25
16	K	301	VNK	N3-C11-C12-C13
16	K	301	VNK	C16-C11-C12-C13
16	K	301	VNK	C11-C16-C17-C23
16	K	301	VNK	C11-C16-C17-C18
16	K	301	VNK	O6-C16-C17-C23
15	V	301	ONK	N3-C11-C12-C13
15	V	301	ONK	C16-C11-C12-C13
16	K	301	VNK	N1-C2-C3-C26
16	Y	301	VNK	C1-C27-C28-C29
16	b	301	VNK	C1-C27-C28-C29
15	V	301	ONK	C1-C27-C28-C29
16	Y	301	VNK	C5-C2-C3-C26
16	K	301	VNK	C5-C2-C3-C4
16	K	301	VNK	N1-C2-C3-C4
15	V	301	ONK	N2-C6-C7-C8
16	N	301	VNK	C1-C27-C28-C29
15	V	301	ONK	C10-C6-C7-C8
16	Y	301	VNK	C6-C7-C8-C9
15	V	301	ONK	C6-C7-C8-C9
16	Y	301	VNK	O6-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
16	b	301	VNK	O6-C16-C17-C23
16	K	301	VNK	O6-C16-C17-C18
16	Y	301	VNK	C5-C2-C3-C4
16	K	301	VNK	C6-C7-C8-C9
16	Y	301	VNK	C27-C28-C29-C30
15	H	301	ONK	C6-C7-C8-C9
15	H	301	ONK	C11-C12-C13-C15
16	Y	301	VNK	N1-C2-C3-C26
15	V	301	ONK	C27-C28-C29-C30
15	V	301	ONK	C11-C12-C13-C15
16	Y	301	VNK	N1-C2-C3-C4
16	N	301	VNK	C28-C29-C30-C31
15	V	301	ONK	C28-C29-C30-C31
16	N	301	VNK	C11-C12-C13-C14
16	b	301	VNK	O6-C16-C17-C18
15	H	301	ONK	N2-C6-C7-C8
16	Y	301	VNK	N3-C11-C12-C13
16	b	301	VNK	N3-C11-C12-C13
16	N	301	VNK	C12-C11-N3-C10
16	N	301	VNK	N3-C11-C16-O6
16	b	301	VNK	C11-C16-C17-C18
16	N	301	VNK	N3-C11-C16-C17
15	H	301	ONK	C16-C11-C12-C13
15	H	301	ONK	C27-C28-C29-C30
16	K	301	VNK	C7-C8-C9-O7
16	K	301	VNK	O2-C10-C6-N2
16	Y	301	VNK	O2-C10-C6-N2
16	b	301	VNK	O2-C10-C6-N2
15	H	301	ONK	C28-C29-C30-C31
16	Y	301	VNK	C28-C29-C30-C31
15	V	301	ONK	O7-C9-N5-C25
16	b	301	VNK	N3-C10-C6-N2
16	Y	301	VNK	N3-C10-C6-N2
15	V	301	ONK	O7-C9-N5-C24
16	K	301	VNK	N3-C10-C6-N2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

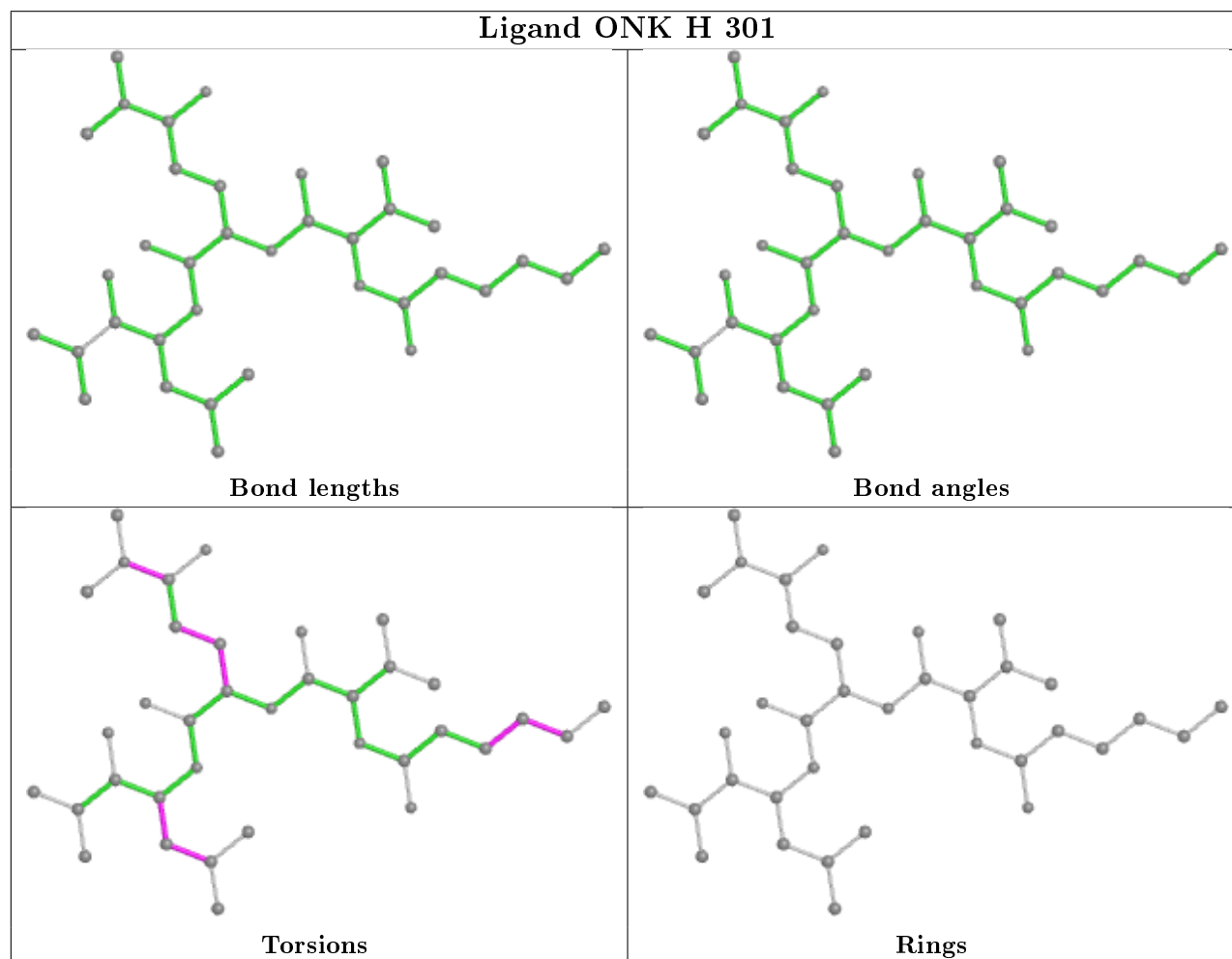
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	H	301	ONK	2	0
16	N	301	VNK	2	0

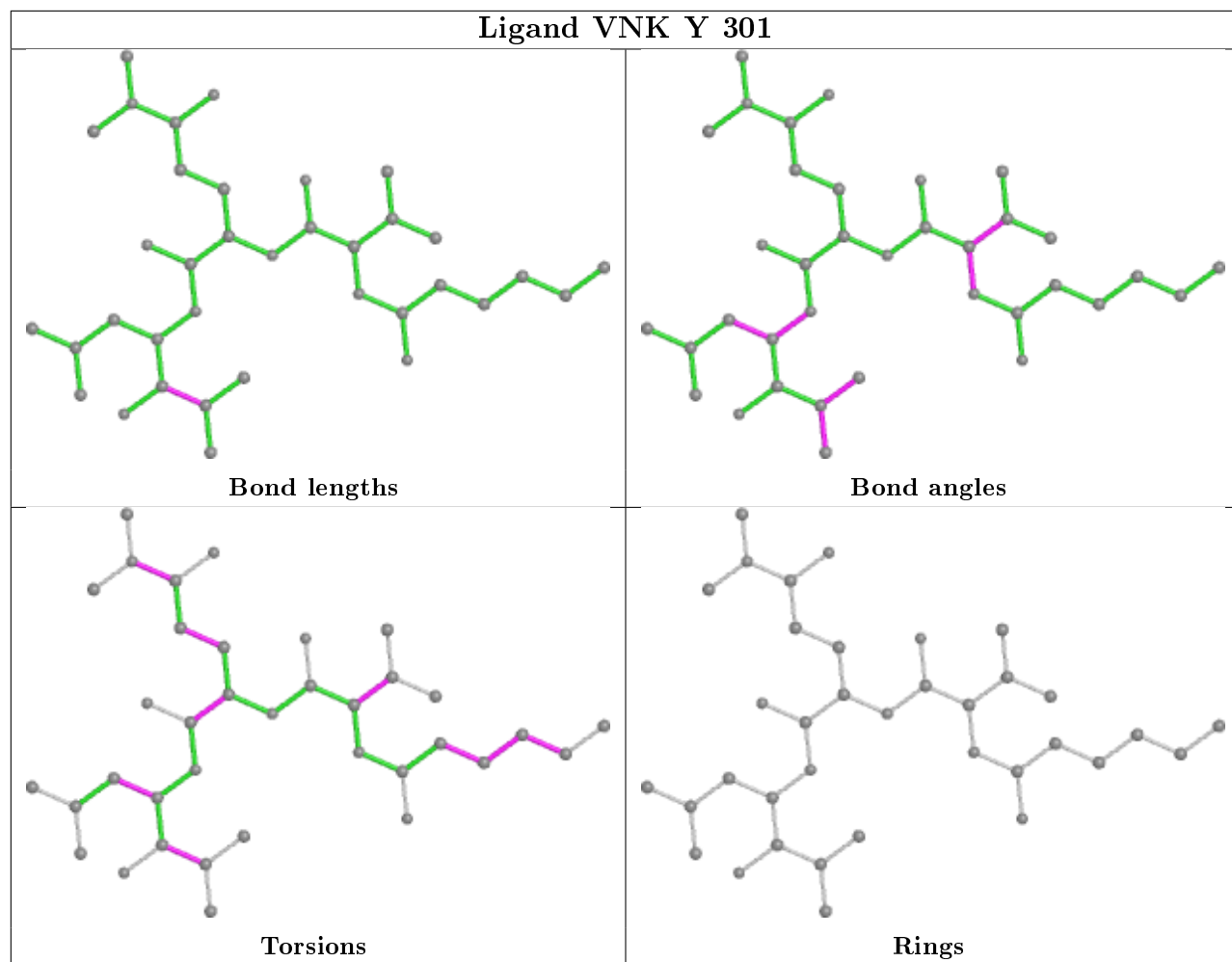
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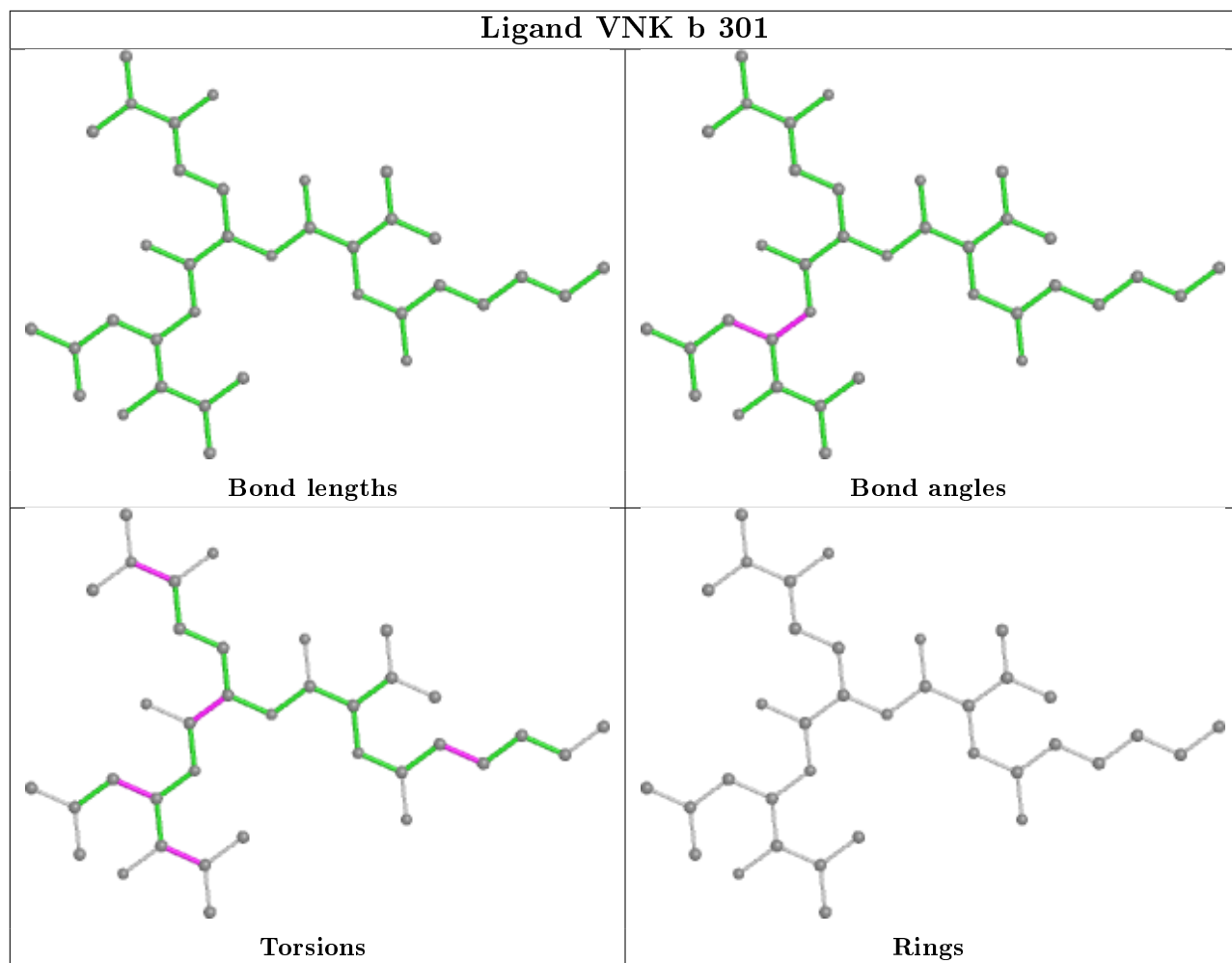
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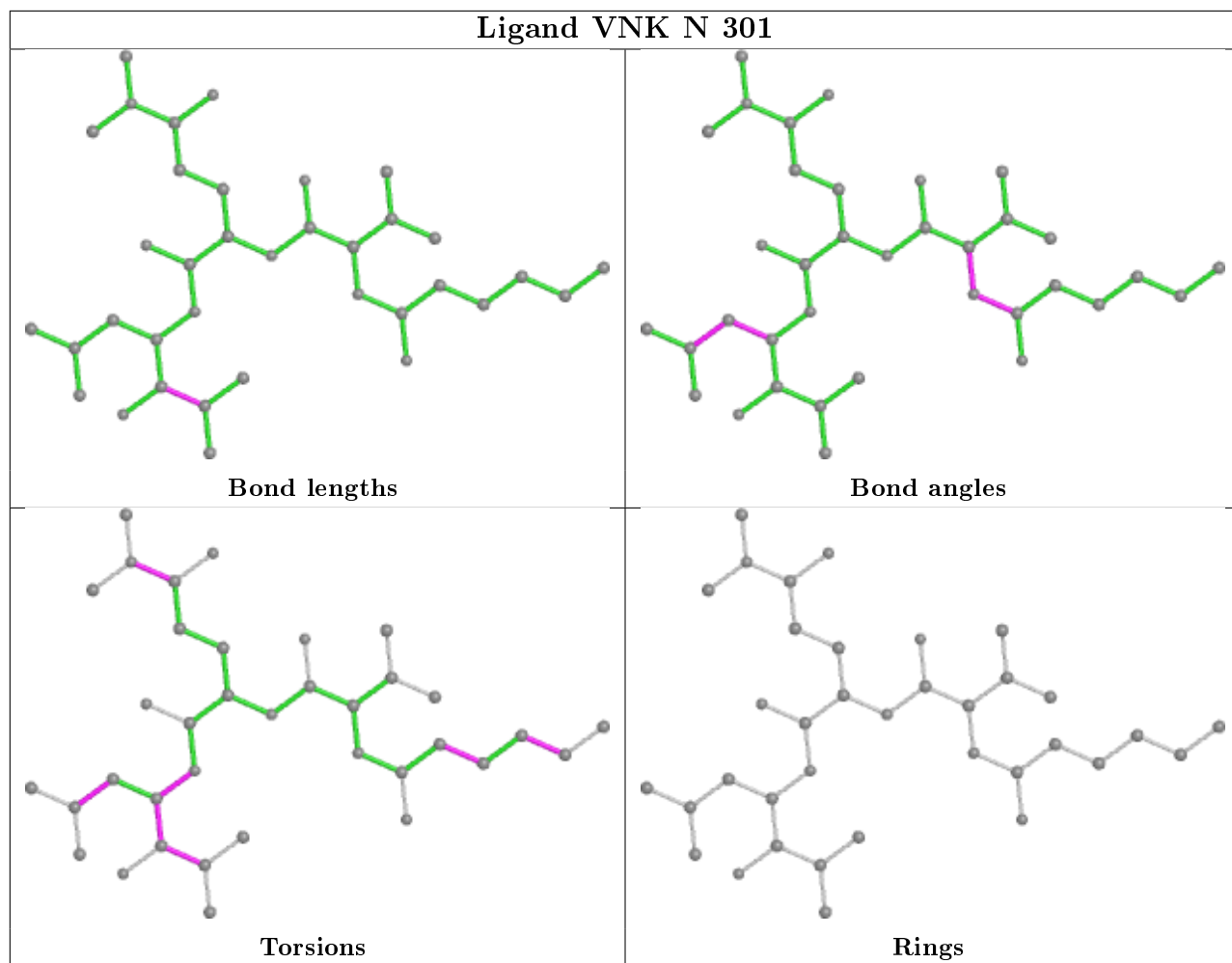
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	K	301	VNK	1	0

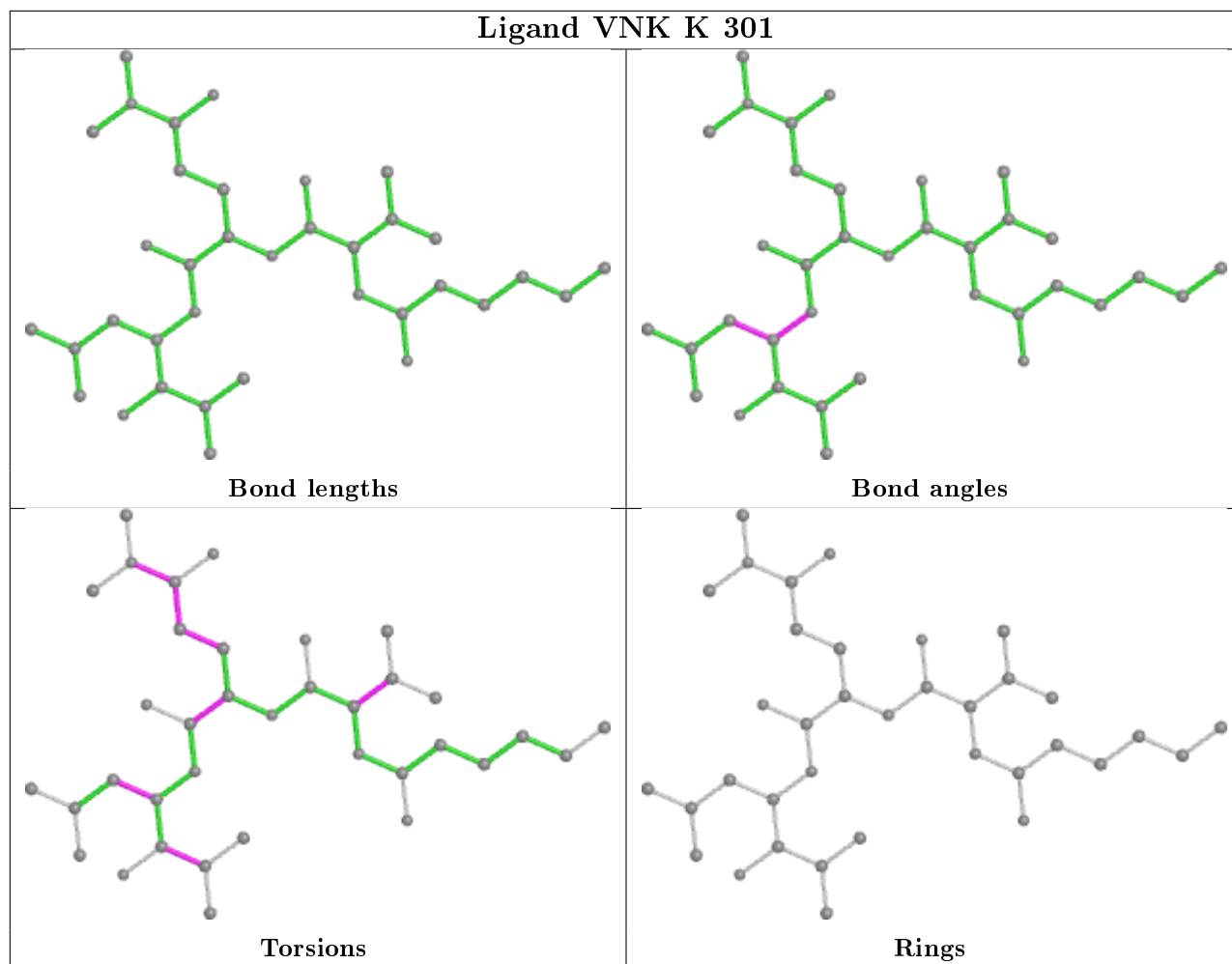
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

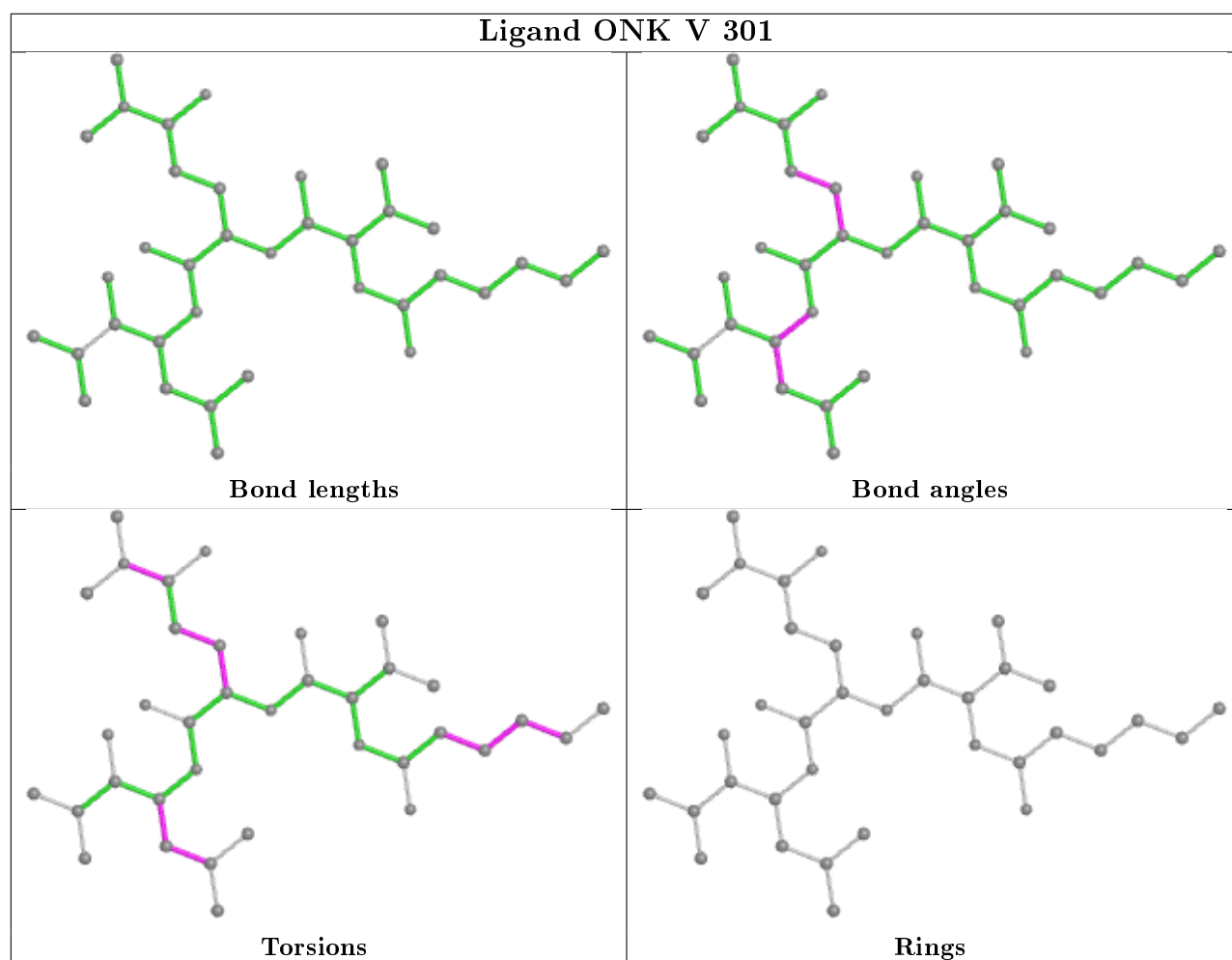












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/250 (100%)	-0.34	4 (1%) 72 66	44, 62, 91, 106	0
1	O	250/250 (100%)	-0.36	5 (2%) 65 56	25, 64, 94, 111	0
2	B	244/244 (100%)	-0.24	4 (1%) 72 66	43, 62, 99, 115	0
2	P	244/244 (100%)	-0.14	6 (2%) 57 47	49, 66, 98, 113	0
3	C	241/241 (100%)	-0.21	7 (2%) 51 41	44, 65, 104, 137	0
3	Q	241/241 (100%)	0.10	15 (6%) 20 13	54, 79, 121, 155	0
4	D	242/242 (100%)	-0.28	5 (2%) 63 54	51, 67, 91, 114	0
4	R	242/242 (100%)	-0.16	7 (2%) 51 41	58, 73, 100, 126	0
5	E	233/233 (100%)	-0.20	5 (2%) 63 54	56, 73, 98, 106	0
5	S	233/233 (100%)	-0.08	4 (1%) 70 63	58, 78, 105, 114	0
6	F	244/244 (100%)	-0.29	2 (0%) 86 81	48, 70, 98, 125	0
6	T	244/244 (100%)	-0.19	4 (1%) 72 66	48, 67, 99, 125	0
7	G	243/243 (100%)	-0.31	3 (1%) 79 73	47, 65, 93, 116	0
7	U	243/243 (100%)	-0.38	2 (0%) 86 81	46, 62, 88, 108	0
8	H	222/222 (100%)	-0.37	2 (0%) 84 80	45, 58, 77, 95	0
8	V	222/222 (100%)	-0.41	2 (0%) 84 80	44, 58, 76, 100	0
9	I	204/204 (100%)	-0.40	1 (0%) 91 88	40, 52, 75, 81	0
9	W	204/204 (100%)	-0.40	1 (0%) 91 88	41, 53, 75, 82	0
10	J	198/198 (100%)	-0.35	3 (1%) 73 68	41, 54, 77, 99	0
10	X	198/198 (100%)	-0.41	4 (2%) 65 56	44, 55, 77, 97	0
11	K	212/212 (100%)	-0.48	2 (0%) 84 80	38, 52, 73, 81	0
11	Y	212/212 (100%)	-0.46	0 100 100	41, 55, 77, 85	0
12	L	222/222 (100%)	-0.50	0 100 100	39, 56, 72, 81	0
12	Z	222/222 (100%)	-0.42	0 100 100	40, 57, 78, 89	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/233 (100%)	-0.42	2 (0%) 84 80	42, 58, 79, 95	0
13	a	233/233 (100%)	-0.49	1 (0%) 92 91	39, 56, 77, 91	0
14	N	196/196 (100%)	-0.46	1 (0%) 91 88	45, 54, 76, 82	0
14	b	196/196 (100%)	-0.38	0 100 100	44, 53, 75, 82	0
All	All	6368/6368 (100%)	-0.32	92 (1%) 75 70	25, 61, 96, 155	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	219	ALA	7.0
1	A	1	MET	6.5
6	T	1	GLY	6.3
2	P	220	ASN	6.0
4	D	120	SER	5.9
6	F	1	GLY	5.8
4	R	120	SER	5.7
10	J	198	GLN	5.7
4	R	121	GLY	5.7
2	B	220	ASN	5.2
4	D	118	GLY	5.0
10	X	197	ALA	5.0
4	D	119	ALA	4.7
7	G	1	ALA	4.5
10	J	197	ALA	4.3
4	R	118	GLY	4.3
2	P	219	ALA	4.3
8	H	221	CYS	4.3
7	U	1	ALA	4.2
6	T	2	THR	4.2
7	G	243	ASP	4.2
4	D	121	GLY	4.2
4	R	119	ALA	4.2
3	Q	241	GLN	4.1
10	X	198	GLN	4.1
3	Q	48	SER	4.0
5	S	1	PHE	4.0
13	M	1	THR	3.9
10	J	196	GLN	3.7
3	Q	49	THR	3.6
13	M	233	ILE	3.6
4	D	125	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
2	P	51	VAL	3.5
3	Q	50	LEU	3.3
3	Q	239	GLN	3.3
7	U	243	ASP	3.2
3	Q	203	THR	3.2
2	P	61	SER	3.2
1	O	1	MET	3.2
3	Q	234	ILE	3.1
9	I	1	SER	3.1
3	C	241	GLN	3.0
3	C	49	THR	3.0
5	E	233	ILE	3.0
3	Q	206	LYS	3.0
8	V	222	ASP	3.0
3	Q	238	LYS	2.9
1	A	250	LEU	2.8
2	B	51	VAL	2.8
5	E	1	PHE	2.8
7	G	242	GLN	2.8
3	Q	235	GLU	2.7
2	B	221	ASP	2.7
8	H	222	ASP	2.7
3	C	50	LEU	2.6
3	C	205	ALA	2.6
3	Q	205	ALA	2.5
1	O	2	THR	2.5
3	C	206	LYS	2.5
3	Q	180	LYS	2.5
3	Q	51	LYS	2.5
10	X	194	ASP	2.5
2	P	60	THR	2.5
2	P	218	GLY	2.5
13	a	1	THR	2.5
3	Q	202	GLN	2.4
1	A	2	THR	2.4
11	K	212	GLY	2.4
8	V	221	CYS	2.4
5	E	202	ASP	2.4
14	N	195	GLN	2.4
3	Q	240	GLU	2.3
5	S	202	ASP	2.3
4	R	228	THR	2.3

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Mol	Chain	Res	Type	RSRZ
6	T	244	ASN	2.3
5	E	207	VAL	2.3
9	W	1	SER	2.3
6	F	202	ASP	2.2
1	O	201	GLU	2.2
1	O	250	LEU	2.2
1	O	248	GLU	2.2
11	K	147	ASP	2.2
4	R	124	ARG	2.1
6	T	241	LYS	2.1
5	S	2	ARG	2.1
10	X	196	GLN	2.1
3	C	234	ILE	2.1
1	A	231	LYS	2.1
4	R	113	LEU	2.1
5	E	173	ARG	2.0
3	C	203	THR	2.0
5	S	204	SER	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

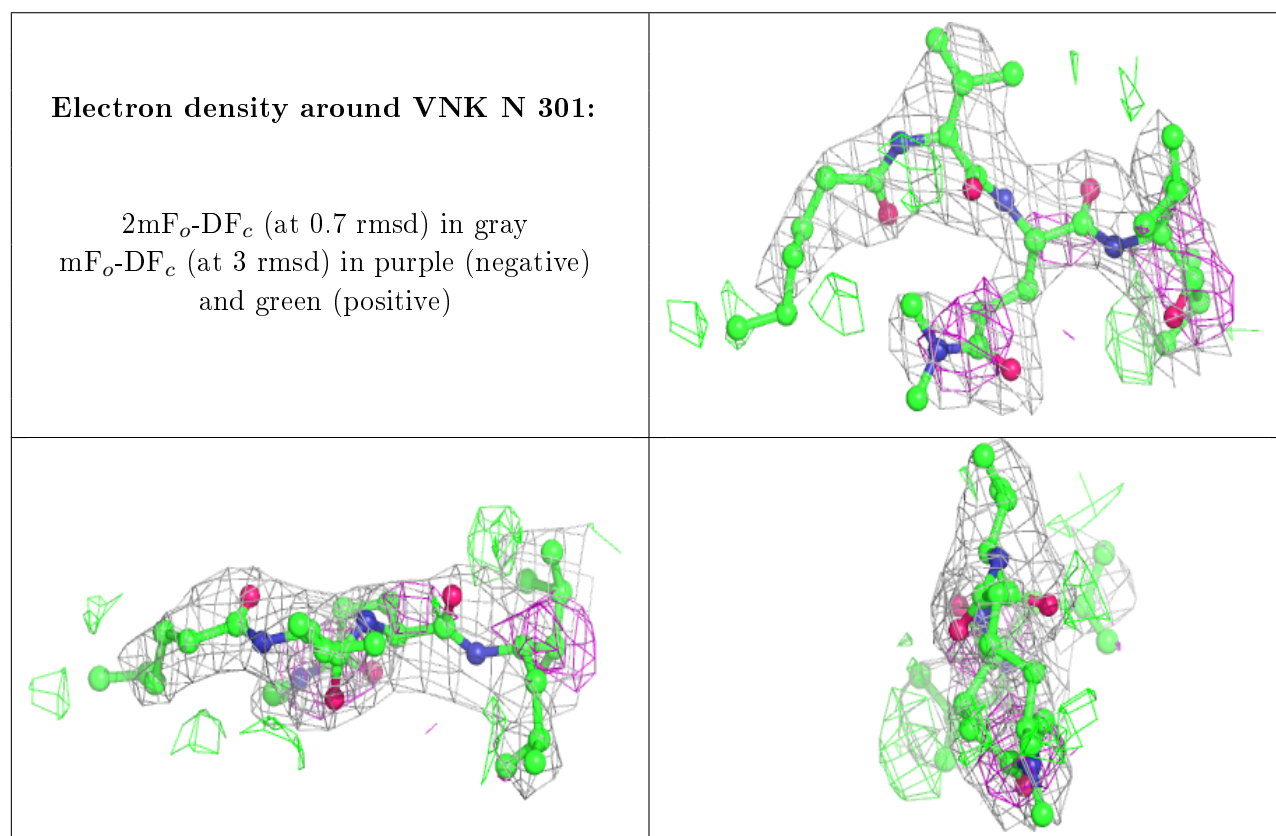
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
16	VNK	N	301	36/36	0.89	0.27	56,67,72,73	0
16	VNK	b	301	36/36	0.90	0.29	56,67,72,72	0
15	ONK	H	301	36/36	0.92	0.20	53,55,60,60	0
15	ONK	V	301	36/36	0.93	0.23	53,55,59,59	0
16	VNK	K	301	36/36	0.94	0.19	43,47,53,54	0

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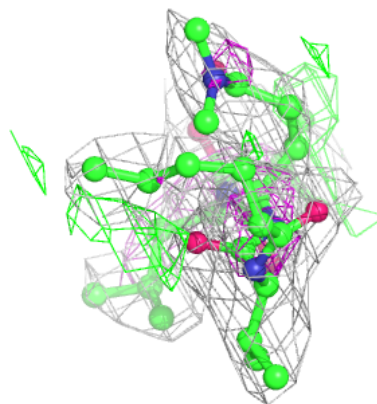
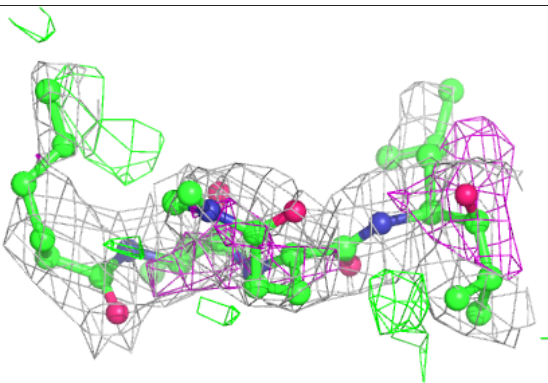
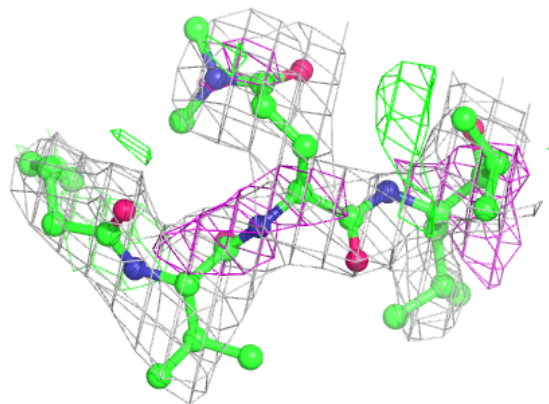
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
16	VNK	Y	301	36/36	0.94	0.19	43,49,54,55	0

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.

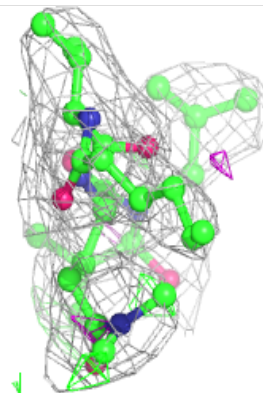
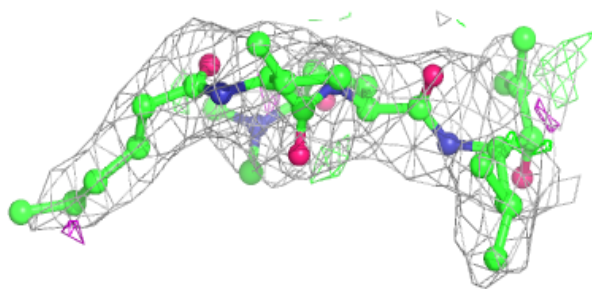
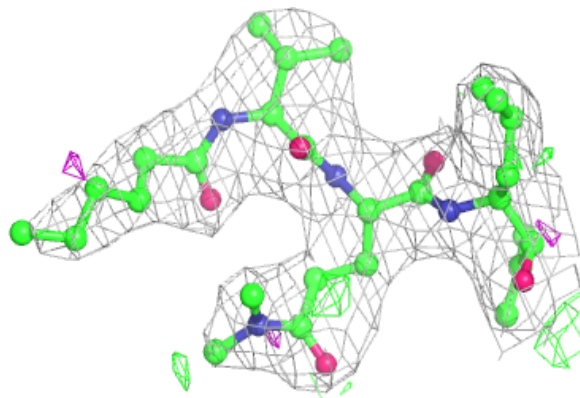


Electron density around VNK b 301:

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

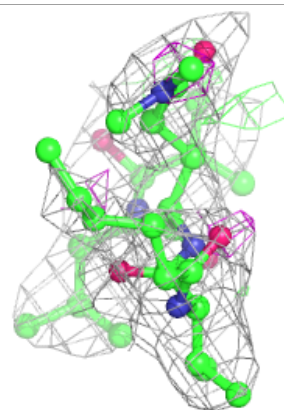
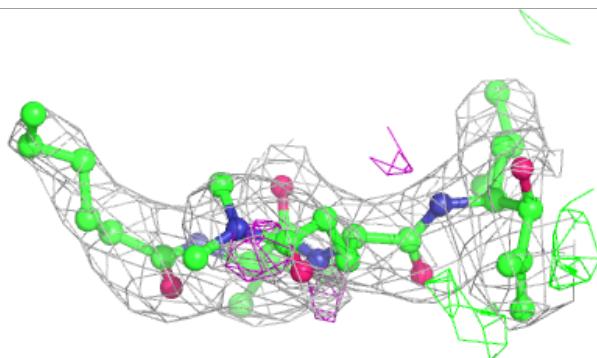
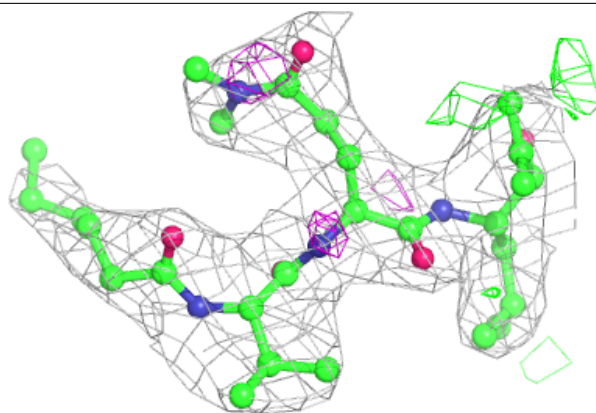
**Electron density around ONK H 301:**

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

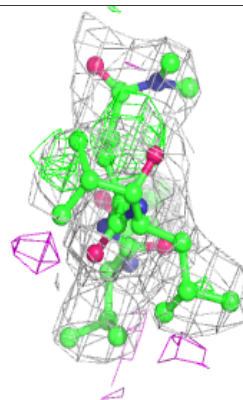
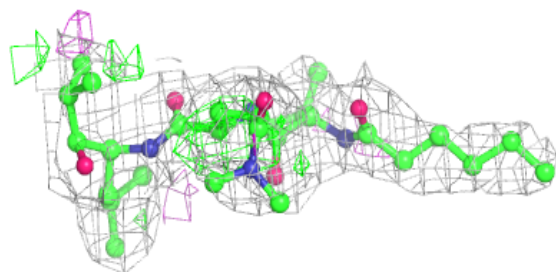
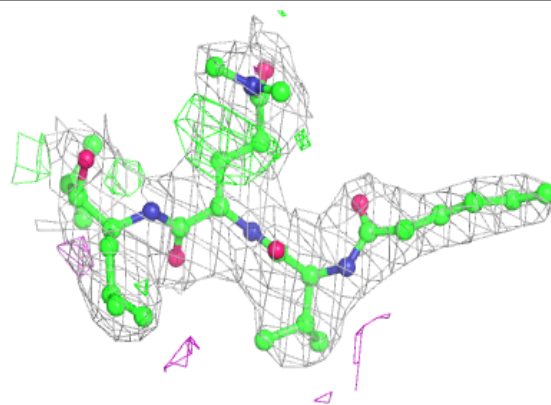


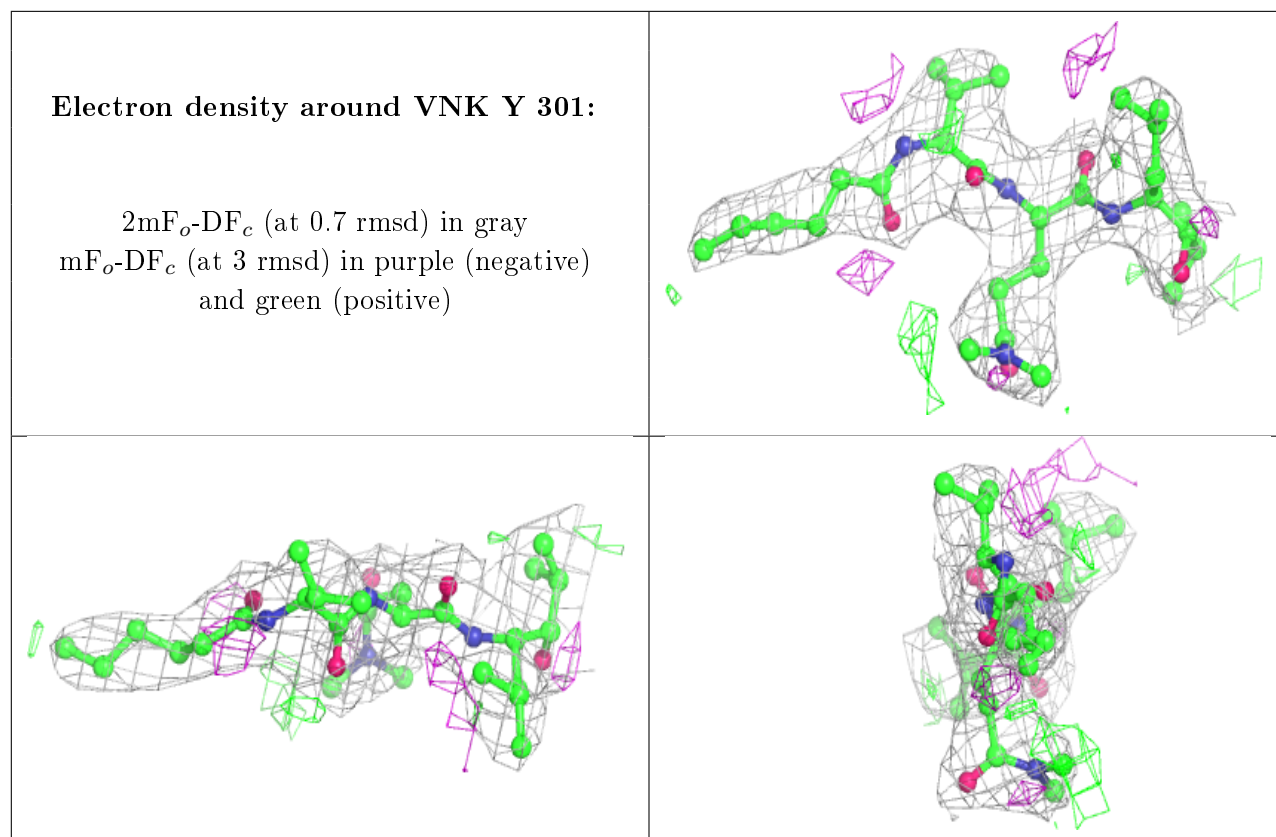
Electron density around ONK V 301:

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

**Electron density around VNK K 301:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.