Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 06:22 PM EDT

PDB ID	:	4R67
Title	:	Human constitutive 20S proteasome in complex with carfilzomib
Authors	:	Sacchettini, J.C.; Harshbarger, W.H.
Deposited on	:	2014-08-22
Resolution	:	2.89 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

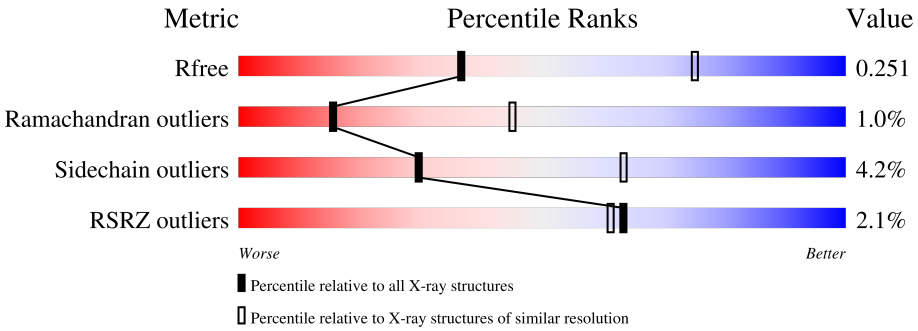
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.89 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	244	2% 94% 6%
1	O	244	2% 95% 5%
1	c	244	3% 95% 5%
1	q	244	2% 94% 5%
2	B	233	2% 97% .
2	P	233	3% 97% .

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Mol	Chain	Length	Quality of chain
2	d	233	2% 97%
2	r	233	2% 97%
3	C	250	4% 97%
3	Q	250	4% 97%
3	e	250	3% 97%
3	s	250	5% 97%
4	D	243	5% 94% 6%
4	R	243	4% 93% 6%
4	f	243	3% 95% 5%
4	t	243	6% 94% 6%
5	E	234	2% 96%
5	S	234	2% 96%
5	g	234	95% 5%
5	u	234	% 95% 5%
6	F	238	2% 97%
6	T	238	4% 96%
6	h	238	3% 97%
6	v	238	3% 96%
7	G	245	3% 96%
7	U	245	3% 97%
7	i	245	5% 96%
7	w	245	4% 97%
8	H	202	2% 97%
8	V	202	97%
8	j	202	3% 97%

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Mol	Chain	Length	Quality of chain
8	x	202	2% 97%
9	I	220	97%
9	W	220	97%
9	k	220	% 97%
9	y	220	97%
10	J	204	92% 8%
10	X	204	% 93% 7%
10	l	204	% 93% 7%
10	z	204	93% 7%
11	0	199	2% 95% 5%
11	K	199	2% 95% 5%
11	Y	199	2% 95% 5%
11	m	199	2% 95% 5%
12	3	201	96%
12	L	201	96%
12	Z	201	97%
12	n	201	2% 96%
13	1	213	2% 98%
13	M	213	% 98%
13	a	213	97%
13	o	213	98%
14	2	217	% 94% 6%
14	N	217	94% 6%
14	b	217	% 94% 6%
14	p	217	% 94% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	3BV	H	301	-	-	-	X
15	3BV	V	301	-	-	-	X

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 96005 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-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	0	0
			1842	1170	309	350	13			
1	O	244	Total	C	N	O	S	0	0	0
			1845	1171	309	352	13			
1	c	244	Total	C	N	O	S	0	0	0
			1842	1170	309	350	13			
1	q	244	Total	C	N	O	S	0	0	0
			1842	1170	309	350	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	233	Total	C	N	O	S	0	0	0
			1713	1087	287	334	5			
2	P	233	Total	C	N	O	S	0	0	0
			1712	1085	287	334	6			
2	d	233	Total	C	N	O	S	0	0	0
			1710	1083	287	334	6			
2	r	233	Total	C	N	O	S	0	0	0
			1716	1090	287	334	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	250	Total	C	N	O	S	0	0	0
			1902	1195	329	370	8			
3	Q	250	Total	C	N	O	S	0	0	0
			1902	1195	329	370	8			
3	e	250	Total	C	N	O	S	0	0	0
			1902	1195	329	370	8			
3	s	250	Total	C	N	O	S	0	0	0
			1902	1195	329	370	8			

- Molecule 4 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	243	Total	C	N	O	S	0	0	0
			1684	1041	310	329	4			
4	R	243	Total	C	N	O	S	0	0	0
			1698	1053	312	329	4			
4	f	243	Total	C	N	O	S	0	0	0
			1668	1033	308	323	4			
4	t	243	Total	C	N	O	S	0	0	0
			1672	1035	309	324	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	234	Total	C	N	O	S	0	0	0
			1759	1102	290	356	11			
5	S	234	Total	C	N	O	S	0	0	0
			1759	1102	290	356	11			
5	g	234	Total	C	N	O	S	0	0	0
			1759	1102	290	356	11			
5	u	234	Total	C	N	O	S	0	0	0
			1763	1105	291	356	11			

- Molecule 6 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	238	Total	C	N	O	S	0	0	0
			1850	1159	334	346	11			
6	T	238	Total	C	N	O	S	0	0	0
			1850	1159	334	346	11			
6	h	238	Total	C	N	O	S	0	0	0
			1850	1159	334	346	11			
6	v	238	Total	C	N	O	S	0	0	0
			1850	1159	334	346	11			

- Molecule 7 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	245	Total	C	N	O	S	0	0	0
			1885	1195	319	360	11			
7	U	245	Total	C	N	O	S	0	0	0
			1885	1195	319	360	11			
7	i	245	Total	C	N	O	S	0	0	0
			1885	1195	319	360	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	w	245	Total	C	N	O	S	0	0	0
			1885	1195	319	360	11			

- Molecule 8 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	202	Total	C	N	O	S	0	0	0
			1509	945	258	294	12			
8	V	202	Total	C	N	O	S	0	0	0
			1509	945	258	294	12			
8	j	202	Total	C	N	O	S	0	0	0
			1509	945	258	294	12			
8	x	202	Total	C	N	O	S	0	0	0
			1509	945	258	294	12			

- Molecule 9 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	220	Total	C	N	O	S	0	0	0
			1643	1033	280	318	12			
9	W	220	Total	C	N	O	S	0	0	0
			1643	1033	280	318	12			
9	k	220	Total	C	N	O	S	0	0	0
			1643	1033	280	318	12			
9	y	220	Total	C	N	O	S	0	0	0
			1647	1035	280	320	12			

- Molecule 10 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	204	Total	C	N	O	S	0	0	0
			1585	1010	262	294	19			
10	X	204	Total	C	N	O	S	0	0	0
			1585	1010	262	294	19			
10	l	204	Total	C	N	O	S	0	0	0
			1585	1010	262	294	19			
10	z	204	Total	C	N	O	S	0	0	0
			1585	1010	262	294	19			

- Molecule 11 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	199	Total	C	N	O	S	0	0	0
			1570	1006	265	290	9			
11	Y	199	Total	C	N	O	S	0	0	0
			1570	1006	265	290	9			
11	m	199	Total	C	N	O	S	0	0	0
			1570	1006	265	290	9			
11	0	199	Total	C	N	O	S	0	0	0
			1570	1006	265	290	9			

- Molecule 12 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	201	Total	C	N	O	S	0	0	0
			1548	974	273	292	9			
12	Z	201	Total	C	N	O	S	0	0	0
			1551	977	273	292	9			
12	n	201	Total	C	N	O	S	0	0	0
			1548	974	273	292	9			
12	3	201	Total	C	N	O	S	0	0	0
			1551	977	273	292	9			

- Molecule 13 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	213	Total	C	N	O	S	0	0	0
			1641	1036	282	313	10			
13	1	213	Total	C	N	O	S	0	0	0
			1639	1034	282	313	10			
13	o	213	Total	C	N	O	S	0	0	0
			1639	1034	282	313	10			
13	a	213	Total	C	N	O	S	0	0	0
			1639	1034	282	313	10			

- Molecule 14 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	217	Total	C	N	O	S	0	0	0
			1676	1057	287	320	12			
14	2	217	Total	C	N	O	S	0	0	0
			1678	1058	290	318	12			
14	p	217	Total	C	N	O	S	0	0	0
			1672	1055	287	318	12			

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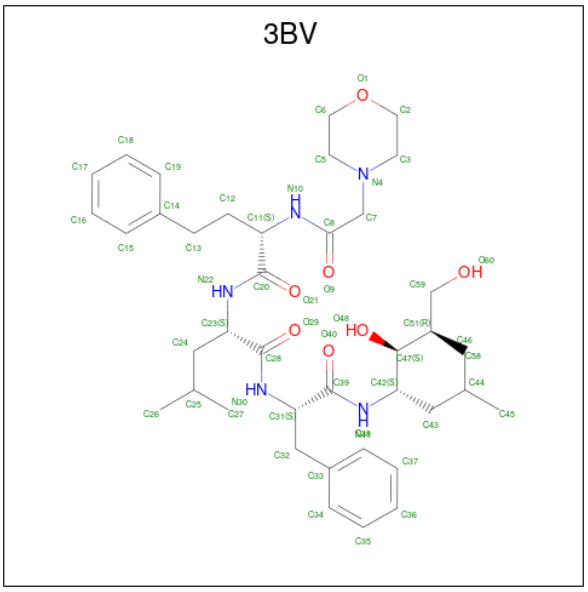
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	b	217	Total	C	N	O	S	0	0	0
			1669	1055	287	315	12			

- Molecule 15 is N-{(2S)-2-[(morpholin-4-ylacetyl)amino]-4-phenylbutanoyl}-L-leucyl-N-[(2R,3S,4S)-1,3-dihydroxy-2,6-dimethylheptan-4-yl]-L-phenylalaninamide (three-letter code: 3BV) (formula: $C_{40}H_{61}N_5O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	H	1	Total	C	N	O	0	0
			52	40	5	7		
15	I	1	Total	C	N	O	0	0
			52	40	5	7		
15	L	1	Total	C	N	O	0	0
			52	40	5	7		
15	V	1	Total	C	N	O	0	0
			52	40	5	7		
15	W	1	Total	C	N	O	0	0
			52	40	5	7		
15	Z	1	Total	C	N	O	0	0
			52	40	5	7		
15	j	1	Total	C	N	O	0	0
			52	40	5	7		
15	k	1	Total	C	N	O	0	0
			52	40	5	7		
15	n	1	Total	C	N	O	0	0
			52	40	5	7		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	y	1	Total C N O 52 40 5 7	0	0
15	3	1	Total C N O 52 40 5 7	0	0

- Molecule 16 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total O 1 1	0	0
16	B	4	Total O 4 4	0	0
16	C	2	Total O 2 2	0	0
16	D	1	Total O 1 1	0	0
16	E	2	Total O 2 2	0	0
16	F	4	Total O 4 4	0	0
16	G	1	Total O 1 1	0	0
16	H	1	Total O 1 1	0	0
16	H	5	Total O 5 5	0	0
16	I	1	Total O 1 1	0	0
16	I	6	Total O 6 6	0	0
16	J	2	Total O 2 2	0	0
16	K	5	Total O 5 5	0	0
16	L	1	Total O 1 1	0	0
16	L	2	Total O 2 2	0	0
16	M	8	Total O 8 8	0	0
16	N	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	O	6	Total O 6 6	0	0
16	P	3	Total O 3 3	0	0
16	Q	9	Total O 9 9	0	0
16	R	2	Total O 2 2	0	0
16	S	1	Total O 1 1	0	0
16	U	2	Total O 2 2	0	0
16	V	1	Total O 1 1	0	0
16	V	3	Total O 3 3	0	0
16	W	1	Total O 1 1	0	0
16	W	4	Total O 4 4	0	0
16	X	9	Total O 9 9	0	0
16	Y	8	Total O 8 8	0	0
16	Z	1	Total O 1 1	0	0
16	Z	7	Total O 7 7	0	0
16	1	5	Total O 5 5	0	0
16	2	5	Total O 5 5	0	0
16	c	3	Total O 3 3	0	0
16	d	1	Total O 1 1	0	0
16	e	5	Total O 5 5	0	0
16	f	1	Total O 1 1	0	0
16	h	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	i	4	Total O 4 4	0	0
16	j	1	Total O 1 1	0	0
16	j	1	Total O 1 1	0	0
16	k	1	Total O 1 1	0	0
16	k	5	Total O 5 5	0	0
16	l	7	Total O 7 7	0	0
16	m	5	Total O 5 5	0	0
16	n	1	Total O 1 1	0	0
16	n	4	Total O 4 4	0	0
16	o	10	Total O 10 10	0	0
16	p	2	Total O 2 2	0	0
16	q	3	Total O 3 3	0	0
16	r	3	Total O 3 3	0	0
16	s	5	Total O 5 5	0	0
16	u	1	Total O 1 1	0	0
16	v	2	Total O 2 2	0	0
16	w	2	Total O 2 2	0	0
16	x	3	Total O 3 3	0	0
16	y	8	Total O 8 8	0	0
16	z	2	Total O 2 2	0	0
16	0	3	Total O 3 3	0	0

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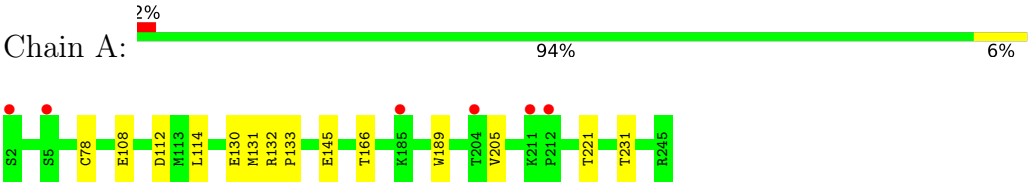
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	3	1	Total O 1 1	0	0
16	3	6	Total O 6 6	0	0
16	a	6	Total O 6 6	0	0
16	b	5	Total O 5 5	0	0

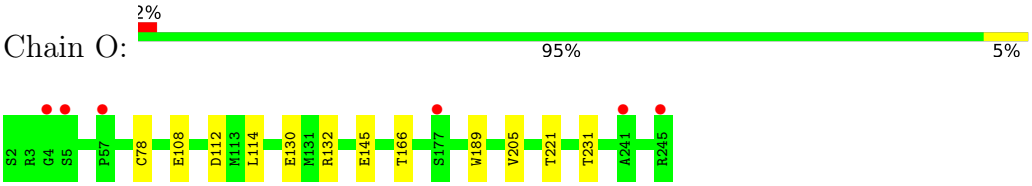
3 Residue-property plots (i)

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.

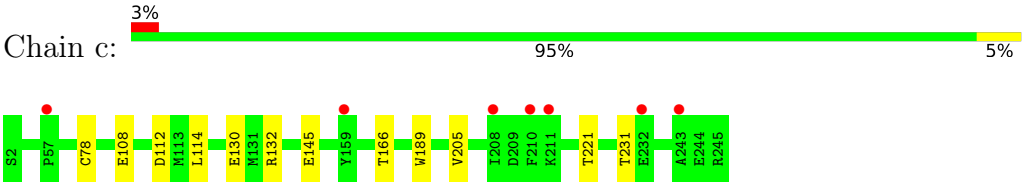
• Molecule 1: Proteasome subunit alpha type-6



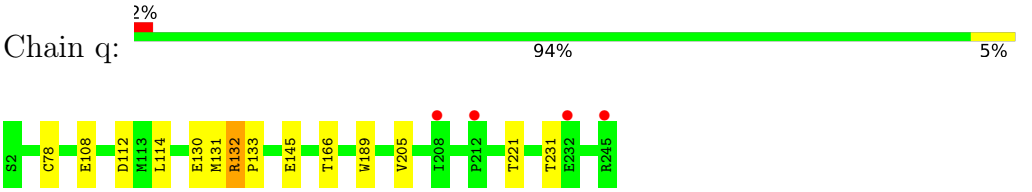
• Molecule 1: Proteasome subunit alpha type-6



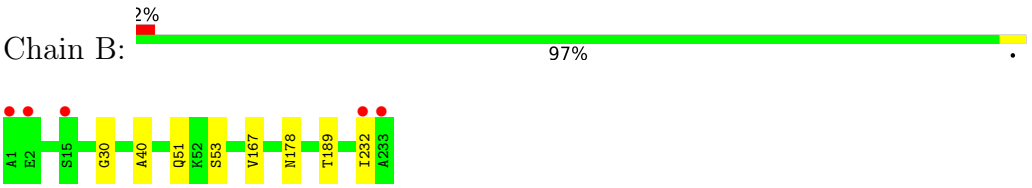
• Molecule 1: Proteasome subunit alpha type-6



• Molecule 1: Proteasome subunit alpha type-6

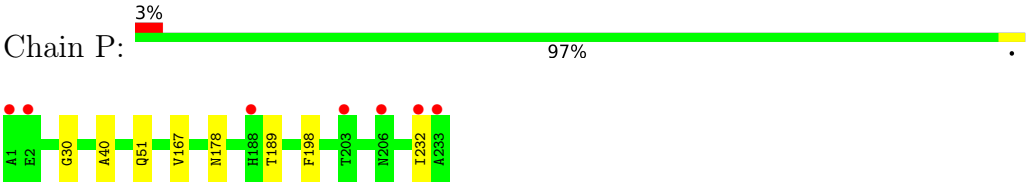


• Molecule 2: Proteasome subunit alpha type-2



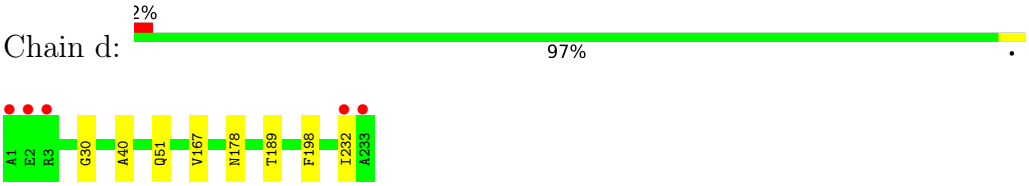
• Molecule 2: Proteasome subunit alpha type-2

Chain P:



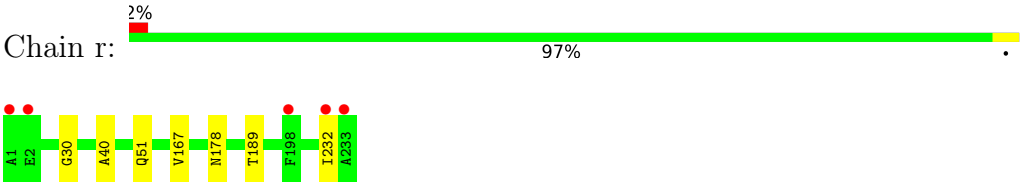
• Molecule 2: Proteasome subunit alpha type-2

Chain d:



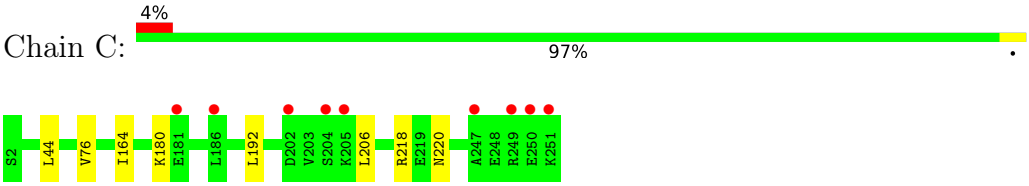
• Molecule 2: Proteasome subunit alpha type-2

Chain r:



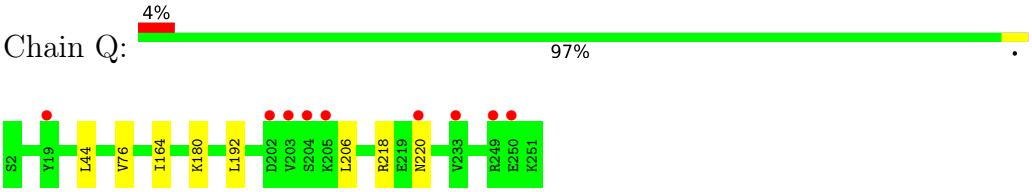
• Molecule 3: Proteasome subunit alpha type-4

Chain C:



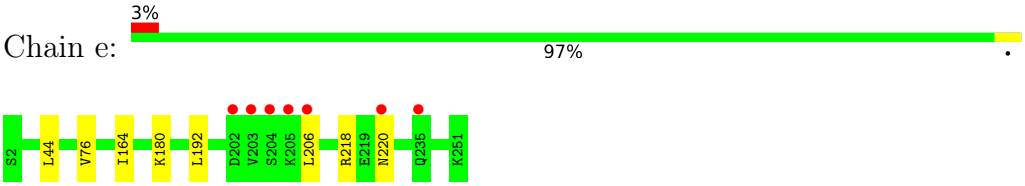
• Molecule 3: Proteasome subunit alpha type-4

Chain Q:



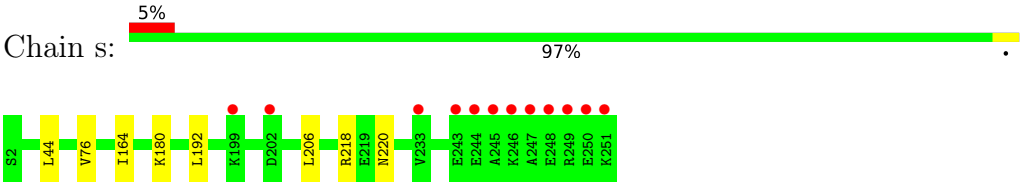
• Molecule 3: Proteasome subunit alpha type-4

Chain e:



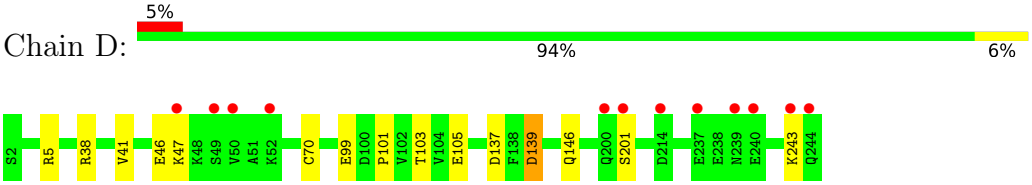
• Molecule 3: Proteasome subunit alpha type-4

Chain s:



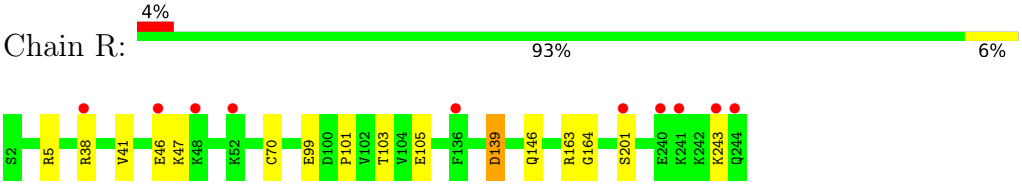
• Molecule 4: Proteasome subunit alpha type-7

Chain D:



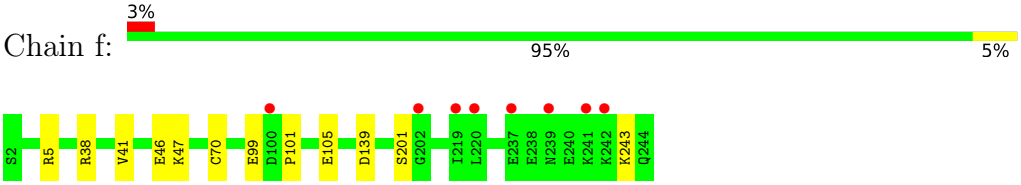
• Molecule 4: Proteasome subunit alpha type-7

Chain R:



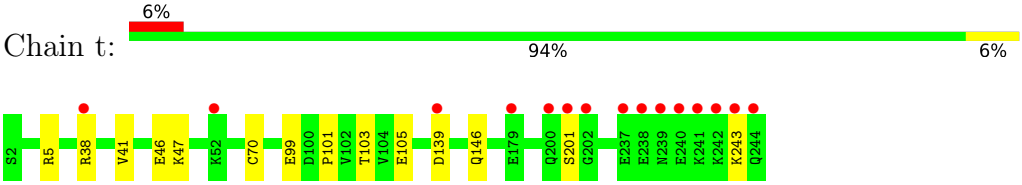
• Molecule 4: Proteasome subunit alpha type-7

Chain f:



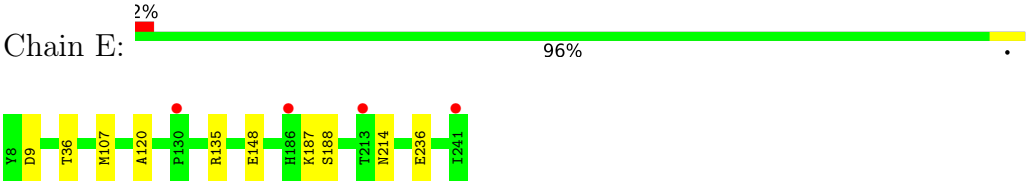
• Molecule 4: Proteasome subunit alpha type-7

Chain t:



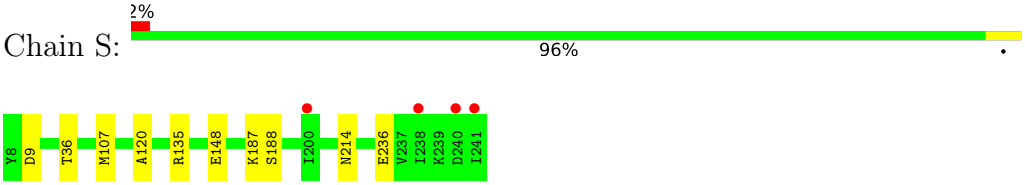
• Molecule 5: Proteasome subunit alpha type-5

Chain E:



• Molecule 5: Proteasome subunit alpha type-5

Chain S:

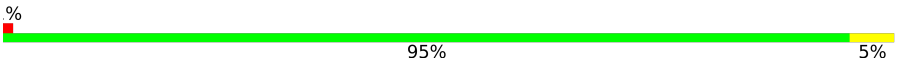


• Molecule 5: Proteasome subunit alpha type-5

Chain g:

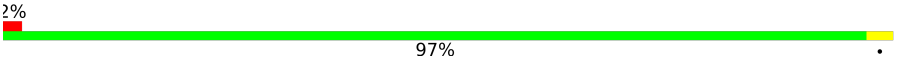
• Molecule 5: Proteasome subunit alpha type-5

Chain u:



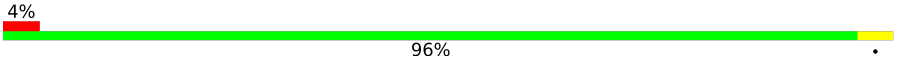
• Molecule 6: Proteasome subunit alpha type-1

Chain F:



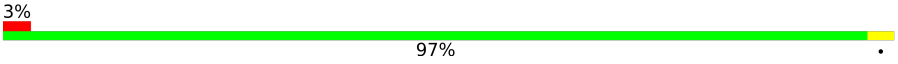
• Molecule 6: Proteasome subunit alpha type-1

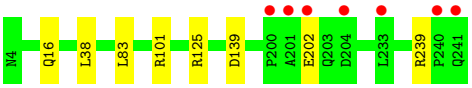
Chain T:



• Molecule 6: Proteasome subunit alpha type-1

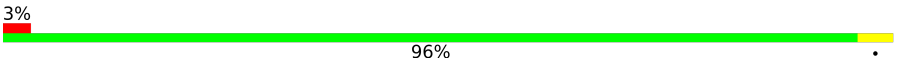
Chain h:

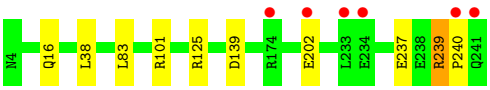




• Molecule 6: Proteasome subunit alpha type-1

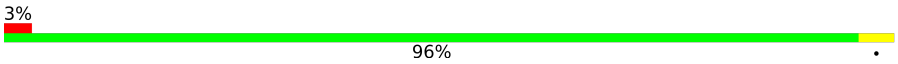
Chain v:





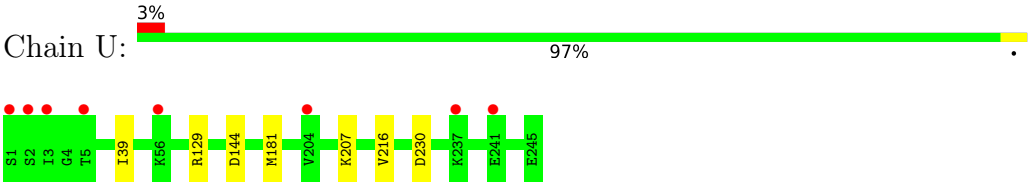
• Molecule 7: Proteasome subunit alpha type-3

Chain G:



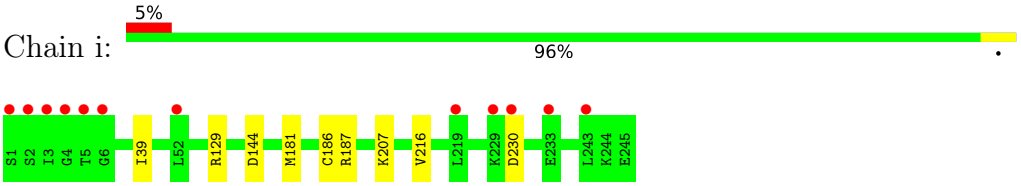
• Molecule 7: Proteasome subunit alpha type-3

Chain U:



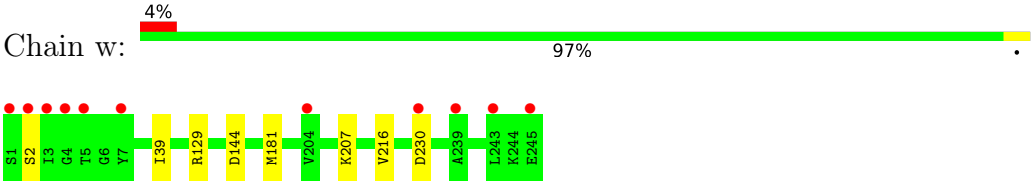
• Molecule 7: Proteasome subunit alpha type-3

Chain i:



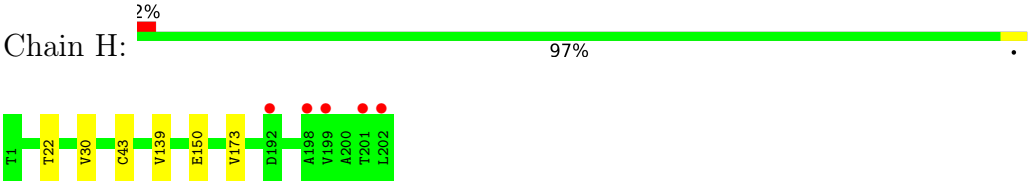
• Molecule 7: Proteasome subunit alpha type-3

Chain w:



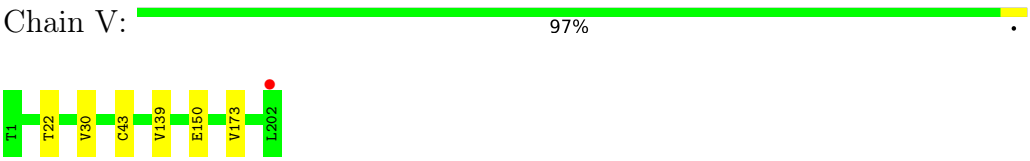
• Molecule 8: Proteasome subunit beta type-6

Chain H:



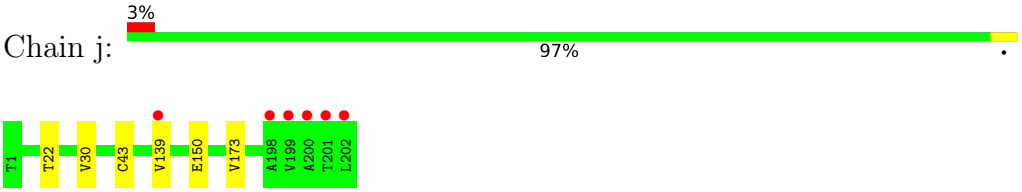
• Molecule 8: Proteasome subunit beta type-6

Chain V:



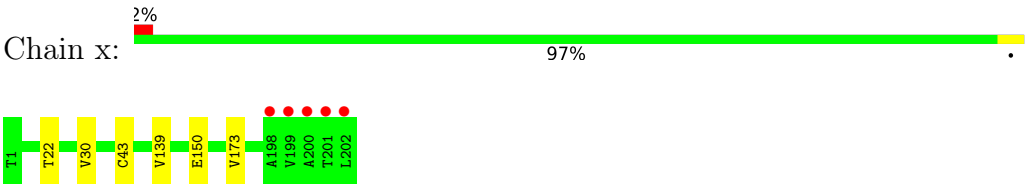
• Molecule 8: Proteasome subunit beta type-6

Chain j:



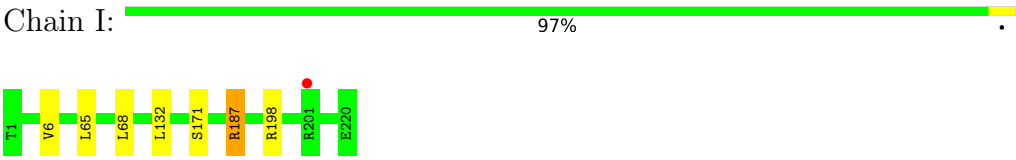
• Molecule 8: Proteasome subunit beta type-6

Chain x:



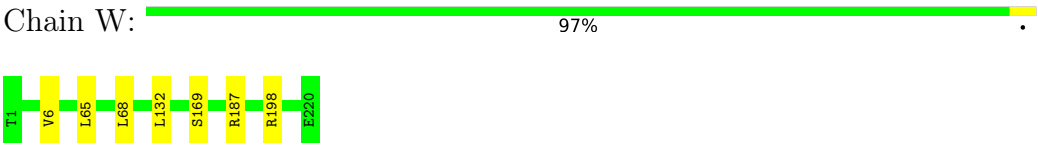
• Molecule 9: Proteasome subunit beta type-7

Chain I:



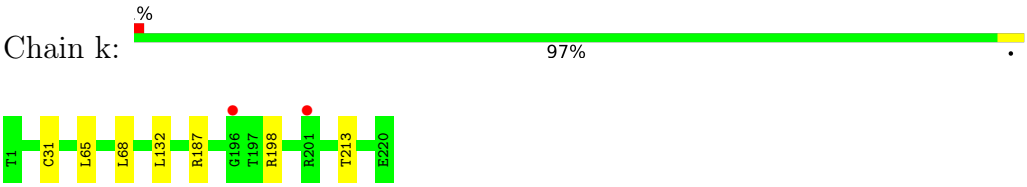
• Molecule 9: Proteasome subunit beta type-7

Chain W:



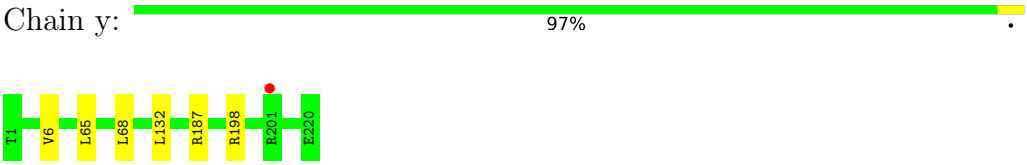
• Molecule 9: Proteasome subunit beta type-7

Chain k:



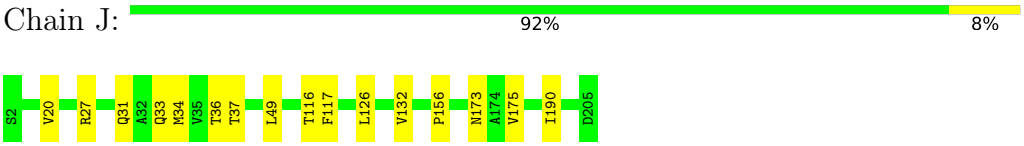
• Molecule 9: Proteasome subunit beta type-7

Chain y:



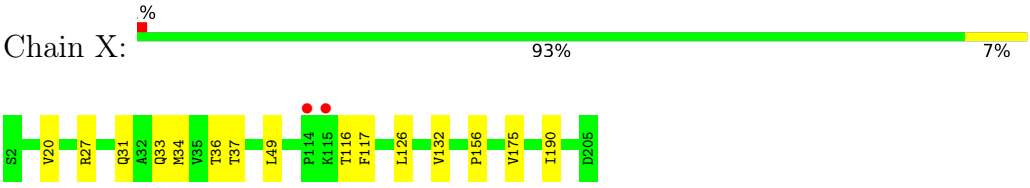
• Molecule 10: Proteasome subunit beta type-3

Chain J:



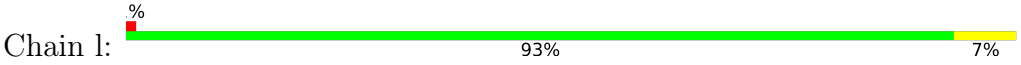
• Molecule 10: Proteasome subunit beta type-3

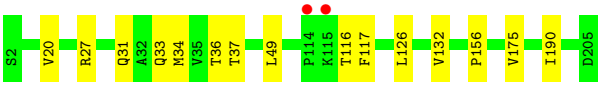
Chain X:



• Molecule 10: Proteasome subunit beta type-3

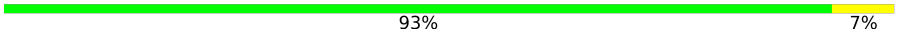
Chain l:

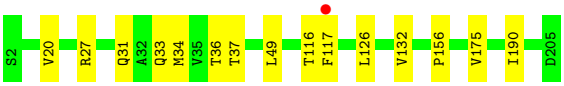




• Molecule 10: Proteasome subunit beta type-3

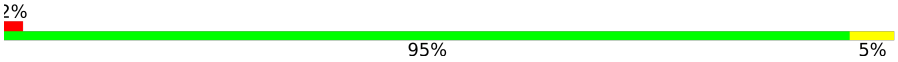
Chain z:

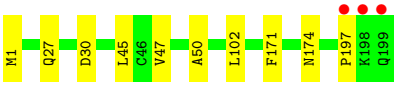




• Molecule 11: Proteasome subunit beta type-2

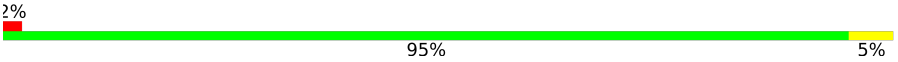
Chain K:

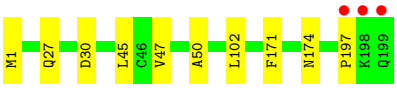




• Molecule 11: Proteasome subunit beta type-2

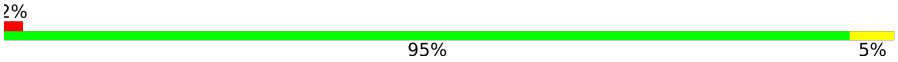
Chain Y:

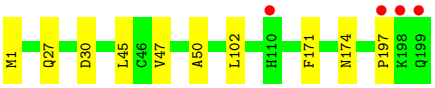




• Molecule 11: Proteasome subunit beta type-2

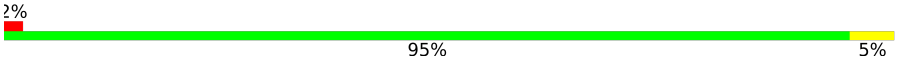
Chain m:

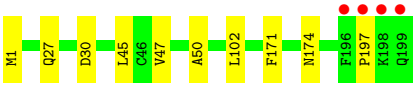




• Molecule 11: Proteasome subunit beta type-2

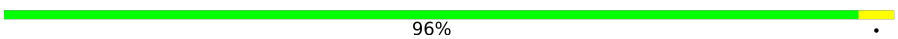
Chain 0:





• Molecule 12: Proteasome subunit beta type-5

Chain L:

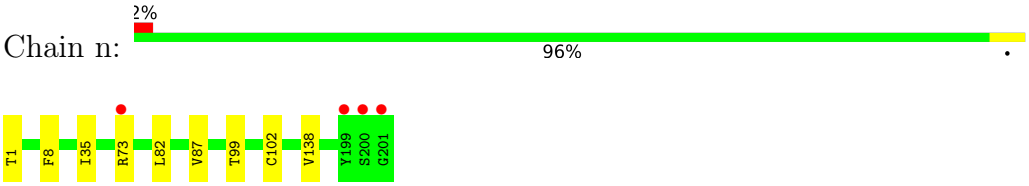


• Molecule 12: Proteasome subunit beta type-5

Chain Z:

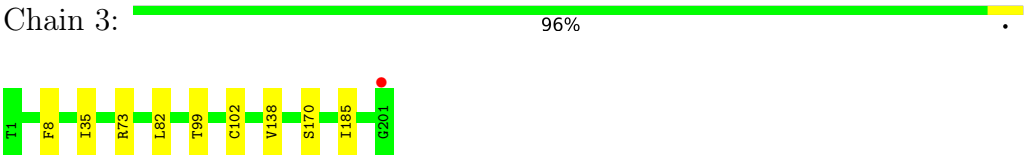
• Molecule 12: Proteasome subunit beta type-5

Chain n:



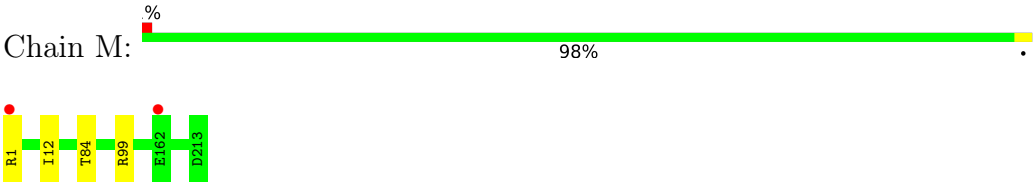
• Molecule 12: Proteasome subunit beta type-5

Chain 3:



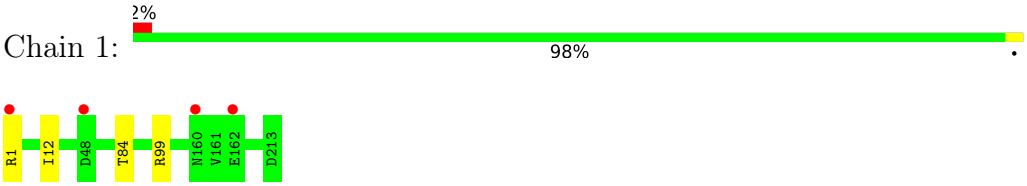
• Molecule 13: Proteasome subunit beta type-1

Chain M:



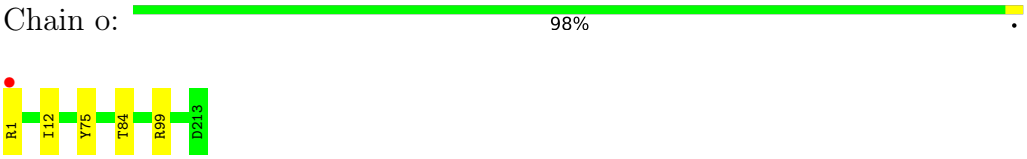
• Molecule 13: Proteasome subunit beta type-1

Chain 1:



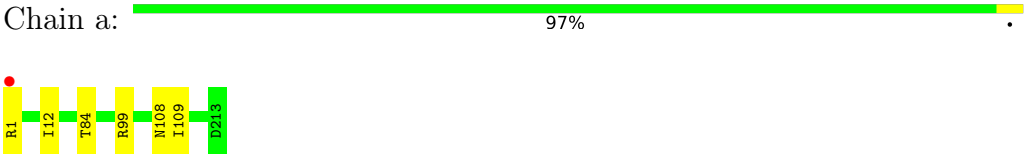
• Molecule 13: Proteasome subunit beta type-1

Chain o:



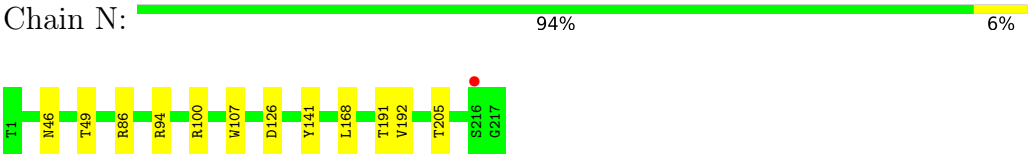
• Molecule 13: Proteasome subunit beta type-1

Chain a:



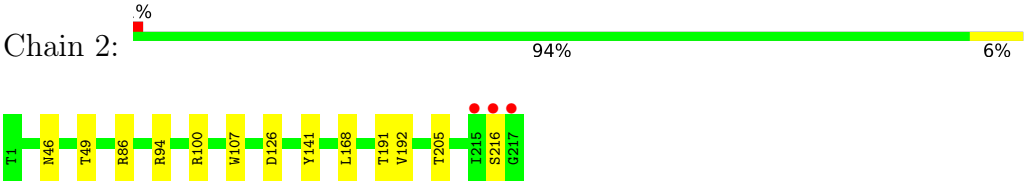
• Molecule 14: Proteasome subunit beta type-4

Chain N:



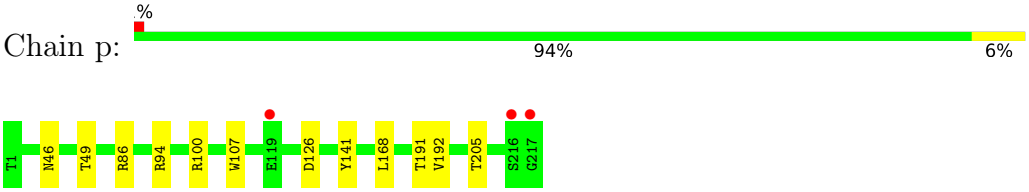
• Molecule 14: Proteasome subunit beta type-4

Chain 2:



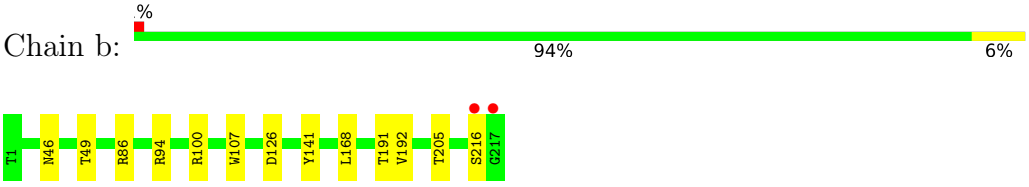
• Molecule 14: Proteasome subunit beta type-4

Chain p:



• Molecule 14: Proteasome subunit beta type-4

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	171.99Å 201.03Å 225.59Å 90.00° 107.93° 90.00°	Depositor
Resolution (Å)	33.51 – 2.89 33.51 – 2.89	Depositor EDS
% Data completeness (in resolution range)	98.6 (33.51-2.89) 98.7 (33.51-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 2.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.215 , 0.245 0.222 , 0.251	Depositor DCC
R_{free} test set	16212 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	72.6	Xtriage
Anisotropy	0.471	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 57.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	96005	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.44% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 3BV

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	0.26	1/1875 (0.1%)	0.43	0/2545
1	O	0.23	0/1878	0.41	0/2549
1	c	0.23	0/1875	0.41	0/2545
1	q	0.27	1/1875 (0.1%)	0.44	1/2545 (0.0%)
2	B	0.23	0/1749	0.41	0/2381
2	P	0.23	0/1747	0.41	0/2378
2	d	0.24	0/1745	0.41	0/2375
2	r	0.25	0/1752	0.41	0/2385
3	C	0.23	0/1931	0.41	0/2613
3	Q	0.23	0/1931	0.41	0/2613
3	e	0.23	0/1931	0.41	0/2613
3	s	0.23	0/1931	0.41	0/2613
4	D	0.22	0/1707	0.41	0/2335
4	R	0.23	0/1723	0.43	0/2355
4	f	0.22	0/1691	0.41	0/2314
4	t	0.21	0/1695	0.41	0/2319
5	E	0.22	0/1786	0.41	0/2419
5	S	0.22	0/1786	0.41	0/2419
5	g	0.23	0/1786	0.42	0/2419
5	u	0.22	0/1790	0.41	0/2423
6	F	0.24	0/1885	0.42	0/2552
6	T	0.26	1/1885 (0.1%)	0.43	0/2552
6	h	0.23	0/1885	0.43	0/2552
6	v	0.23	0/1885	0.43	0/2552
7	G	0.32	0/1920	0.42	0/2591
7	U	0.22	0/1920	0.39	0/2591
7	i	0.22	0/1920	0.39	0/2591
7	w	0.22	0/1920	0.39	0/2591
8	H	0.27	0/1535	0.43	0/2078
8	V	0.23	0/1535	0.42	0/2078
8	j	0.23	0/1535	0.42	0/2078
8	x	0.23	0/1535	0.42	0/2078

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
9	I	0.28	0/1670	0.43	0/2265
9	W	0.24	0/1670	0.43	0/2265
9	k	0.23	0/1670	0.43	0/2265
9	y	0.23	0/1674	0.43	0/2270
10	J	0.28	1/1614 (0.1%)	0.42	0/2177
10	X	0.25	0/1614	0.43	0/2177
10	l	0.25	0/1614	0.42	0/2177
10	z	0.32	0/1614	0.44	0/2177
11	0	0.22	0/1603	0.42	0/2174
11	K	0.22	0/1603	0.42	0/2174
11	Y	0.22	0/1603	0.42	0/2174
11	m	0.23	0/1603	0.41	0/2174
12	3	0.23	0/1582	0.44	2/2138 (0.1%)
12	L	0.27	1/1579 (0.1%)	0.44	2/2134 (0.1%)
12	Z	0.23	0/1582	0.40	0/2138
12	n	0.28	0/1579	0.45	2/2134 (0.1%)
13	1	0.24	0/1669	0.43	0/2250
13	M	0.24	0/1671	0.43	0/2253
13	a	0.27	0/1669	0.45	0/2250
13	o	0.32	1/1669 (0.1%)	0.45	0/2250
14	2	0.23	0/1711	0.42	0/2319
14	N	0.23	0/1709	0.42	0/2317
14	b	0.23	0/1702	0.42	0/2306
14	p	0.23	0/1705	0.42	0/2312
All	All	0.24	6/96923 (0.0%)	0.42	7/131312 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	3	THR	C-N	-5.74	1.20	1.34
1	q	133	PRO	N-CD	5.28	1.55	1.47
1	A	133	PRO	N-CD	5.28	1.55	1.47
6	T	240	PRO	N-CD	5.25	1.55	1.47
10	J	173	ASN	CG-ND2	-5.05	1.20	1.32
13	o	75	TYR	CE2-CZ	-5.01	1.32	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	n	73	ARG	NE-CZ-NH2	-5.93	117.34	120.30
12	3	73	ARG	NE-CZ-NH2	-5.89	117.35	120.30
12	L	73	ARG	NE-CZ-NH2	-5.88	117.36	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	q	132	ARG	C-N-CD	5.59	140.15	128.40
12	L	73	ARG	NE-CZ-NH1	5.58	123.09	120.30
12	3	73	ARG	NE-CZ-NH1	5.46	123.03	120.30
12	n	73	ARG	NE-CZ-NH1	5.42	123.01	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	242/244 (99%)	229 (95%)	12 (5%)	1 (0%)	34	66
1	O	242/244 (99%)	228 (94%)	13 (5%)	1 (0%)	34	66
1	c	242/244 (99%)	229 (95%)	12 (5%)	1 (0%)	34	66
1	q	242/244 (99%)	229 (95%)	12 (5%)	1 (0%)	34	66
2	B	231/233 (99%)	209 (90%)	17 (7%)	5 (2%)	6	24
2	P	231/233 (99%)	208 (90%)	18 (8%)	5 (2%)	6	24
2	d	231/233 (99%)	209 (90%)	17 (7%)	5 (2%)	6	24
2	r	231/233 (99%)	208 (90%)	19 (8%)	4 (2%)	9	31
3	C	248/250 (99%)	236 (95%)	11 (4%)	1 (0%)	34	66
3	Q	248/250 (99%)	236 (95%)	11 (4%)	1 (0%)	34	66
3	e	248/250 (99%)	236 (95%)	11 (4%)	1 (0%)	34	66
3	s	248/250 (99%)	236 (95%)	11 (4%)	1 (0%)	34	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	241/243 (99%)	225 (93%)	10 (4%)	6 (2%)	5	21
4	R	241/243 (99%)	222 (92%)	13 (5%)	6 (2%)	5	21
4	f	241/243 (99%)	225 (93%)	10 (4%)	6 (2%)	5	21
4	t	241/243 (99%)	225 (93%)	10 (4%)	6 (2%)	5	21
5	E	232/234 (99%)	220 (95%)	9 (4%)	3 (1%)	12	37
5	S	232/234 (99%)	220 (95%)	9 (4%)	3 (1%)	12	37
5	g	232/234 (99%)	219 (94%)	10 (4%)	3 (1%)	12	37
5	u	232/234 (99%)	220 (95%)	9 (4%)	3 (1%)	12	37
6	F	236/238 (99%)	227 (96%)	9 (4%)	0	100	100
6	T	236/238 (99%)	228 (97%)	6 (2%)	2 (1%)	19	51
6	h	236/238 (99%)	229 (97%)	6 (2%)	1 (0%)	34	66
6	v	236/238 (99%)	227 (96%)	6 (2%)	3 (1%)	12	37
7	G	243/245 (99%)	229 (94%)	12 (5%)	2 (1%)	19	51
7	U	243/245 (99%)	230 (95%)	11 (4%)	2 (1%)	19	51
7	i	243/245 (99%)	229 (94%)	12 (5%)	2 (1%)	19	51
7	w	243/245 (99%)	231 (95%)	9 (4%)	3 (1%)	13	40
8	H	200/202 (99%)	194 (97%)	5 (2%)	1 (0%)	29	61
8	V	200/202 (99%)	194 (97%)	5 (2%)	1 (0%)	29	61
8	j	200/202 (99%)	192 (96%)	7 (4%)	1 (0%)	29	61
8	x	200/202 (99%)	194 (97%)	5 (2%)	1 (0%)	29	61
9	I	218/220 (99%)	205 (94%)	11 (5%)	2 (1%)	17	48
9	W	218/220 (99%)	204 (94%)	13 (6%)	1 (0%)	29	61
9	k	218/220 (99%)	206 (94%)	11 (5%)	1 (0%)	29	61
9	y	218/220 (99%)	206 (94%)	11 (5%)	1 (0%)	29	61
10	J	202/204 (99%)	191 (95%)	7 (4%)	4 (2%)	7	27
10	X	202/204 (99%)	191 (95%)	7 (4%)	4 (2%)	7	27
10	l	202/204 (99%)	191 (95%)	7 (4%)	4 (2%)	7	27
10	z	202/204 (99%)	190 (94%)	8 (4%)	4 (2%)	7	27
11	0	197/199 (99%)	187 (95%)	7 (4%)	3 (2%)	10	34
11	K	197/199 (99%)	187 (95%)	7 (4%)	3 (2%)	10	34
11	Y	197/199 (99%)	187 (95%)	7 (4%)	3 (2%)	10	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
11	m	197/199 (99%)	187 (95%)	7 (4%)	3 (2%)	10 34
12	3	199/201 (99%)	185 (93%)	14 (7%)	0	100 100
12	L	199/201 (99%)	186 (94%)	12 (6%)	1 (0%)	29 61
12	Z	199/201 (99%)	186 (94%)	13 (6%)	0	100 100
12	n	199/201 (99%)	184 (92%)	15 (8%)	0	100 100
13	1	211/213 (99%)	207 (98%)	4 (2%)	0	100 100
13	M	211/213 (99%)	206 (98%)	5 (2%)	0	100 100
13	a	211/213 (99%)	207 (98%)	4 (2%)	0	100 100
13	o	211/213 (99%)	206 (98%)	5 (2%)	0	100 100
14	2	215/217 (99%)	199 (93%)	13 (6%)	3 (1%)	11 36
14	N	215/217 (99%)	199 (93%)	14 (6%)	2 (1%)	17 48
14	b	215/217 (99%)	199 (93%)	13 (6%)	3 (1%)	11 36
14	p	215/217 (99%)	199 (93%)	14 (6%)	2 (1%)	17 48
All	All	12460/12572 (99%)	11768 (94%)	566 (4%)	126 (1%)	15 45

All (126) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	232	ILE
4	D	47	LYS
9	I	187	ARG
10	J	117	PHE
10	J	156	PRO
2	P	232	ILE
4	R	47	LYS
6	T	237	GLU
6	T	239	ARG
10	X	117	PHE
10	X	156	PRO
2	d	232	ILE
4	f	47	LYS
10	l	117	PHE
10	l	156	PRO
2	r	232	ILE
4	t	47	LYS
6	v	237	GLU
6	v	239	ARG

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Mol	Chain	Res	Type
10	z	117	PHE
10	z	156	PRO
2	B	51	GLN
4	D	101	PRO
5	E	120	ALA
9	I	171	SER
4	R	101	PRO
5	S	120	ALA
4	f	101	PRO
5	g	120	ALA
4	t	101	PRO
5	u	120	ALA
6	v	240	PRO
7	w	2	SER
2	B	30	GLY
4	D	46	GLU
4	D	139	ASP
4	D	201	SER
10	J	116	THR
11	K	50	ALA
12	L	2	THR
14	N	46	ASN
2	P	30	GLY
2	P	51	GLN
2	P	198	PHE
4	R	139	ASP
4	R	164	GLY
4	R	201	SER
10	X	116	THR
11	Y	50	ALA
14	2	46	ASN
2	d	30	GLY
2	d	198	PHE
4	f	46	GLU
4	f	139	ASP
4	f	201	SER
10	l	116	THR
11	m	50	ALA
14	p	46	ASN
2	r	30	GLY
4	t	46	GLU
4	t	139	ASP

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Mol	Chain	Res	Type
4	t	201	SER
10	z	116	THR
11	0	50	ALA
14	b	46	ASN
2	B	40	ALA
3	C	206	LEU
5	E	187	LYS
5	E	188	SER
7	G	207	LYS
11	K	174	ASN
14	N	107	TRP
2	P	40	ALA
3	Q	206	LEU
5	S	187	LYS
7	U	207	LYS
11	Y	174	ASN
14	2	107	TRP
2	d	40	ALA
2	d	51	GLN
3	e	206	LEU
5	g	187	LYS
5	g	188	SER
6	h	239	ARG
7	i	207	LYS
14	p	107	TRP
2	r	51	GLN
3	s	206	LEU
5	u	187	LYS
5	u	188	SER
7	w	207	LYS
11	0	174	ASN
14	b	107	TRP
1	A	189	TRP
2	B	53	SER
10	J	31	GLN
1	O	189	TRP
4	R	243	LYS
5	S	188	SER
9	W	187	ARG
10	X	31	GLN
1	c	189	TRP
9	k	187	ARG

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Mol	Chain	Res	Type
10	l	31	GLN
11	m	174	ASN
1	q	189	TRP
2	r	40	ALA
9	y	187	ARG
10	z	31	GLN
4	D	243	LYS
11	Y	197	PRO
14	2	216	SER
4	f	243	LYS
4	t	243	LYS
11	0	197	PRO
14	b	216	SER
11	K	197	PRO
11	m	197	PRO
8	j	30	VAL
8	H	30	VAL
8	V	30	VAL
8	x	30	VAL
7	G	216	VAL
7	U	216	VAL
7	i	216	VAL
7	w	216	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	192/208 (92%)	180 (94%)	12 (6%)	18 46
1	O	193/208 (93%)	182 (94%)	11 (6%)	20 51
1	c	192/208 (92%)	181 (94%)	11 (6%)	20 51
1	q	192/208 (92%)	180 (94%)	12 (6%)	18 46
2	B	164/190 (86%)	161 (98%)	3 (2%)	59 85
2	P	165/190 (87%)	162 (98%)	3 (2%)	59 85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	d	164/190 (86%)	161 (98%)	3 (2%)	59	85
2	r	165/190 (87%)	162 (98%)	3 (2%)	59	85
3	C	191/210 (91%)	184 (96%)	7 (4%)	34	68
3	Q	191/210 (91%)	184 (96%)	7 (4%)	34	68
3	e	191/210 (91%)	184 (96%)	7 (4%)	34	68
3	s	191/210 (91%)	184 (96%)	7 (4%)	34	68
4	D	142/207 (69%)	132 (93%)	10 (7%)	15	41
4	R	143/207 (69%)	132 (92%)	11 (8%)	13	35
4	f	137/207 (66%)	131 (96%)	6 (4%)	28	61
4	t	138/207 (67%)	130 (94%)	8 (6%)	20	50
5	E	189/196 (96%)	182 (96%)	7 (4%)	34	68
5	S	189/196 (96%)	182 (96%)	7 (4%)	34	68
5	g	189/196 (96%)	181 (96%)	8 (4%)	30	63
5	u	190/196 (97%)	182 (96%)	8 (4%)	30	63
6	F	198/204 (97%)	190 (96%)	8 (4%)	31	65
6	T	198/204 (97%)	190 (96%)	8 (4%)	31	65
6	h	198/204 (97%)	191 (96%)	7 (4%)	36	70
6	v	198/204 (97%)	190 (96%)	8 (4%)	31	65
7	G	195/202 (96%)	186 (95%)	9 (5%)	27	60
7	U	195/202 (96%)	190 (97%)	5 (3%)	46	77
7	i	195/202 (96%)	188 (96%)	7 (4%)	35	69
7	w	195/202 (96%)	190 (97%)	5 (3%)	46	77
8	H	155/157 (99%)	150 (97%)	5 (3%)	39	73
8	V	155/157 (99%)	150 (97%)	5 (3%)	39	73
8	j	155/157 (99%)	150 (97%)	5 (3%)	39	73
8	x	155/157 (99%)	150 (97%)	5 (3%)	39	73
9	I	177/181 (98%)	171 (97%)	6 (3%)	37	71
9	W	177/181 (98%)	171 (97%)	6 (3%)	37	71
9	k	177/181 (98%)	171 (97%)	6 (3%)	37	71
9	y	178/181 (98%)	173 (97%)	5 (3%)	43	76
10	J	172/173 (99%)	161 (94%)	11 (6%)	17	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	X	172/173 (99%)	161 (94%)	11 (6%)	17 45
10	l	172/173 (99%)	161 (94%)	11 (6%)	17 45
10	z	172/173 (99%)	161 (94%)	11 (6%)	17 45
11	0	164/170 (96%)	157 (96%)	7 (4%)	29 62
11	K	164/170 (96%)	157 (96%)	7 (4%)	29 62
11	Y	164/170 (96%)	157 (96%)	7 (4%)	29 62
11	m	164/170 (96%)	157 (96%)	7 (4%)	29 62
12	3	154/156 (99%)	146 (95%)	8 (5%)	23 55
12	L	153/156 (98%)	147 (96%)	6 (4%)	32 66
12	Z	154/156 (99%)	147 (96%)	7 (4%)	27 61
12	n	153/156 (98%)	145 (95%)	8 (5%)	23 55
13	1	173/178 (97%)	169 (98%)	4 (2%)	50 80
13	M	174/178 (98%)	170 (98%)	4 (2%)	50 80
13	a	173/178 (97%)	167 (96%)	6 (4%)	36 70
13	o	173/178 (97%)	169 (98%)	4 (2%)	50 80
14	2	175/179 (98%)	165 (94%)	10 (6%)	20 51
14	N	175/179 (98%)	165 (94%)	10 (6%)	20 51
14	b	174/179 (97%)	164 (94%)	10 (6%)	20 51
14	p	174/179 (97%)	164 (94%)	10 (6%)	20 51
All	All	9758/10444 (93%)	9348 (96%)	410 (4%)	30 63

All (410) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	CYS
1	A	108	GLU
1	A	112	ASP
1	A	114	LEU
1	A	130	GLU
1	A	131	MET
1	A	132	ARG
1	A	145	GLU
1	A	166	THR
1	A	205	VAL
1	A	221	THR

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Mol	Chain	Res	Type
1	A	231	THR
2	B	167	VAL
2	B	178	ASN
2	B	189	THR
3	C	44	LEU
3	C	76	VAL
3	C	164	ILE
3	C	180	LYS
3	C	192	LEU
3	C	218	ARG
3	C	220	ASN
4	D	5	ARG
4	D	38	ARG
4	D	41	VAL
4	D	70	CYS
4	D	99	GLU
4	D	103	THR
4	D	105	GLU
4	D	137	ASP
4	D	139	ASP
4	D	146	GLN
5	E	9	ASP
5	E	36	THR
5	E	107	MET
5	E	135	ARG
5	E	148	GLU
5	E	214	ASN
5	E	236	GLU
6	F	16	GLN
6	F	38	LEU
6	F	83	LEU
6	F	101	ARG
6	F	125	ARG
6	F	139	ASP
6	F	202	GLU
6	F	239	ARG
7	G	39	ILE
7	G	41	CYS
7	G	42	LYS
7	G	125	TYR
7	G	129	ARG
7	G	144	ASP

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Mol	Chain	Res	Type
7	G	181	MET
7	G	187	ARG
7	G	230	ASP
8	H	22	THR
8	H	43	CYS
8	H	139	VAL
8	H	150	GLU
8	H	173	VAL
9	I	6	VAL
9	I	65	LEU
9	I	68	LEU
9	I	132	LEU
9	I	187	ARG
9	I	198	ARG
10	J	20	VAL
10	J	27	ARG
10	J	33	GLN
10	J	34	MET
10	J	36	THR
10	J	37	THR
10	J	49	LEU
10	J	126	LEU
10	J	132	VAL
10	J	175	VAL
10	J	190	ILE
11	K	1	MET
11	K	27	GLN
11	K	30	ASP
11	K	45	LEU
11	K	47	VAL
11	K	102	LEU
11	K	171	PHE
12	L	8	PHE
12	L	35	ILE
12	L	82	LEU
12	L	99	THR
12	L	102	CYS
12	L	138	VAL
13	M	1	ARG
13	M	12	ILE
13	M	84	THR
13	M	99	ARG

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Mol	Chain	Res	Type
14	N	49	THR
14	N	86	ARG
14	N	94	ARG
14	N	100	ARG
14	N	126	ASP
14	N	141	TYR
14	N	168	LEU
14	N	191	THR
14	N	192	VAL
14	N	205	THR
1	O	78	CYS
1	O	108	GLU
1	O	112	ASP
1	O	114	LEU
1	O	130	GLU
1	O	132	ARG
1	O	145	GLU
1	O	166	THR
1	O	205	VAL
1	O	221	THR
1	O	231	THR
2	P	167	VAL
2	P	178	ASN
2	P	189	THR
3	Q	44	LEU
3	Q	76	VAL
3	Q	164	ILE
3	Q	180	LYS
3	Q	192	LEU
3	Q	218	ARG
3	Q	220	ASN
4	R	5	ARG
4	R	38	ARG
4	R	41	VAL
4	R	46	GLU
4	R	70	CYS
4	R	99	GLU
4	R	103	THR
4	R	105	GLU
4	R	139	ASP
4	R	146	GLN
4	R	163	ARG

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Mol	Chain	Res	Type
5	S	9	ASP
5	S	36	THR
5	S	107	MET
5	S	135	ARG
5	S	148	GLU
5	S	214	ASN
5	S	236	GLU
6	T	16	GLN
6	T	38	LEU
6	T	83	LEU
6	T	101	ARG
6	T	125	ARG
6	T	139	ASP
6	T	202	GLU
6	T	239	ARG
7	U	39	ILE
7	U	129	ARG
7	U	144	ASP
7	U	181	MET
7	U	230	ASP
8	V	22	THR
8	V	43	CYS
8	V	139	VAL
8	V	150	GLU
8	V	173	VAL
9	W	6	VAL
9	W	65	LEU
9	W	68	LEU
9	W	132	LEU
9	W	169	SER
9	W	198	ARG
10	X	20	VAL
10	X	27	ARG
10	X	33	GLN
10	X	34	MET
10	X	36	THR
10	X	37	THR
10	X	49	LEU
10	X	126	LEU
10	X	132	VAL
10	X	175	VAL
10	X	190	ILE

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Mol	Chain	Res	Type
11	Y	1	MET
11	Y	27	GLN
11	Y	30	ASP
11	Y	45	LEU
11	Y	47	VAL
11	Y	102	LEU
11	Y	171	PHE
12	Z	8	PHE
12	Z	35	ILE
12	Z	82	LEU
12	Z	87	VAL
12	Z	99	THR
12	Z	102	CYS
12	Z	138	VAL
13	1	1	ARG
13	1	12	ILE
13	1	84	THR
13	1	99	ARG
14	2	49	THR
14	2	86	ARG
14	2	94	ARG
14	2	100	ARG
14	2	126	ASP
14	2	141	TYR
14	2	168	LEU
14	2	191	THR
14	2	192	VAL
14	2	205	THR
1	c	78	CYS
1	c	108	GLU
1	c	112	ASP
1	c	114	LEU
1	c	130	GLU
1	c	132	ARG
1	c	145	GLU
1	c	166	THR
1	c	205	VAL
1	c	221	THR
1	c	231	THR
2	d	167	VAL
2	d	178	ASN
2	d	189	THR

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Mol	Chain	Res	Type
3	e	44	LEU
3	e	76	VAL
3	e	164	ILE
3	e	180	LYS
3	e	192	LEU
3	e	218	ARG
3	e	220	ASN
4	f	5	ARG
4	f	38	ARG
4	f	41	VAL
4	f	70	CYS
4	f	99	GLU
4	f	105	GLU
5	g	9	ASP
5	g	36	THR
5	g	107	MET
5	g	135	ARG
5	g	148	GLU
5	g	168	ARG
5	g	214	ASN
5	g	236	GLU
6	h	16	GLN
6	h	38	LEU
6	h	83	LEU
6	h	101	ARG
6	h	125	ARG
6	h	139	ASP
6	h	202	GLU
7	i	39	ILE
7	i	129	ARG
7	i	144	ASP
7	i	181	MET
7	i	186	CYS
7	i	187	ARG
7	i	230	ASP
8	j	22	THR
8	j	43	CYS
8	j	139	VAL
8	j	150	GLU
8	j	173	VAL
9	k	31	CYS
9	k	65	LEU

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Mol	Chain	Res	Type
9	k	68	LEU
9	k	132	LEU
9	k	198	ARG
9	k	213	THR
10	l	20	VAL
10	l	27	ARG
10	l	33	GLN
10	l	34	MET
10	l	36	THR
10	l	37	THR
10	l	49	LEU
10	l	126	LEU
10	l	132	VAL
10	l	175	VAL
10	l	190	ILE
11	m	1	MET
11	m	27	GLN
11	m	30	ASP
11	m	45	LEU
11	m	47	VAL
11	m	102	LEU
11	m	171	PHE
12	n	1	THR
12	n	8	PHE
12	n	35	ILE
12	n	82	LEU
12	n	87	VAL
12	n	99	THR
12	n	102	CYS
12	n	138	VAL
13	o	1	ARG
13	o	12	ILE
13	o	84	THR
13	o	99	ARG
14	p	49	THR
14	p	86	ARG
14	p	94	ARG
14	p	100	ARG
14	p	126	ASP
14	p	141	TYR
14	p	168	LEU
14	p	191	THR

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Mol	Chain	Res	Type
14	p	192	VAL
14	p	205	THR
1	q	78	CYS
1	q	108	GLU
1	q	112	ASP
1	q	114	LEU
1	q	130	GLU
1	q	131	MET
1	q	132	ARG
1	q	145	GLU
1	q	166	THR
1	q	205	VAL
1	q	221	THR
1	q	231	THR
2	r	167	VAL
2	r	178	ASN
2	r	189	THR
3	s	44	LEU
3	s	76	VAL
3	s	164	ILE
3	s	180	LYS
3	s	192	LEU
3	s	218	ARG
3	s	220	ASN
4	t	5	ARG
4	t	38	ARG
4	t	41	VAL
4	t	70	CYS
4	t	99	GLU
4	t	103	THR
4	t	105	GLU
4	t	146	GLN
5	u	9	ASP
5	u	36	THR
5	u	107	MET
5	u	135	ARG
5	u	148	GLU
5	u	214	ASN
5	u	231	LYS
5	u	236	GLU
6	v	16	GLN
6	v	38	LEU

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Mol	Chain	Res	Type
6	v	83	LEU
6	v	101	ARG
6	v	125	ARG
6	v	139	ASP
6	v	202	GLU
6	v	239	ARG
7	w	39	ILE
7	w	129	ARG
7	w	144	ASP
7	w	181	MET
7	w	230	ASP
8	x	22	THR
8	x	43	CYS
8	x	139	VAL
8	x	150	GLU
8	x	173	VAL
9	y	6	VAL
9	y	65	LEU
9	y	68	LEU
9	y	132	LEU
9	y	198	ARG
10	z	20	VAL
10	z	27	ARG
10	z	33	GLN
10	z	34	MET
10	z	36	THR
10	z	37	THR
10	z	49	LEU
10	z	126	LEU
10	z	132	VAL
10	z	175	VAL
10	z	190	ILE
11	0	1	MET
11	0	27	GLN
11	0	30	ASP
11	0	45	LEU
11	0	47	VAL
11	0	102	LEU
11	0	171	PHE
12	3	8	PHE
12	3	35	ILE
12	3	82	LEU

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Mol	Chain	Res	Type
12	3	99	THR
12	3	102	CYS
12	3	138	VAL
12	3	170	SER
12	3	185	ILE
13	a	1	ARG
13	a	12	ILE
13	a	84	THR
13	a	99	ARG
13	a	108	ASN
13	a	109	ILE
14	b	49	THR
14	b	86	ARG
14	b	94	ARG
14	b	100	ARG
14	b	126	ASP
14	b	141	TYR
14	b	168	LEU
14	b	191	THR
14	b	192	VAL
14	b	205	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	206	ASN
5	E	152	GLN
13	M	146	GLN
2	P	147	GLN
10	X	173	ASN
13	1	146	GLN
2	d	206	ASN
10	l	173	ASN
13	o	146	GLN
13	o	152	GLN
5	u	152	GLN
10	z	173	ASN
13	a	146	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)

11 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	3BV	y	301	9	54,54,54	2.72	13 (24%)	68,71,71	1.91	11 (16%)
15	3BV	3	301	12	54,54,54	2.39	11 (20%)	68,71,71	1.64	11 (16%)
15	3BV	n	301	12	54,54,54	2.65	11 (20%)	68,71,71	2.19	20 (29%)
15	3BV	L	301	-	54,54,54	2.41	12 (22%)	68,71,71	1.93	16 (23%)
15	3BV	V	301	8	54,54,54	2.37	11 (20%)	68,71,71	1.58	9 (13%)
15	3BV	H	301	8	54,54,54	2.63	11 (20%)	68,71,71	1.58	11 (16%)
15	3BV	j	301	8	54,54,54	2.42	10 (18%)	68,71,71	2.35	20 (29%)
15	3BV	W	301	-	54,54,54	2.41	12 (22%)	68,71,71	1.98	19 (27%)
15	3BV	k	301	9	54,54,54	2.54	11 (20%)	68,71,71	1.82	17 (25%)
15	3BV	Z	301	12	54,54,54	2.96	15 (27%)	68,71,71	3.11	22 (32%)
15	3BV	I	301	-	54,54,54	2.69	12 (22%)	68,71,71	2.08	16 (23%)

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	3BV	y	301	9	-	22/59/67/67	0/3/3/3
15	3BV	3	301	12	-	19/59/67/67	0/3/3/3
15	3BV	n	301	12	-	18/59/67/67	0/3/3/3
15	3BV	L	301	-	-	17/59/67/67	0/3/3/3
15	3BV	V	301	8	-	26/59/67/67	0/3/3/3
15	3BV	H	301	8	-	22/59/67/67	0/3/3/3
15	3BV	j	301	8	-	29/59/67/67	0/3/3/3
15	3BV	W	301	-	-	24/59/67/67	0/3/3/3
15	3BV	k	301	9	-	15/59/67/67	0/3/3/3
15	3BV	Z	301	12	-	22/59/67/67	0/3/3/3
15	3BV	I	301	-	-	18/59/67/67	0/3/3/3

All (129) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	I	301	3BV	O48-C47	-12.97	1.12	1.43
15	n	301	3BV	O48-C47	-12.02	1.14	1.43
15	Z	301	3BV	O48-C47	-10.97	1.17	1.43
15	k	301	3BV	O48-C47	-10.60	1.18	1.43
15	Z	301	3BV	C43-C42	-10.47	1.37	1.52
15	H	301	3BV	O48-C47	-9.99	1.19	1.43
15	W	301	3BV	O48-C47	-9.70	1.20	1.43
15	y	301	3BV	O48-C47	-9.09	1.21	1.43
15	L	301	3BV	O48-C47	-8.83	1.22	1.43
15	j	301	3BV	O48-C47	-8.54	1.22	1.43
15	H	301	3BV	C8-N10	8.27	1.51	1.34
15	y	301	3BV	C8-N10	8.26	1.51	1.34
15	3	301	3BV	C8-N10	8.25	1.51	1.34
15	V	301	3BV	C8-N10	8.23	1.51	1.34
15	j	301	3BV	C8-N10	7.74	1.50	1.34
15	k	301	3BV	C8-N10	7.67	1.50	1.34
15	y	301	3BV	C39-N41	7.42	1.50	1.34
15	3	301	3BV	C39-N41	7.42	1.50	1.34
15	V	301	3BV	C39-N41	7.40	1.50	1.34
15	H	301	3BV	C39-N41	7.40	1.50	1.34
15	I	301	3BV	C8-N10	7.03	1.49	1.34
15	n	301	3BV	C8-N10	6.99	1.49	1.34
15	L	301	3BV	C8-N10	6.88	1.48	1.34
15	W	301	3BV	C8-N10	6.78	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	y	301	3BV	C31-N30	6.60	1.59	1.45
15	3	301	3BV	C31-N30	6.59	1.59	1.45
15	j	301	3BV	C39-N41	6.57	1.48	1.34
15	H	301	3BV	C31-N30	6.57	1.59	1.45
15	V	301	3BV	C31-N30	6.56	1.59	1.45
15	Z	301	3BV	C8-N10	6.34	1.47	1.34
15	y	301	3BV	C59-C51	-6.19	1.45	1.52
15	W	301	3BV	C39-N41	6.14	1.47	1.34
15	k	301	3BV	C39-N41	5.83	1.46	1.34
15	j	301	3BV	C31-N30	5.76	1.58	1.45
15	3	301	3BV	O48-C47	-5.65	1.29	1.43
15	V	301	3BV	C28-N30	5.62	1.46	1.34
15	k	301	3BV	C31-N30	5.62	1.57	1.45
15	3	301	3BV	C28-N30	5.61	1.46	1.34
15	H	301	3BV	C28-N30	5.60	1.46	1.34
15	y	301	3BV	C28-N30	5.56	1.46	1.34
15	Z	301	3BV	C43-C44	-5.50	1.28	1.52
15	V	301	3BV	O48-C47	-5.37	1.30	1.43
15	n	301	3BV	C39-N41	5.33	1.45	1.34
15	I	301	3BV	C39-N41	5.31	1.45	1.34
15	L	301	3BV	C31-N30	5.18	1.56	1.45
15	W	301	3BV	C31-N30	5.15	1.56	1.45
15	L	301	3BV	C39-N41	5.12	1.45	1.34
15	I	301	3BV	C31-N30	4.85	1.56	1.45
15	Z	301	3BV	C39-N41	4.82	1.44	1.34
15	n	301	3BV	C31-N30	4.80	1.56	1.45
15	k	301	3BV	C28-N30	4.76	1.44	1.34
15	j	301	3BV	C28-N30	4.71	1.44	1.34
15	Z	301	3BV	O40-C39	-4.69	1.14	1.23
15	L	301	3BV	O40-C39	-4.43	1.14	1.23
15	W	301	3BV	C28-N30	4.42	1.43	1.34
15	L	301	3BV	C28-N30	4.37	1.43	1.34
15	n	301	3BV	O40-C39	-4.19	1.15	1.23
15	I	301	3BV	O40-C39	-4.18	1.15	1.23
15	Z	301	3BV	C31-N30	4.07	1.54	1.45
15	L	301	3BV	O29-C28	-3.95	1.15	1.23
15	I	301	3BV	C28-N30	3.91	1.42	1.34
15	k	301	3BV	O40-C39	-3.88	1.15	1.23
15	n	301	3BV	C28-N30	3.86	1.42	1.34
15	n	301	3BV	C43-C42	-3.79	1.47	1.52
15	I	301	3BV	C43-C42	-3.71	1.47	1.52
15	Z	301	3BV	O29-C28	-3.67	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	y	301	3BV	C31-C39	3.65	1.62	1.52
15	3	301	3BV	C31-C39	3.63	1.62	1.52
15	V	301	3BV	C31-C39	3.62	1.62	1.52
15	H	301	3BV	C31-C39	3.61	1.62	1.52
15	n	301	3BV	O29-C28	-3.61	1.16	1.23
15	L	301	3BV	C43-C42	-3.53	1.47	1.52
15	W	301	3BV	O40-C39	-3.52	1.16	1.23
15	I	301	3BV	O29-C28	-3.46	1.16	1.23
15	j	301	3BV	O40-C39	-3.42	1.16	1.23
15	W	301	3BV	O29-C28	-3.37	1.16	1.23
15	Z	301	3BV	C28-N30	3.31	1.41	1.34
15	n	301	3BV	C47-C42	-3.31	1.47	1.53
15	Z	301	3BV	C47-C42	-3.27	1.47	1.53
15	y	301	3BV	C20-N22	3.27	1.41	1.34
15	W	301	3BV	C43-C42	-3.25	1.48	1.52
15	H	301	3BV	C20-N22	3.24	1.41	1.34
15	V	301	3BV	C20-N22	3.24	1.41	1.34
15	3	301	3BV	C20-N22	3.23	1.41	1.34
15	k	301	3BV	O29-C28	-3.10	1.17	1.23
15	j	301	3BV	O29-C28	-3.02	1.17	1.23
15	k	301	3BV	C43-C42	-2.97	1.48	1.52
15	j	301	3BV	C31-C39	2.94	1.60	1.52
15	Z	301	3BV	C42-N41	-2.93	1.41	1.46
15	Z	301	3BV	C23-N22	-2.86	1.39	1.45
15	j	301	3BV	C43-C42	-2.83	1.48	1.52
15	Z	301	3BV	C46-C44	-2.80	1.36	1.51
15	y	301	3BV	C16-C15	2.67	1.44	1.38
15	3	301	3BV	C16-C15	2.66	1.44	1.38
15	H	301	3BV	C16-C15	2.66	1.44	1.38
15	V	301	3BV	C16-C15	2.66	1.44	1.38
15	Z	301	3BV	C23-C28	-2.49	1.46	1.52
15	L	301	3BV	C23-C28	-2.41	1.46	1.52
15	Z	301	3BV	C35-C34	-2.40	1.33	1.38
15	k	301	3BV	C31-C39	2.35	1.59	1.52
15	W	301	3BV	C47-C42	-2.33	1.49	1.53
15	k	301	3BV	C20-N22	2.33	1.39	1.34
15	L	301	3BV	C23-N22	-2.30	1.41	1.45
15	W	301	3BV	C31-C39	2.29	1.58	1.52
15	I	301	3BV	C23-N22	-2.27	1.41	1.45
15	y	301	3BV	O40-C39	-2.26	1.18	1.23
15	j	301	3BV	C16-C15	2.25	1.43	1.38
15	V	301	3BV	C43-C42	-2.24	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	3	301	3BV	C43-C42	-2.23	1.49	1.52
15	3	301	3BV	O40-C39	-2.22	1.19	1.23
15	V	301	3BV	O40-C39	-2.21	1.19	1.23
15	W	301	3BV	C35-C34	-2.21	1.34	1.38
15	W	301	3BV	C20-N22	2.20	1.38	1.34
15	I	301	3BV	C42-N41	-2.19	1.42	1.46
15	L	301	3BV	C42-N41	-2.19	1.42	1.46
15	H	301	3BV	C43-C42	-2.18	1.49	1.52
15	H	301	3BV	O40-C39	-2.18	1.19	1.23
15	y	301	3BV	C43-C42	-2.18	1.49	1.52
15	y	301	3BV	O60-C59	-2.14	1.33	1.42
15	n	301	3BV	C31-C39	2.13	1.58	1.52
15	L	301	3BV	O21-C20	-2.12	1.19	1.23
15	k	301	3BV	C35-C34	-2.08	1.34	1.38
15	3	301	3BV	O29-C28	-2.08	1.19	1.23
15	I	301	3BV	C31-C39	2.07	1.58	1.52
15	H	301	3BV	O29-C28	-2.05	1.19	1.23
15	V	301	3BV	O29-C28	-2.03	1.19	1.23
15	n	301	3BV	C35-C34	-2.03	1.34	1.38
15	y	301	3BV	O29-C28	-2.03	1.19	1.23
15	I	301	3BV	C16-C15	2.01	1.43	1.38

All (172) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	Z	301	3BV	C44-C43-C42	10.34	136.42	115.84
15	j	301	3BV	O48-C47-C51	-10.06	90.93	109.83
15	Z	301	3BV	C58-C51-C59	-9.55	97.33	109.88
15	y	301	3BV	O48-C47-C51	9.25	127.20	109.83
15	Z	301	3BV	O48-C47-C42	8.72	129.84	108.98
15	L	301	3BV	C58-C51-C59	-8.30	98.97	109.88
15	I	301	3BV	C58-C51-C59	-8.19	99.12	109.88
15	Z	301	3BV	C43-C42-N41	-7.79	100.11	110.18
15	n	301	3BV	C58-C51-C59	-7.56	99.95	109.88
15	Z	301	3BV	C46-C44-C43	7.53	138.80	111.11
15	I	301	3BV	O48-C47-C51	7.40	123.72	109.83
15	Z	301	3BV	C20-C11-N10	-6.79	92.68	111.16
15	W	301	3BV	O48-C47-C42	6.40	124.29	108.98
15	j	301	3BV	C7-N4-C5	5.97	120.36	111.09
15	n	301	3BV	O48-C47-C42	5.82	122.90	108.98
15	Z	301	3BV	C7-N4-C5	5.72	119.96	111.09
15	j	301	3BV	C32-C31-C39	5.33	124.08	110.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	W	301	3BV	C58-C51-C59	-5.30	102.91	109.88
15	3	301	3BV	C7-N4-C5	5.15	119.08	111.09
15	V	301	3BV	C7-N4-C5	5.14	119.07	111.09
15	y	301	3BV	C7-N4-C5	5.14	119.06	111.09
15	H	301	3BV	C7-N4-C5	5.12	119.04	111.09
15	j	301	3BV	C8-C7-N4	4.71	124.28	113.36
15	k	301	3BV	C58-C51-C59	-4.67	103.74	109.88
15	I	301	3BV	C7-N4-C5	4.67	118.33	111.09
15	3	301	3BV	O48-C47-C42	4.65	120.10	108.98
15	j	301	3BV	C43-C42-N41	-4.60	104.24	110.18
15	3	301	3BV	C32-C31-C39	4.51	121.96	110.25
15	V	301	3BV	C32-C31-C39	4.50	121.94	110.25
15	y	301	3BV	C32-C31-C39	4.50	121.94	110.25
15	H	301	3BV	C32-C31-C39	4.49	121.90	110.25
15	n	301	3BV	C24-C23-N22	4.47	120.88	110.58
15	L	301	3BV	C7-N4-C5	4.44	117.98	111.09
15	Z	301	3BV	C13-C12-C11	4.41	121.91	113.21
15	j	301	3BV	C58-C51-C59	-4.40	104.09	109.88
15	I	301	3BV	C7-N4-C3	4.20	117.60	111.09
15	n	301	3BV	C24-C23-C28	4.18	120.53	110.57
15	n	301	3BV	C3-N4-C5	4.18	118.23	108.83
15	V	301	3BV	O48-C47-C51	4.17	117.66	109.83
15	Z	301	3BV	C42-N41-C39	-4.10	115.83	123.07
15	I	301	3BV	C3-N4-C5	4.04	117.93	108.83
15	3	301	3BV	C7-N4-C3	3.98	117.26	111.09
15	V	301	3BV	C7-N4-C3	3.98	117.26	111.09
15	H	301	3BV	C7-N4-C3	3.97	117.25	111.09
15	Z	301	3BV	O48-C47-C51	-3.96	102.38	109.83
15	y	301	3BV	C7-N4-C3	3.96	117.23	111.09
15	W	301	3BV	C12-C11-C20	3.95	119.42	110.20
15	k	301	3BV	O48-C47-C51	3.94	117.23	109.83
15	k	301	3BV	C13-C12-C11	3.93	120.95	113.21
15	L	301	3BV	C3-N4-C5	3.91	117.62	108.83
15	n	301	3BV	C7-N4-C5	3.89	117.13	111.09
15	n	301	3BV	O60-C59-C51	3.83	119.15	111.33
15	W	301	3BV	C13-C12-C11	3.77	120.65	113.21
15	L	301	3BV	O60-C59-C51	3.70	118.89	111.33
15	L	301	3BV	C7-C8-N10	3.67	123.59	115.31
15	k	301	3BV	C7-N4-C5	3.63	116.72	111.09
15	j	301	3BV	O60-C59-C51	3.59	118.67	111.33
15	W	301	3BV	C3-N4-C5	3.57	116.87	108.83
15	k	301	3BV	C8-C7-N4	3.47	121.40	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	k	301	3BV	C3-N4-C5	3.44	116.57	108.83
15	Z	301	3BV	O60-C59-C51	3.44	118.36	111.33
15	W	301	3BV	O60-C59-C51	3.35	118.18	111.33
15	y	301	3BV	O60-C59-C51	3.34	118.15	111.33
15	k	301	3BV	O60-C59-C51	3.31	118.10	111.33
15	k	301	3BV	C44-C43-C42	3.30	122.42	115.84
15	Z	301	3BV	C3-N4-C5	3.28	116.21	108.83
15	n	301	3BV	C7-C8-N10	3.27	122.69	115.31
15	j	301	3BV	C20-C11-N10	-3.24	102.34	111.16
15	Z	301	3BV	C38-C33-C34	3.22	123.23	118.17
15	n	301	3BV	C39-C31-N30	-3.20	102.44	111.16
15	k	301	3BV	C32-C31-C39	3.18	118.50	110.25
15	k	301	3BV	C7-N4-C3	3.14	115.97	111.09
15	Z	301	3BV	C39-C31-N30	-3.14	102.62	111.16
15	H	301	3BV	O60-C59-C51	3.11	117.68	111.33
15	H	301	3BV	O48-C47-C42	3.11	116.41	108.98
15	V	301	3BV	O60-C59-C51	3.10	117.67	111.33
15	3	301	3BV	O60-C59-C51	3.09	117.65	111.33
15	H	301	3BV	C3-N4-C5	3.07	115.75	108.83
15	n	301	3BV	C58-C51-C47	3.07	117.23	111.54
15	y	301	3BV	C3-N4-C5	3.07	115.73	108.83
15	W	301	3BV	O48-C47-C51	-3.06	104.08	109.83
15	3	301	3BV	C3-N4-C5	3.05	115.69	108.83
15	Z	301	3BV	C7-N4-C3	3.05	115.82	111.09
15	j	301	3BV	C24-C23-N22	3.03	117.56	110.58
15	W	301	3BV	C7-N4-C5	3.03	115.79	111.09
15	j	301	3BV	C32-C31-N30	3.02	117.14	110.79
15	Z	301	3BV	C37-C38-C33	-3.01	116.01	120.63
15	n	301	3BV	O9-C8-N10	-3.01	117.88	122.95
15	W	301	3BV	C38-C33-C34	2.98	122.84	118.17
15	3	301	3BV	C58-C51-C59	-2.96	105.99	109.88
15	I	301	3BV	C59-C51-C47	-2.94	105.43	110.99
15	H	301	3BV	C58-C51-C59	-2.93	106.03	109.88
15	j	301	3BV	C42-N41-C39	-2.92	117.91	123.07
15	V	301	3BV	C58-C51-C59	-2.91	106.05	109.88
15	n	301	3BV	C8-C7-N4	2.85	119.98	113.36
15	k	301	3BV	C7-C8-N10	2.82	121.68	115.31
15	I	301	3BV	O60-C59-C51	2.80	117.06	111.33
15	y	301	3BV	C58-C51-C59	-2.80	106.20	109.88
15	W	301	3BV	O9-C8-N10	-2.79	118.24	122.95
15	L	301	3BV	C7-N4-C3	2.79	115.42	111.09
15	I	301	3BV	C43-C42-N41	-2.78	106.58	110.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	H	301	3BV	C8-C7-N4	2.78	119.81	113.36
15	V	301	3BV	C8-C7-N4	2.78	119.80	113.36
15	y	301	3BV	C8-C7-N4	2.78	119.80	113.36
15	n	301	3BV	C32-C31-C39	2.77	117.44	110.25
15	I	301	3BV	C32-C31-C39	2.77	117.44	110.25
15	3	301	3BV	C8-C7-N4	2.77	119.78	113.36
15	j	301	3BV	C44-C43-C42	2.76	121.34	115.84
15	L	301	3BV	O9-C8-N10	-2.76	118.30	122.95
15	W	301	3BV	C11-C20-N22	2.75	122.73	116.70
15	Z	301	3BV	C58-C51-C47	2.73	116.60	111.54
15	L	301	3BV	C32-C31-C39	2.73	117.33	110.25
15	L	301	3BV	O48-C47-C42	2.73	115.50	108.98
15	L	301	3BV	C38-C33-C34	2.70	122.42	118.17
15	Z	301	3BV	C2-O1-C6	2.68	118.86	109.89
15	k	301	3BV	C23-N22-C20	2.68	127.41	121.67
15	W	301	3BV	C32-C31-C39	2.63	117.07	110.25
15	n	301	3BV	C42-N41-C39	-2.62	118.45	123.07
15	j	301	3BV	O9-C8-N10	-2.61	118.54	122.95
15	j	301	3BV	C3-N4-C5	2.59	114.65	108.83
15	L	301	3BV	C42-N41-C39	-2.56	118.56	123.07
15	j	301	3BV	C7-N4-C3	2.53	115.02	111.09
15	Z	301	3BV	O9-C8-N10	-2.52	118.70	122.95
15	I	301	3BV	O9-C8-N10	-2.49	118.74	122.95
15	I	301	3BV	C39-C31-N30	-2.49	104.40	111.16
15	I	301	3BV	C42-N41-C39	-2.47	118.71	123.07
15	Z	301	3BV	C36-C35-C34	-2.46	116.44	120.19
15	n	301	3BV	C20-C11-N10	-2.45	104.49	111.16
15	I	301	3BV	C7-C8-N10	2.45	120.83	115.31
15	n	301	3BV	C15-C14-C19	2.43	121.99	118.17
15	L	301	3BV	C8-C7-N4	2.42	118.98	113.36
15	n	301	3BV	C38-C33-C34	2.42	121.97	118.17
15	W	301	3BV	C58-C51-C47	2.39	115.97	111.54
15	k	301	3BV	C12-C11-C20	-2.38	104.64	110.20
15	n	301	3BV	C7-N4-C3	2.37	114.77	111.09
15	j	301	3BV	C39-C31-N30	-2.35	104.77	111.16
15	W	301	3BV	C7-C8-N10	2.33	120.57	115.31
15	W	301	3BV	C7-N4-C3	2.33	114.70	111.09
15	L	301	3BV	O1-C6-C5	-2.32	106.68	111.80
15	k	301	3BV	C15-C14-C19	2.31	121.80	118.17
15	y	301	3BV	C59-C51-C47	-2.28	106.68	110.99
15	k	301	3BV	C2-O1-C6	2.28	117.49	109.89
15	I	301	3BV	C13-C12-C11	2.24	117.63	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	j	301	3BV	C33-C32-C31	2.24	119.57	113.39
15	I	301	3BV	C25-C24-C23	2.23	121.57	115.43
15	V	301	3BV	C13-C12-C11	2.22	117.59	113.21
15	H	301	3BV	C13-C12-C11	2.22	117.58	113.21
15	I	301	3BV	C24-C23-C28	-2.20	105.32	110.57
15	y	301	3BV	C13-C12-C11	2.20	117.55	113.21
15	W	301	3BV	C2-C3-N4	2.20	113.44	110.10
15	3	301	3BV	C13-C12-C11	2.20	117.54	113.21
15	W	301	3BV	C8-C7-N4	2.19	118.44	113.36
15	L	301	3BV	C2-O1-C6	2.19	117.19	109.89
15	L	301	3BV	C15-C14-C19	2.18	121.59	118.17
15	W	301	3BV	C15-C14-C19	2.18	121.59	118.17
15	W	301	3BV	C20-C11-N10	-2.18	105.24	111.16
15	k	301	3BV	C38-C33-C34	2.14	121.53	118.17
15	Z	301	3BV	C23-C28-N30	-2.14	112.01	116.70
15	y	301	3BV	C7-C8-N10	2.13	120.12	115.31
15	n	301	3BV	C35-C34-C33	-2.13	117.36	120.63
15	H	301	3BV	C7-C8-N10	2.13	120.11	115.31
15	V	301	3BV	C7-C8-N10	2.13	120.11	115.31
15	j	301	3BV	C2-O1-C6	2.13	116.99	109.89
15	3	301	3BV	C7-C8-N10	2.13	120.11	115.31
15	k	301	3BV	C25-C24-C23	2.12	121.28	115.43
15	n	301	3BV	C2-O1-C6	2.12	116.97	109.89
15	j	301	3BV	C11-C20-N22	2.12	121.35	116.70
15	j	301	3BV	C7-C8-N10	2.09	120.02	115.31
15	Z	301	3BV	C7-C8-N10	2.06	119.96	115.31
15	H	301	3BV	O9-C8-N10	-2.02	119.54	122.95
15	3	301	3BV	O9-C8-N10	-2.02	119.55	122.95
15	L	301	3BV	C37-C38-C33	-2.01	117.55	120.63

There are no chirality outliers.

All (232) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	H	301	3BV	C11-C12-C13-C14
15	H	301	3BV	N41-C42-C43-C44
15	H	301	3BV	C47-C42-C43-C44
15	H	301	3BV	N41-C42-C47-C51
15	H	301	3BV	N41-C42-C47-O48
15	H	301	3BV	C43-C42-C47-C51
15	H	301	3BV	C43-C42-C47-O48
15	H	301	3BV	C42-C47-C51-C58

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Mol	Chain	Res	Type	Atoms
15	H	301	3BV	C42-C47-C51-C59
15	H	301	3BV	C47-C51-C59-O60
15	H	301	3BV	C58-C51-C59-O60
15	I	301	3BV	N41-C42-C47-C51
15	I	301	3BV	C43-C42-C47-C51
15	I	301	3BV	C42-C47-C51-C58
15	I	301	3BV	C42-C47-C51-C59
15	L	301	3BV	C8-C7-N4-C5
15	L	301	3BV	N41-C42-C47-C51
15	L	301	3BV	N41-C42-C47-O48
15	L	301	3BV	C43-C42-C47-C51
15	L	301	3BV	C43-C42-C47-O48
15	L	301	3BV	C42-C47-C51-C58
15	L	301	3BV	C42-C47-C51-C59
15	V	301	3BV	C8-C7-N4-C3
15	V	301	3BV	C11-C12-C13-C14
15	V	301	3BV	N22-C23-C24-C25
15	V	301	3BV	N41-C42-C47-C51
15	V	301	3BV	C43-C42-C47-C51
15	V	301	3BV	C42-C47-C51-C58
15	V	301	3BV	C42-C47-C51-C59
15	V	301	3BV	C47-C51-C59-O60
15	V	301	3BV	C58-C51-C59-O60
15	W	301	3BV	C8-C7-N4-C5
15	W	301	3BV	N41-C42-C47-C51
15	W	301	3BV	N41-C42-C47-O48
15	W	301	3BV	C43-C42-C47-C51
15	W	301	3BV	C43-C42-C47-O48
15	W	301	3BV	C42-C47-C51-C58
15	W	301	3BV	C42-C47-C51-C59
15	Z	301	3BV	C8-C7-N4-C5
15	Z	301	3BV	N41-C42-C47-C51
15	Z	301	3BV	N41-C42-C47-O48
15	Z	301	3BV	C43-C42-C47-C51
15	Z	301	3BV	C43-C42-C47-O48
15	Z	301	3BV	C42-C47-C51-C58
15	Z	301	3BV	C42-C47-C51-C59
15	j	301	3BV	C8-C7-N4-C5
15	j	301	3BV	C11-C12-C13-C14
15	j	301	3BV	N41-C42-C47-O48
15	j	301	3BV	C47-C51-C59-O60
15	k	301	3BV	C8-C7-N4-C3

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Mol	Chain	Res	Type	Atoms
15	k	301	3BV	N41-C42-C47-C51
15	k	301	3BV	C43-C42-C47-C51
15	k	301	3BV	C47-C51-C59-O60
15	k	301	3BV	C58-C51-C59-O60
15	n	301	3BV	C8-C7-N4-C5
15	n	301	3BV	N41-C42-C47-C51
15	n	301	3BV	N41-C42-C47-O48
15	n	301	3BV	C43-C42-C47-C51
15	n	301	3BV	C43-C42-C47-O48
15	n	301	3BV	C42-C47-C51-C58
15	n	301	3BV	C42-C47-C51-C59
15	y	301	3BV	N41-C42-C47-C51
15	y	301	3BV	C43-C42-C47-C51
15	y	301	3BV	C42-C47-C51-C58
15	y	301	3BV	C42-C47-C51-C59
15	y	301	3BV	C47-C51-C59-O60
15	y	301	3BV	C58-C51-C59-O60
15	3	301	3BV	C8-C7-N4-C5
15	3	301	3BV	N10-C11-C12-C13
15	3	301	3BV	C43-C42-C47-C51
15	3	301	3BV	C42-C47-C51-C58
15	3	301	3BV	C42-C47-C51-C59
15	y	301	3BV	C39-C31-C32-C33
15	k	301	3BV	N10-C11-C12-C13
15	n	301	3BV	C39-C31-C32-C33
15	H	301	3BV	O9-C8-N10-C11
15	I	301	3BV	N22-C23-C24-C25
15	n	301	3BV	N30-C31-C32-C33
15	k	301	3BV	C20-C11-C12-C13
15	y	301	3BV	C20-C11-C12-C13
15	k	301	3BV	N22-C23-C24-C25
15	j	301	3BV	C32-C31-C39-N41
15	j	301	3BV	C23-C24-C25-C27
15	I	301	3BV	C28-C23-C24-C25
15	k	301	3BV	C28-C23-C24-C25
15	j	301	3BV	C32-C31-C39-O40
15	y	301	3BV	N10-C11-C12-C13
15	V	301	3BV	C23-C24-C25-C26
15	Z	301	3BV	C28-C23-C24-C25
15	n	301	3BV	C23-C24-C25-C26
15	j	301	3BV	C23-C24-C25-C26
15	Z	301	3BV	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
15	y	301	3BV	C23-C24-C25-C26
15	k	301	3BV	C23-C24-C25-C27
15	n	301	3BV	C23-C24-C25-C27
15	H	301	3BV	C42-C43-C44-C45
15	j	301	3BV	C42-C43-C44-C45
15	H	301	3BV	C7-C8-N10-C11
15	V	301	3BV	C42-C43-C44-C46
15	W	301	3BV	C42-C43-C44-C46
15	I	301	3BV	C23-C24-C25-C27
15	y	301	3BV	N22-C23-C24-C25
15	V	301	3BV	C23-C24-C25-C27
15	n	301	3BV	C28-C23-C24-C25
15	y	301	3BV	C28-C23-C24-C25
15	Z	301	3BV	N30-C31-C32-C33
15	V	301	3BV	C20-C11-N10-C8
15	I	301	3BV	C42-C43-C44-C45
15	V	301	3BV	C32-C31-C39-O40
15	L	301	3BV	O48-C47-C51-C59
15	V	301	3BV	O48-C47-C51-C58
15	Z	301	3BV	O48-C47-C51-C58
15	Z	301	3BV	O48-C47-C51-C59
15	y	301	3BV	C32-C31-C39-O40
15	V	301	3BV	C42-C43-C44-C45
15	k	301	3BV	C23-C24-C25-C26
15	y	301	3BV	C32-C31-C39-N41
15	Z	301	3BV	C23-C24-C25-C27
15	Z	301	3BV	N22-C23-C24-C25
15	V	301	3BV	C32-C31-C39-N41
15	j	301	3BV	C42-C47-C51-C58
15	k	301	3BV	C42-C47-C51-C58
15	y	301	3BV	N30-C31-C32-C33
15	V	301	3BV	C28-C23-C24-C25
15	L	301	3BV	C28-C23-C24-C25
15	j	301	3BV	C42-C43-C44-C46
15	H	301	3BV	C23-C24-C25-C26
15	I	301	3BV	O48-C47-C51-C58
15	L	301	3BV	O48-C47-C51-C58
15	W	301	3BV	O48-C47-C51-C58
15	j	301	3BV	O48-C47-C51-C58
15	n	301	3BV	O48-C47-C51-C58
15	n	301	3BV	O48-C47-C51-C59
15	Z	301	3BV	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
15	I	301	3BV	C8-C7-N4-C5
15	Z	301	3BV	C8-C7-N4-C3
15	I	301	3BV	N10-C11-C12-C13
15	j	301	3BV	N22-C23-C24-C25
15	Z	301	3BV	N4-C7-C8-O9
15	W	301	3BV	C23-C24-C25-C27
15	L	301	3BV	N22-C23-C24-C25
15	j	301	3BV	N41-C42-C43-C44
15	3	301	3BV	N41-C42-C43-C44
15	V	301	3BV	N30-C31-C39-O40
15	y	301	3BV	N30-C31-C39-O40
15	W	301	3BV	C28-C23-C24-C25
15	y	301	3BV	C23-C24-C25-C27
15	H	301	3BV	C8-C7-N4-C5
15	I	301	3BV	C8-C7-N4-C3
15	n	301	3BV	C8-C7-N4-C3
15	Z	301	3BV	N10-C11-C12-C13
15	H	301	3BV	C42-C43-C44-C46
15	j	301	3BV	C31-C32-C33-C34
15	V	301	3BV	C12-C11-N10-C8
15	y	301	3BV	N4-C7-C8-N10
15	y	301	3BV	N30-C31-C39-N41
15	j	301	3BV	C31-C32-C33-C38
15	V	301	3BV	N30-C31-C39-N41
15	H	301	3BV	O48-C47-C51-C58
15	V	301	3BV	O48-C47-C51-C59
15	W	301	3BV	O48-C47-C51-C59
15	j	301	3BV	N4-C7-C8-O9
15	y	301	3BV	N4-C7-C8-O9
15	V	301	3BV	C43-C42-C47-O48
15	j	301	3BV	C43-C42-C47-O48
15	W	301	3BV	N30-C31-C39-O40
15	j	301	3BV	N30-C31-C39-O40
15	W	301	3BV	N30-C31-C39-N41
15	3	301	3BV	C28-C23-C24-C25
15	j	301	3BV	N22-C23-C28-O29
15	3	301	3BV	C20-C11-C12-C13
15	W	301	3BV	N22-C23-C24-C25
15	V	301	3BV	N22-C23-C28-O29
15	3	301	3BV	N41-C42-C47-C51
15	j	301	3BV	N4-C7-C8-N10
15	3	301	3BV	N22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
15	j	301	3BV	C47-C42-C43-C44
15	V	301	3BV	N22-C23-C28-N30
15	j	301	3BV	N22-C23-C28-N30
15	Z	301	3BV	N4-C7-C8-N10
15	I	301	3BV	C20-C11-C12-C13
15	H	301	3BV	C23-C24-C25-C27
15	L	301	3BV	C42-C43-C44-C45
15	Z	301	3BV	C39-C31-C32-C33
15	H	301	3BV	C20-C11-C12-C13
15	H	301	3BV	N10-C11-C12-C13
15	n	301	3BV	N10-C11-C12-C13
15	L	301	3BV	C23-C24-C25-C26
15	W	301	3BV	C12-C13-C14-C19
15	3	301	3BV	C12-C13-C14-C15
15	W	301	3BV	C20-C11-C12-C13
15	j	301	3BV	N30-C31-C39-N41
15	j	301	3BV	C12-C13-C14-C19
15	3	301	3BV	N10-C11-C20-O21
15	3	301	3BV	C12-C13-C14-C19
15	W	301	3BV	C12-C13-C14-C15
15	Z	301	3BV	C12-C13-C14-C19
15	j	301	3BV	C12-C13-C14-C15
15	3	301	3BV	C32-C31-C39-O40
15	n	301	3BV	C12-C13-C14-C15
15	L	301	3BV	N4-C7-C8-O9
15	I	301	3BV	N30-C31-C39-O40
15	Z	301	3BV	C12-C13-C14-C15
15	I	301	3BV	C12-C13-C14-C15
15	n	301	3BV	C12-C13-C14-C19
15	W	301	3BV	C42-C43-C44-C45
15	3	301	3BV	N4-C7-C8-O9
15	3	301	3BV	C23-C24-C25-C27
15	3	301	3BV	N10-C11-C20-N22
15	I	301	3BV	C23-C24-C25-C26
15	W	301	3BV	C32-C31-C39-O40
15	I	301	3BV	C12-C13-C14-C19
15	k	301	3BV	N30-C31-C39-O40
15	I	301	3BV	N30-C31-C39-N41
15	H	301	3BV	C8-C7-N4-C3
15	V	301	3BV	N41-C42-C47-O48
15	3	301	3BV	C32-C31-C39-N41
15	j	301	3BV	O48-C47-C51-C59

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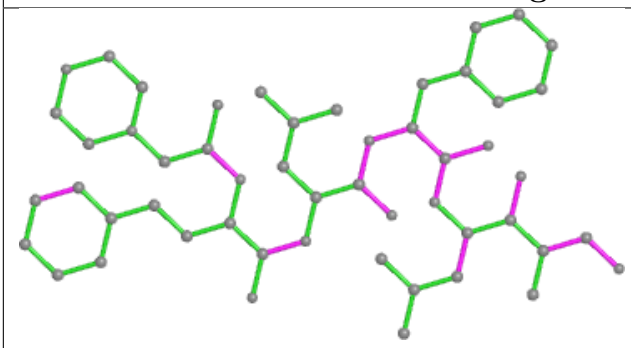
Mol	Chain	Res	Type	Atoms
15	j	301	3BV	N30-C31-C32-C33
15	L	301	3BV	N30-C31-C39-O40
15	W	301	3BV	C32-C31-C39-N41
15	W	301	3BV	N10-C11-C12-C13
15	j	301	3BV	C43-C42-N41-C39
15	k	301	3BV	N30-C31-C39-N41
15	3	301	3BV	N30-C31-C39-O40
15	W	301	3BV	N4-C7-C8-O9
15	k	301	3BV	C42-C47-C51-C59
15	L	301	3BV	N30-C31-C39-N41
15	y	301	3BV	C12-C13-C14-C15
15	W	301	3BV	C8-C7-N4-C3
15	L	301	3BV	C12-C13-C14-C15
15	y	301	3BV	C12-C13-C14-C19

There are no ring outliers.

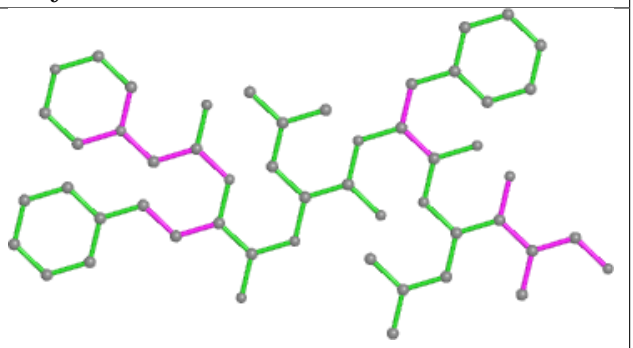
No monomer is involved in short contacts.

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.

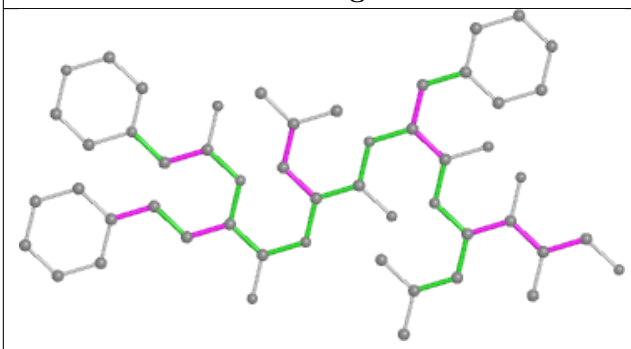
Ligand 3BV y 301



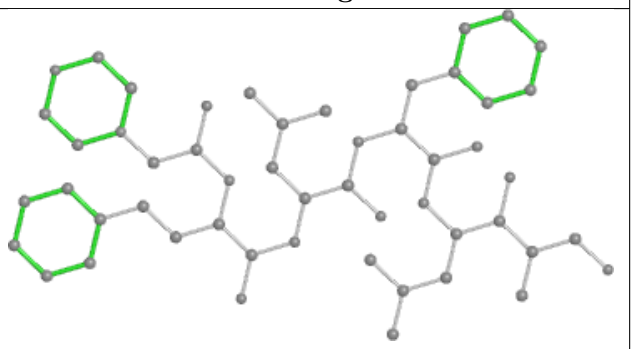
Bond lengths



Bond angles

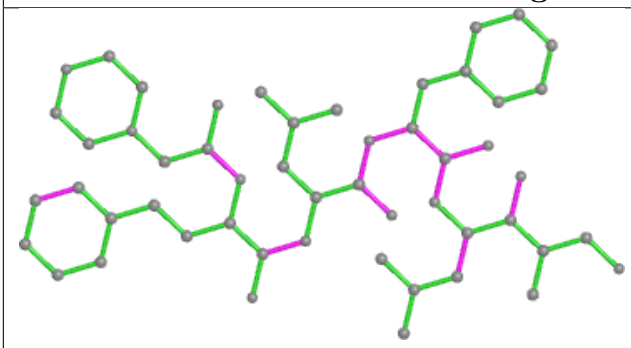


Torsions

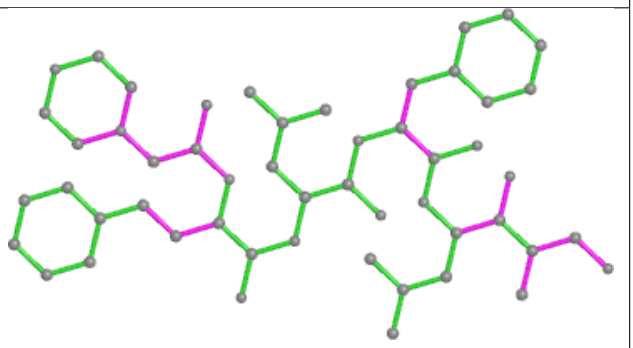


Rings

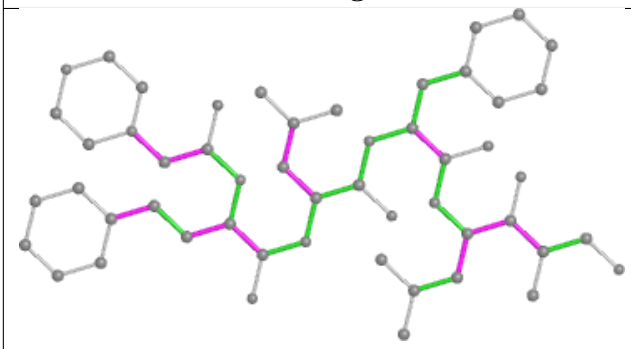
Ligand 3BV 3 301



Bond lengths



Bond angles



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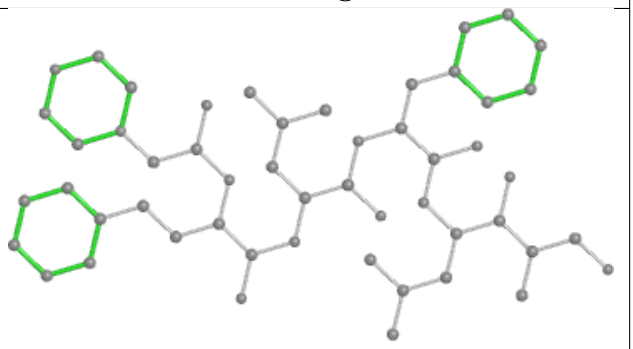
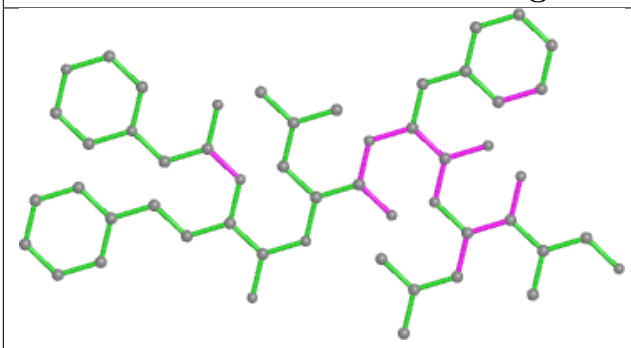
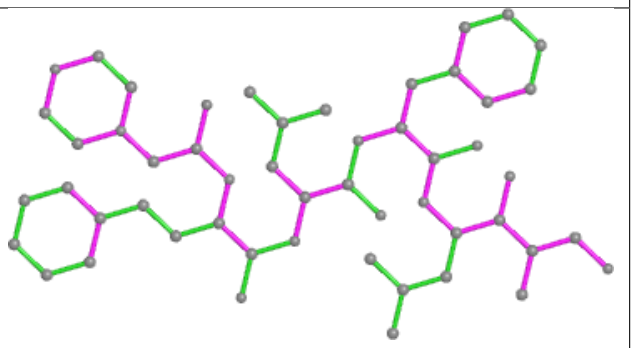


Rings

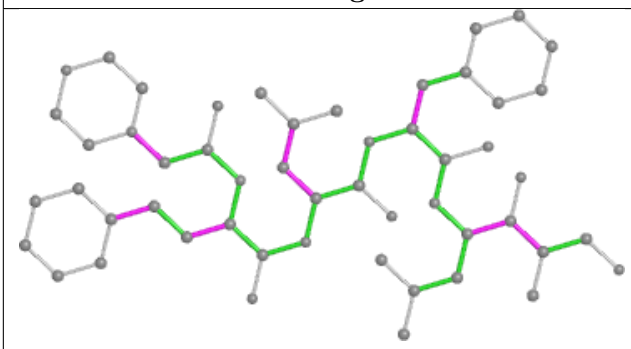
Ligand 3BV n 301



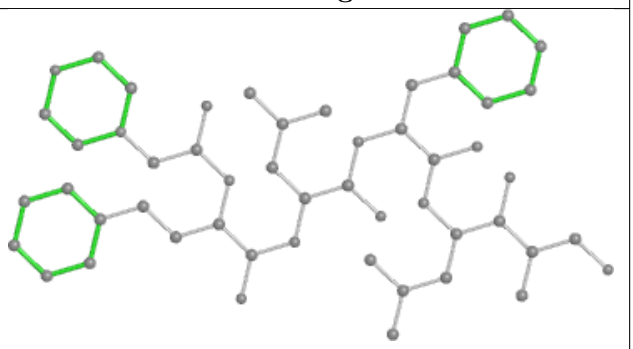
Bond lengths



Bond angles

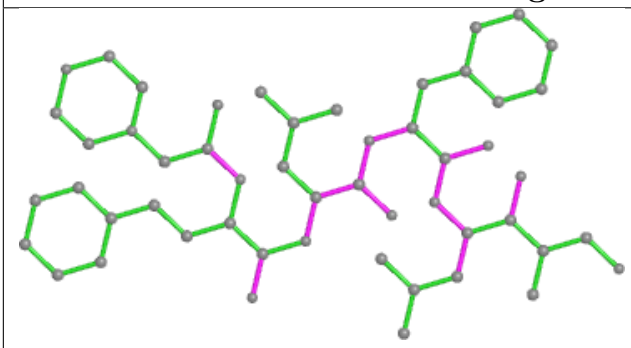


Torsions

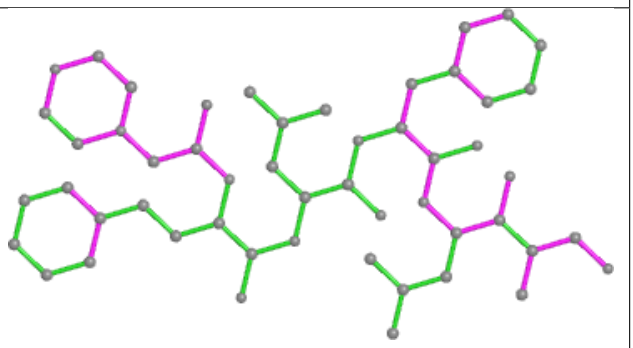


Rings

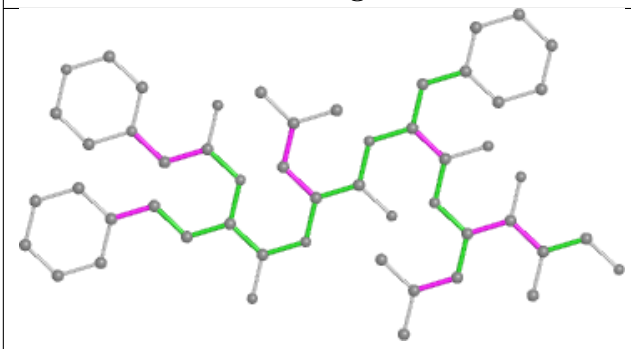
Ligand 3BV L 301



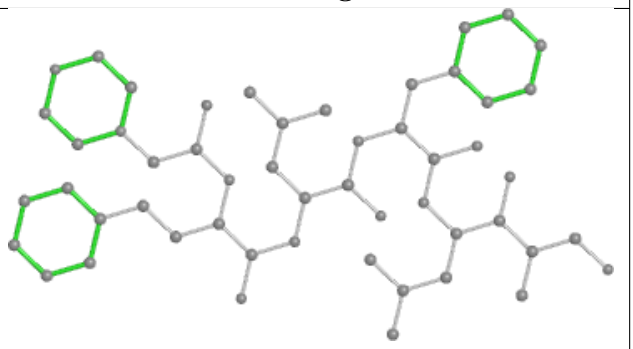
Bond lengths



Bond angles

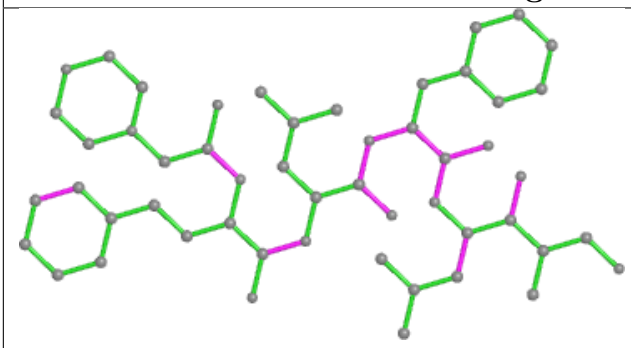


Torsions

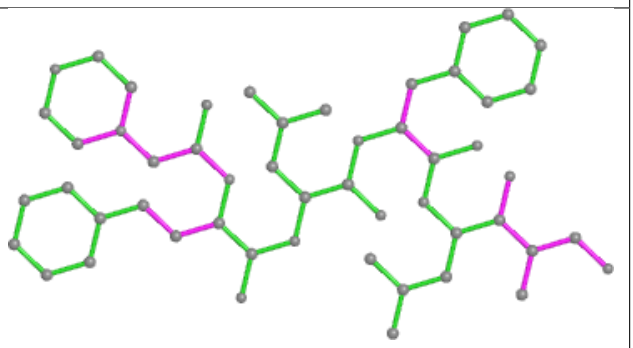


Rings

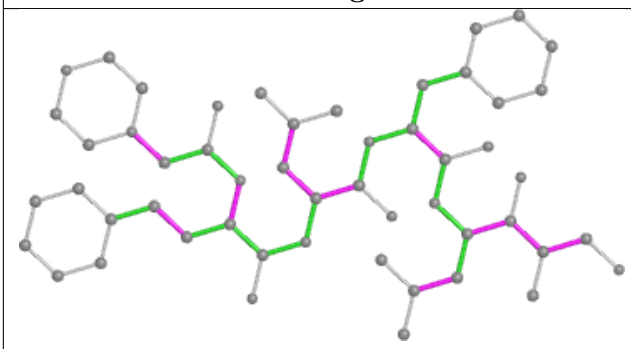
Ligand 3BV V 301



Bond lengths



Bond angles



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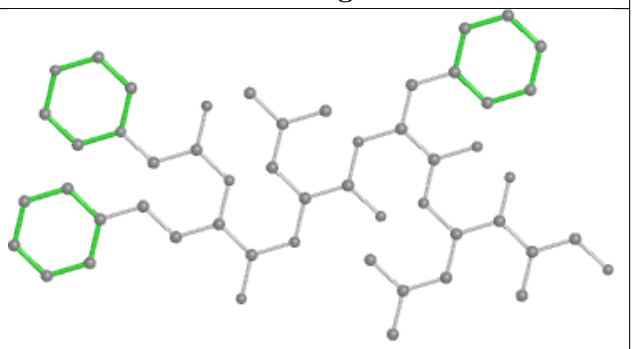
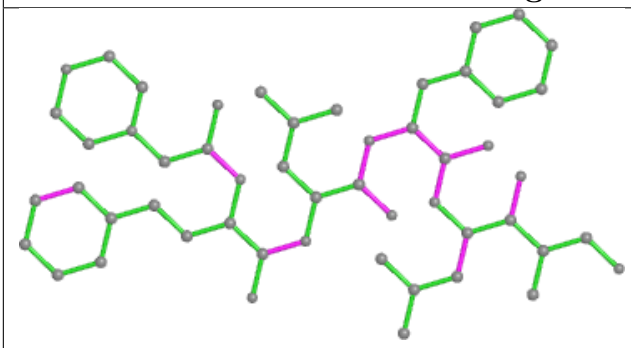


Rings

Ligand 3BV H 301



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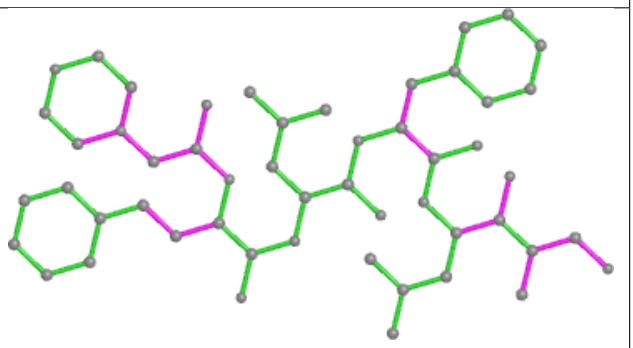
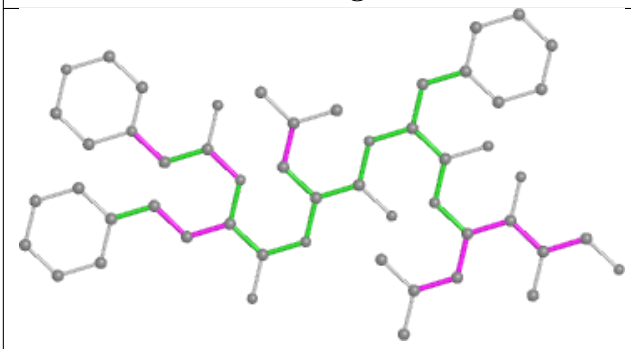


Bond angles



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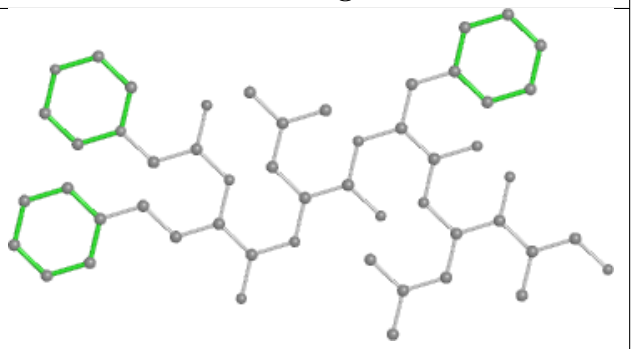
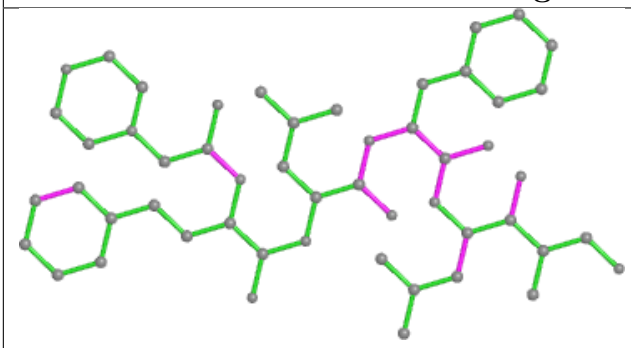
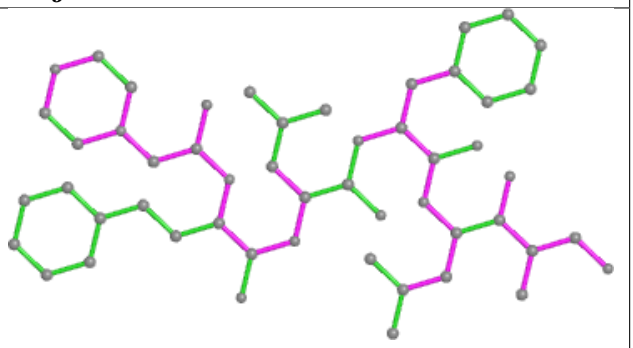


Rings

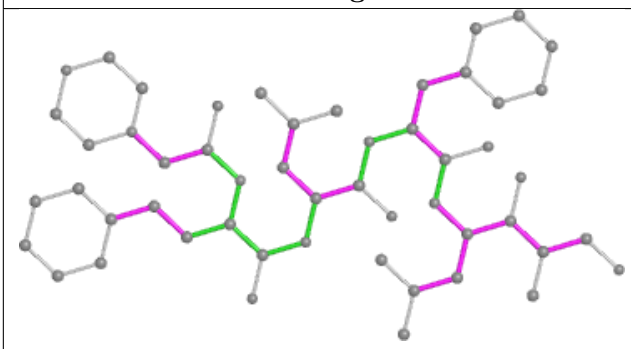
Ligand 3BV j 301



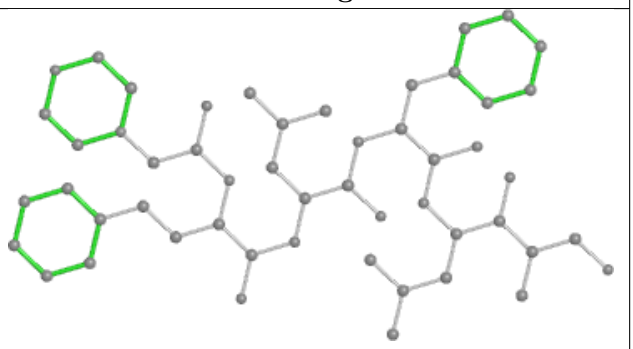
Bond lengths



Bond angles

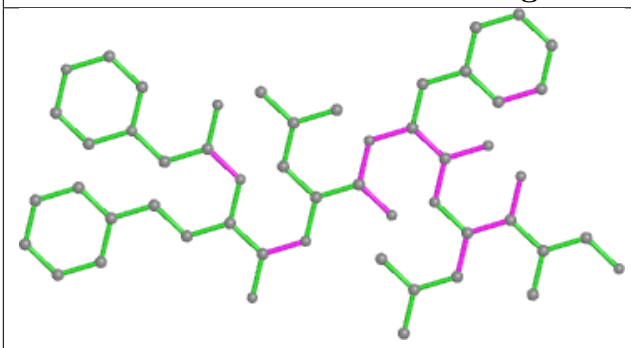


Torsions

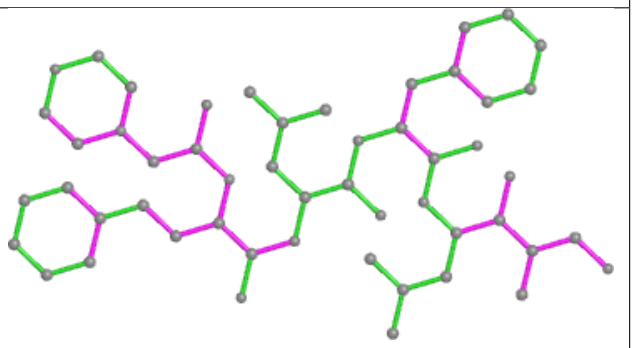


Rings

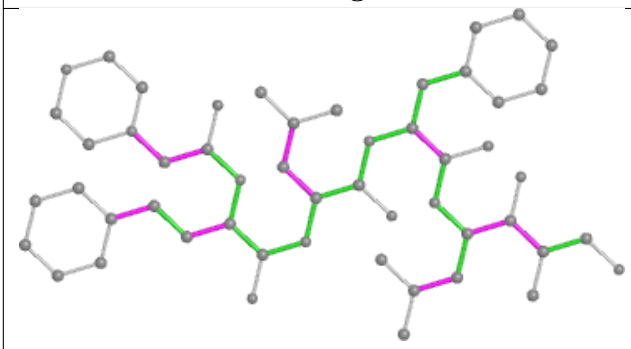
Ligand 3BV W 301



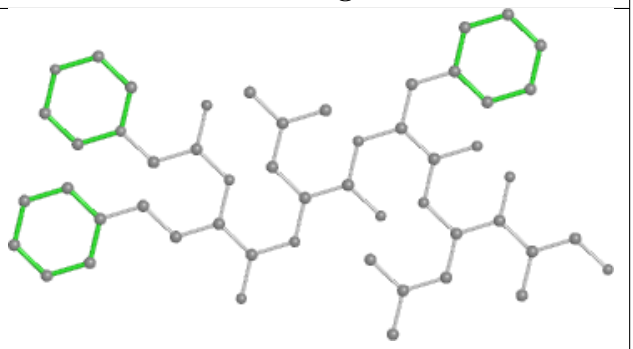
Bond lengths



Bond angles

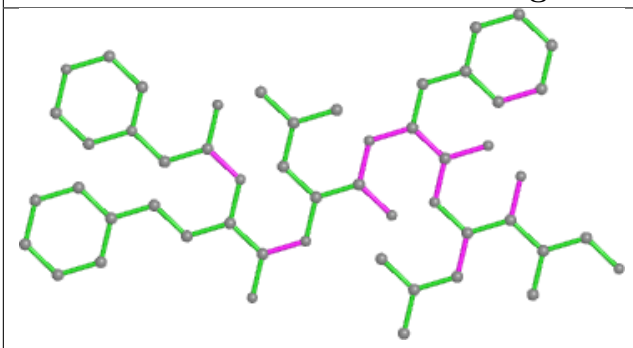


Torsions

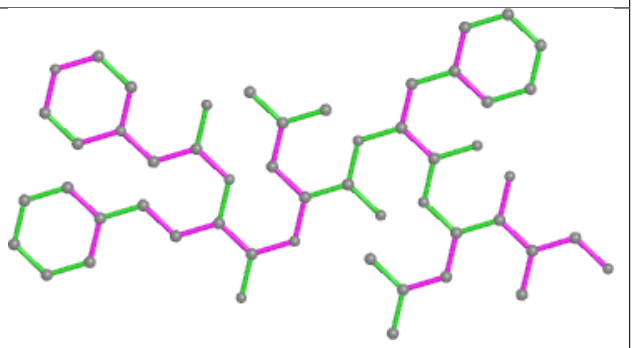


Rings

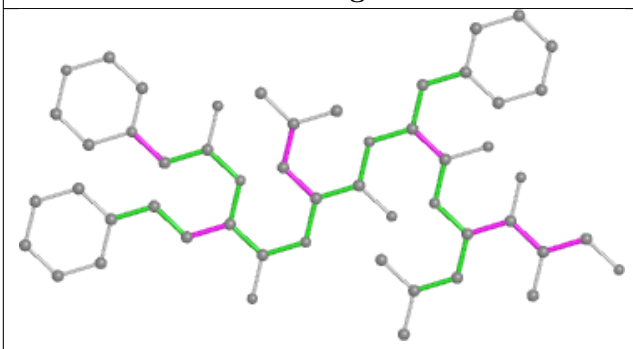
Ligand 3BV k 301



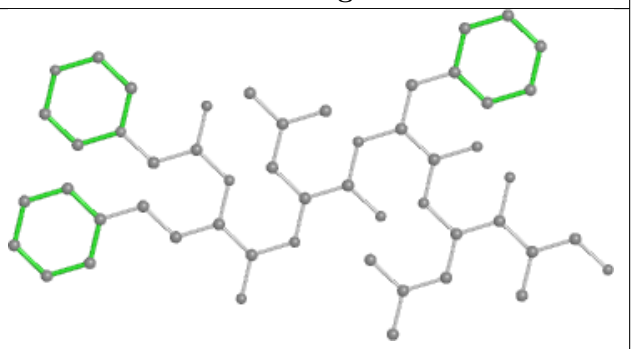
Bond lengths



Bond angles

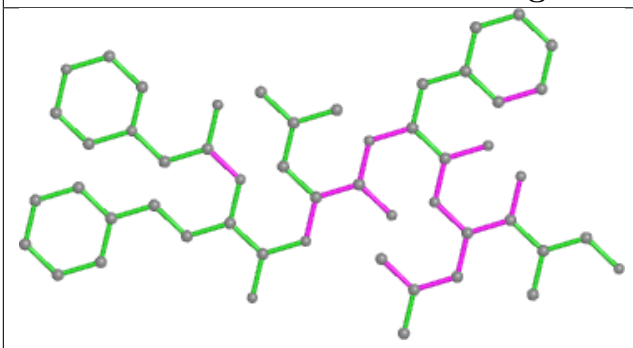


Torsions

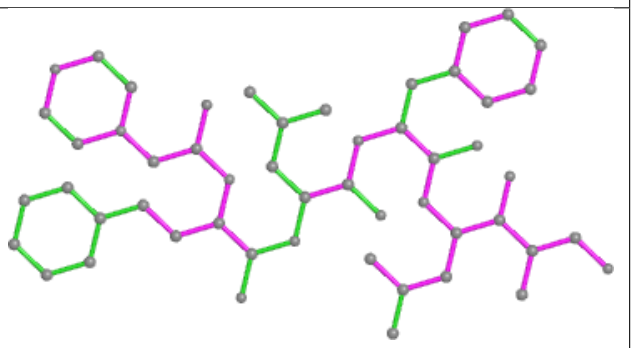


Rings

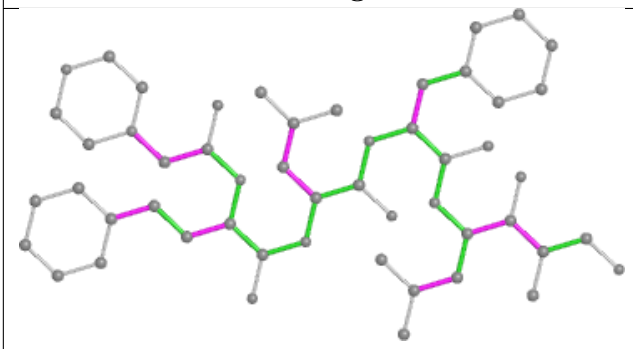
Ligand 3BV Z 301



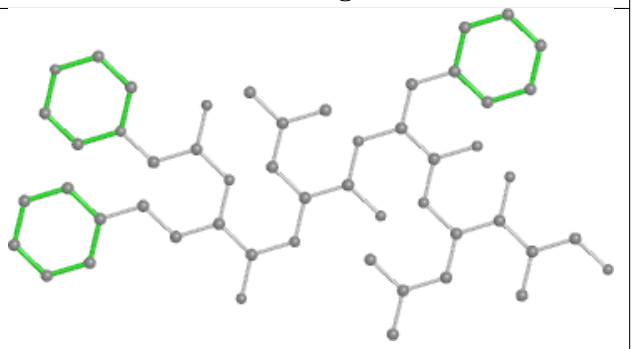
Bond lengths



Bond angles

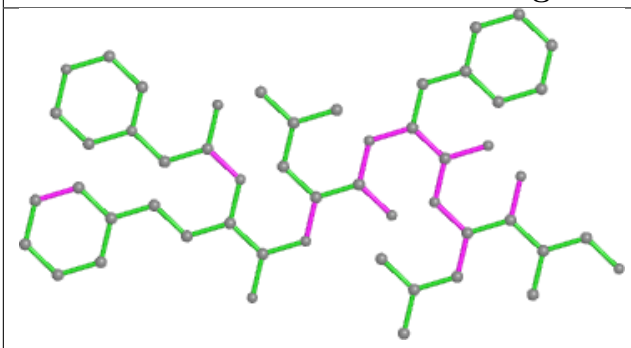


Torsions

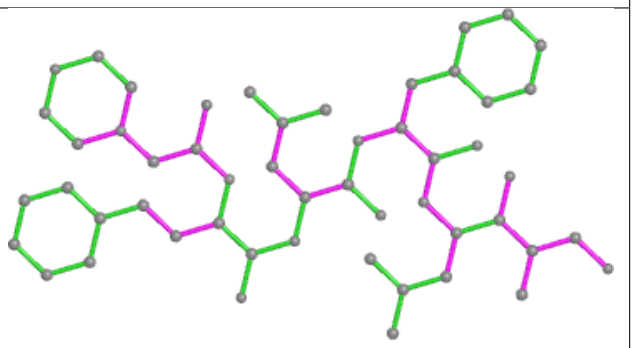


Rings

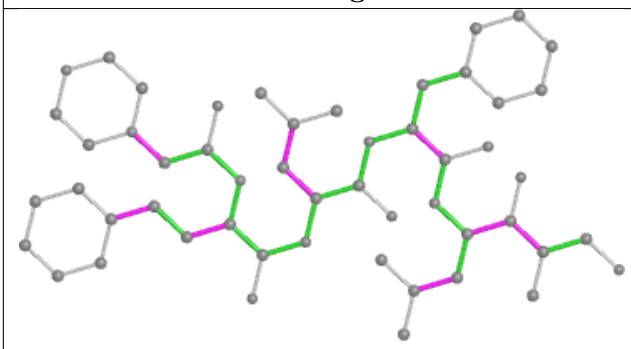
Ligand 3BV I 301



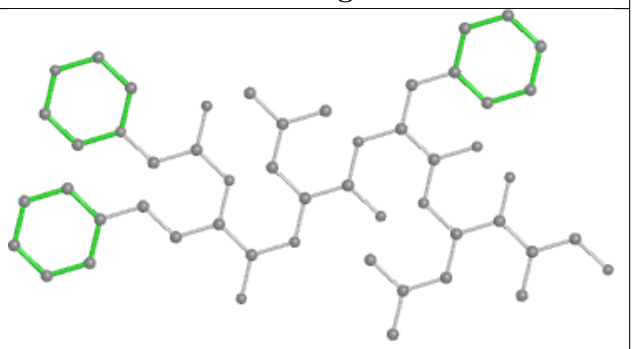
Bond lengths



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	244/244 (100%)	0.04	6 (2%)	57	55	48, 84, 133, 170	0
1	O	244/244 (100%)	0.01	6 (2%)	57	55	48, 80, 118, 153	0
1	c	244/244 (100%)	-0.00	7 (2%)	51	47	52, 89, 131, 180	0
1	q	244/244 (100%)	0.04	4 (1%)	72	71	55, 87, 130, 178	0
2	B	233/233 (100%)	-0.03	5 (2%)	63	61	48, 72, 123, 252	0
2	P	233/233 (100%)	-0.06	7 (3%)	50	45	47, 77, 121, 237	0
2	d	233/233 (100%)	-0.15	5 (2%)	63	61	46, 77, 120, 234	0
2	r	233/233 (100%)	-0.03	5 (2%)	63	61	50, 76, 119, 248	0
3	C	250/250 (100%)	-0.10	9 (3%)	42	37	50, 79, 135, 232	0
3	Q	250/250 (100%)	0.05	9 (3%)	42	37	48, 77, 127, 221	0
3	e	250/250 (100%)	-0.00	7 (2%)	53	49	32, 77, 124, 193	0
3	s	250/250 (100%)	0.17	12 (4%)	30	27	55, 86, 152, 251	0
4	D	243/243 (100%)	0.11	12 (4%)	29	26	53, 94, 180, 223	0
4	R	243/243 (100%)	0.16	10 (4%)	37	32	42, 86, 174, 239	0
4	f	243/243 (100%)	0.06	8 (3%)	46	41	51, 91, 162, 233	0
4	t	243/243 (100%)	0.17	15 (6%)	20	16	54, 95, 184, 221	0
5	E	234/234 (100%)	-0.19	4 (1%)	70	69	49, 83, 118, 173	0
5	S	234/234 (100%)	-0.03	4 (1%)	70	69	50, 86, 127, 169	0
5	g	234/234 (100%)	-0.08	0	100	100	49, 88, 127, 163	0
5	u	234/234 (100%)	-0.09	2 (0%)	84	84	59, 87, 126, 164	0
6	F	238/238 (100%)	-0.12	5 (2%)	63	61	46, 73, 125, 231	0
6	T	238/238 (100%)	0.10	10 (4%)	36	32	46, 81, 135, 205	0
6	h	238/238 (100%)	0.19	7 (2%)	51	47	48, 83, 135, 225	0
6	v	238/238 (100%)	0.03	6 (2%)	57	55	53, 80, 135, 208	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
7	G	245/245 (100%)	0.10	8 (3%) 46 41	48, 82, 133, 254	0
7	U	245/245 (100%)	0.06	8 (3%) 46 41	44, 83, 139, 261	0
7	i	245/245 (100%)	0.09	12 (4%) 29 26	57, 87, 133, 235	0
7	w	245/245 (100%)	0.27	11 (4%) 33 29	57, 87, 131, 274	0
8	H	202/202 (100%)	-0.14	5 (2%) 57 55	43, 65, 114, 206	0
8	V	202/202 (100%)	-0.22	1 (0%) 91 91	46, 69, 110, 177	0
8	j	202/202 (100%)	-0.03	6 (2%) 50 45	48, 74, 116, 186	0
8	x	202/202 (100%)	-0.05	5 (2%) 57 55	43, 72, 115, 193	0
9	I	220/220 (100%)	-0.38	1 (0%) 91 91	44, 61, 92, 139	0
9	W	220/220 (100%)	-0.20	0 100 100	40, 63, 98, 134	0
9	k	220/220 (100%)	-0.16	2 (0%) 84 84	45, 65, 98, 126	0
9	y	220/220 (100%)	-0.21	1 (0%) 91 91	45, 68, 99, 139	0
10	J	204/204 (100%)	-0.22	0 100 100	42, 64, 93, 156	0
10	X	204/204 (100%)	-0.14	2 (0%) 82 82	41, 64, 99, 150	0
10	l	204/204 (100%)	-0.24	2 (0%) 82 82	42, 66, 90, 143	0
10	z	204/204 (100%)	-0.28	1 (0%) 91 91	42, 68, 93, 148	0
11	0	199/199 (100%)	-0.24	4 (2%) 65 63	50, 71, 111, 201	0
11	K	199/199 (100%)	-0.24	3 (1%) 73 73	50, 70, 106, 194	0
11	Y	199/199 (100%)	-0.18	3 (1%) 73 73	40, 70, 102, 218	0
11	m	199/199 (100%)	-0.27	4 (2%) 65 63	40, 71, 100, 184	0
12	3	201/201 (100%)	-0.13	1 (0%) 91 91	38, 68, 103, 134	0
12	L	201/201 (100%)	-0.15	1 (0%) 91 91	45, 67, 106, 158	0
12	Z	201/201 (100%)	-0.14	1 (0%) 91 91	45, 68, 98, 164	0
12	n	201/201 (100%)	-0.10	4 (1%) 65 63	44, 69, 97, 158	0
13	1	213/213 (100%)	-0.26	4 (1%) 66 65	38, 60, 94, 181	0
13	M	213/213 (100%)	-0.34	2 (0%) 84 84	37, 58, 91, 180	0
13	a	213/213 (100%)	-0.28	1 (0%) 91 91	40, 63, 98, 161	0
13	o	213/213 (100%)	-0.15	1 (0%) 91 91	37, 67, 98, 145	0
14	2	217/217 (100%)	-0.30	3 (1%) 75 75	36, 63, 100, 177	0
14	N	217/217 (100%)	-0.25	1 (0%) 91 91	39, 62, 102, 159	0
14	b	217/217 (100%)	-0.21	2 (0%) 84 84	45, 68, 104, 189	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
14	p	217/217 (100%)	-0.10	3 (1%) 75 75	45, 70, 99, 172	0
All	All	12572/12572 (100%)	-0.08	268 (2%) 63 61	32, 75, 126, 274	0

All (268) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	Y	199	GLN	20.1
7	w	1	SER	19.2
2	B	233	ALA	17.9
2	P	233	ALA	15.5
2	B	232	ILE	14.5
7	G	2	SER	13.5
7	w	2	SER	12.8
3	s	249	ARG	12.6
4	R	244	GLN	12.5
2	r	233	ALA	12.1
3	s	247	ALA	11.9
11	m	199	GLN	11.2
3	s	250	GLU	11.0
3	s	251	LYS	10.7
2	r	232	ILE	10.4
11	0	199	GLN	10.4
7	U	2	SER	10.4
11	K	199	GLN	10.2
7	G	1	SER	9.6
4	D	244	GLN	9.4
7	w	3	ILE	9.2
3	Q	204	SER	8.2
14	b	217	GLY	8.1
14	p	217	GLY	8.0
6	v	241	GLN	7.3
3	s	248	GLU	7.2
14	2	217	GLY	7.1
11	0	198	LYS	6.7
4	f	242	LYS	6.7
8	j	202	LEU	6.6
6	h	241	GLN	6.4
7	i	1	SER	6.4
4	R	243	LYS	6.3
8	x	201	THR	6.2
2	d	232	ILE	6.1
7	i	2	SER	6.0

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Mol	Chain	Res	Type	RSRZ
2	d	233	ALA	6.0
4	t	243	LYS	6.0
4	f	241	LYS	5.8
8	V	202	LEU	5.7
7	U	5	THR	5.7
4	t	240	GLU	5.6
4	t	244	GLN	5.6
8	x	202	LEU	5.4
3	s	243	GLU	5.4
2	P	232	ILE	5.3
4	t	242	LYS	5.1
7	U	1	SER	5.1
4	t	239	ASN	5.0
11	K	198	LYS	5.0
3	e	204	SER	5.0
8	j	200	ALA	4.9
3	Q	205	LYS	4.8
7	i	3	ILE	4.8
6	h	201	ALA	4.8
6	T	241	GLN	4.8
4	D	243	LYS	4.8
10	X	114	PRO	4.7
4	D	52	LYS	4.6
11	m	198	LYS	4.6
7	G	3	ILE	4.6
14	p	216	SER	4.6
3	s	244	GLU	4.6
11	0	197	PRO	4.5
2	B	2	GLU	4.5
8	j	201	THR	4.5
13	M	1	ARG	4.5
3	e	203	VAL	4.4
4	D	50	VAL	4.4
4	R	240	GLU	4.3
5	E	241	ILE	4.3
3	Q	203	VAL	4.3
6	v	240	PRO	4.1
4	D	49	SER	4.1
7	i	5	THR	4.1
12	L	201	GLY	4.1
4	f	237	GLU	4.0
6	F	239	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
10	X	115	LYS	4.0
4	D	200	GLN	4.0
8	x	198	ALA	3.9
8	H	198	ALA	3.9
3	C	205	LYS	3.9
4	t	52	LYS	3.9
4	t	201	SER	3.9
8	H	201	THR	3.8
12	n	200	SER	3.8
5	u	241	ILE	3.8
13	a	1	ARG	3.8
6	F	241	GLN	3.7
8	x	200	ALA	3.7
11	m	197	PRO	3.7
4	R	38	ARG	3.6
10	l	115	LYS	3.6
1	O	57	PRO	3.6
2	d	3	ARG	3.6
4	f	219	ILE	3.6
2	P	2	GLU	3.5
2	r	2	GLU	3.5
12	n	199	TYR	3.5
4	R	241	LYS	3.4
7	U	241	GLU	3.4
7	w	243	LEU	3.4
5	E	186	HIS	3.4
3	s	245	ALA	3.4
6	T	240	PRO	3.4
4	D	47	LYS	3.3
5	S	240	ASP	3.3
14	2	216	SER	3.3
7	i	4	GLY	3.3
1	q	208	ILE	3.3
12	3	201	GLY	3.2
3	s	246	LYS	3.2
4	f	220	LEU	3.2
6	h	200	PRO	3.2
7	w	239	ALA	3.2
6	T	202	GLU	3.1
8	H	199	VAL	3.1
4	t	200	GLN	3.1
14	2	215	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
7	w	5	THR	3.1
14	b	216	SER	3.1
3	Q	202	ASP	3.0
1	A	212	PRO	3.0
4	D	239	ASN	3.0
1	c	210	PHE	3.0
4	f	239	ASN	3.0
12	n	201	GLY	3.0
7	U	3	ILE	3.0
6	T	234	GLU	3.0
8	x	199	VAL	3.0
3	e	220	ASN	3.0
6	h	204	ASP	2.9
7	G	199	ILE	2.9
7	G	198	TYR	2.9
9	y	201	ARG	2.9
7	i	229	LYS	2.9
7	w	4	GLY	2.8
5	S	241	ILE	2.8
3	e	202	ASP	2.8
4	D	201	SER	2.8
4	t	38	ARG	2.8
6	T	239	ARG	2.8
6	v	174	ARG	2.8
1	c	57	PRO	2.8
5	S	200	ILE	2.8
3	C	181	GLU	2.8
11	K	197	PRO	2.7
3	C	202	ASP	2.7
7	G	244	LYS	2.7
2	P	1	ALA	2.7
8	j	198	ALA	2.7
5	S	238	ILE	2.7
11	Y	198	LYS	2.7
6	T	189	LYS	2.7
9	k	201	ARG	2.7
1	c	211	LYS	2.7
4	t	241	LYS	2.7
7	G	5	THR	2.7
3	s	202	ASP	2.7
14	p	119	GLU	2.7
5	E	130	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
7	w	245	GLU	2.6
6	h	233	LEU	2.6
13	1	160	ASN	2.6
3	Q	19	TYR	2.6
3	C	251	LYS	2.6
6	v	233	LEU	2.6
8	j	199	VAL	2.6
4	D	240	GLU	2.6
2	B	1	ALA	2.6
1	q	232	GLU	2.6
1	A	211	LYS	2.6
6	F	5	GLN	2.5
6	F	193	ARG	2.5
7	w	204	VAL	2.5
2	d	1	ALA	2.5
2	r	198	PHE	2.5
14	N	216	SER	2.5
4	D	237	GLU	2.5
3	s	199	LYS	2.5
3	Q	233	VAL	2.5
1	A	204	THR	2.5
3	e	205	LYS	2.5
9	I	201	ARG	2.5
2	d	2	GLU	2.5
6	h	240	PRO	2.5
3	Q	249	ARG	2.5
4	R	52	LYS	2.5
1	O	5	SER	2.4
1	q	245	ARG	2.4
2	P	206	ASN	2.4
1	c	159	TYR	2.4
4	t	237	GLU	2.4
3	e	206	LEU	2.4
6	T	236	LEU	2.4
5	E	213	THR	2.4
6	T	174	ARG	2.4
6	h	202	GLU	2.4
2	r	1	ALA	2.4
7	G	245	GLU	2.4
8	H	192	ASP	2.3
1	A	5	SER	2.3
7	i	230	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	c	232	GLU	2.3
9	k	196	GLY	2.3
11	m	110	HIS	2.3
4	D	214	ASP	2.3
1	c	243	ALA	2.3
1	O	177	SER	2.3
3	e	235	GLN	2.3
1	A	2	SER	2.3
7	U	237	LYS	2.3
7	i	233	GLU	2.3
7	w	7	TYR	2.3
3	C	204	SER	2.3
12	Z	197	GLU	2.3
6	F	240	PRO	2.2
7	i	219	LEU	2.2
7	i	243	LEU	2.2
6	v	234	GLU	2.2
10	z	117	PHE	2.2
6	v	202	GLU	2.2
3	C	247	ALA	2.2
7	U	204	VAL	2.2
4	t	238	GLU	2.2
4	t	139	ASP	2.2
13	o	1	ARG	2.2
1	c	208	ILE	2.2
10	l	114	PRO	2.2
11	Y	197	PRO	2.2
4	R	136	PHE	2.2
1	A	185	LYS	2.2
13	M	162	GLU	2.2
4	R	48	LYS	2.2
13	1	48	ASP	2.1
1	q	212	PRO	2.1
4	R	201	SER	2.1
13	1	162	GLU	2.1
4	t	179	GLU	2.1
2	P	188	HIS	2.1
6	T	41	LYS	2.1
7	U	56	LYS	2.1
7	i	52	LEU	2.1
4	f	202	GLY	2.1
8	j	139	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
13	1	1	ARG	2.1
3	C	250	GLU	2.1
4	f	100	ASP	2.1
4	R	46	GLU	2.1
1	O	241	ALA	2.1
3	Q	220	ASN	2.1
3	Q	250	GLU	2.1
2	B	15	SER	2.1
2	P	203	THR	2.1
5	u	207	GLU	2.1
7	w	230	ASP	2.0
1	O	4	GLY	2.0
3	C	186	LEU	2.0
6	T	233	LEU	2.0
11	0	196	PHE	2.0
1	O	245	ARG	2.0
4	t	202	GLY	2.0
7	i	6	GLY	2.0
3	C	249	ARG	2.0
3	s	233	VAL	2.0
12	n	73	ARG	2.0
8	H	202	LEU	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	3BV	H	301	52/52	0.70	0.47	55,115,155,162	0

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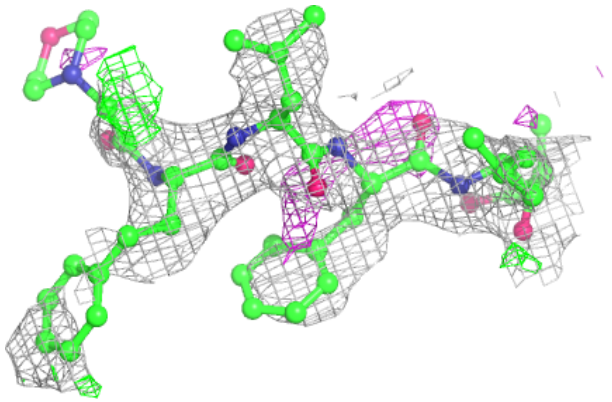
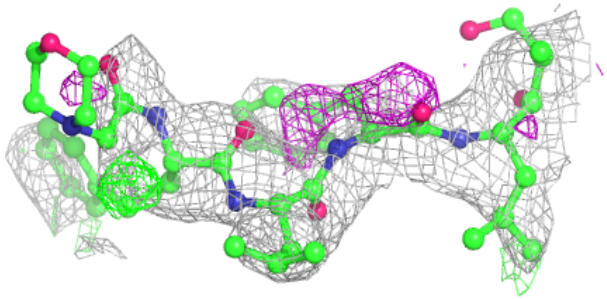
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	3BV	V	301	52/52	0.76	0.41	67,120,158,160	0
15	3BV	j	301	52/52	0.80	0.36	43,141,173,181	0
15	3BV	3	301	52/52	0.85	0.27	42,72,95,102	0
15	3BV	y	301	52/52	0.89	0.27	55,81,141,146	0
15	3BV	n	301	52/52	0.89	0.23	41,72,103,124	0
15	3BV	Z	301	52/52	0.90	0.23	45,62,91,103	0
15	3BV	I	301	52/52	0.91	0.24	51,80,119,132	0
15	3BV	W	301	52/52	0.91	0.24	44,78,127,140	0
15	3BV	k	301	52/52	0.91	0.24	39,88,123,130	0
15	3BV	L	301	52/52	0.92	0.19	33,63,97,106	0

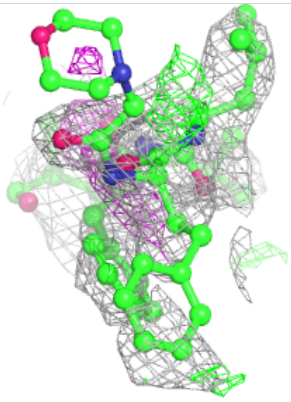
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 3BV 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)

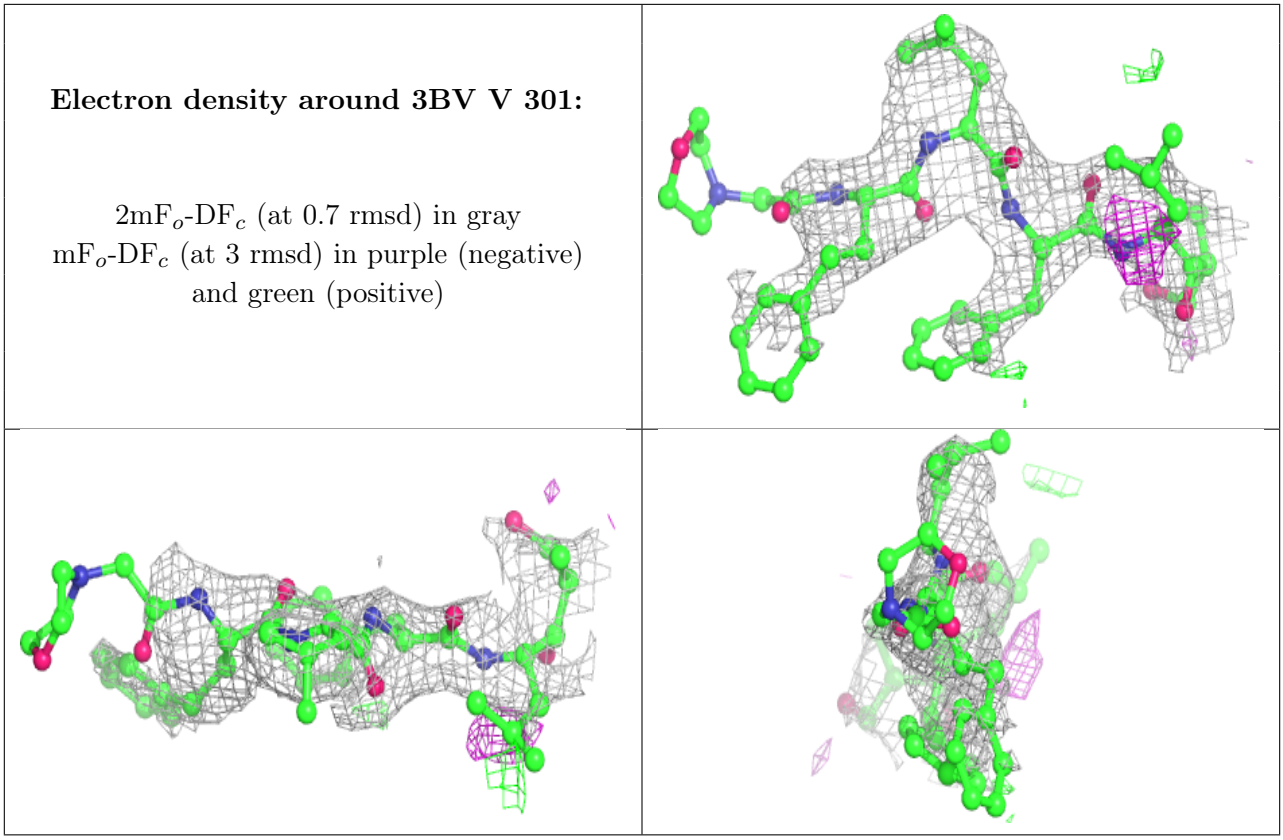






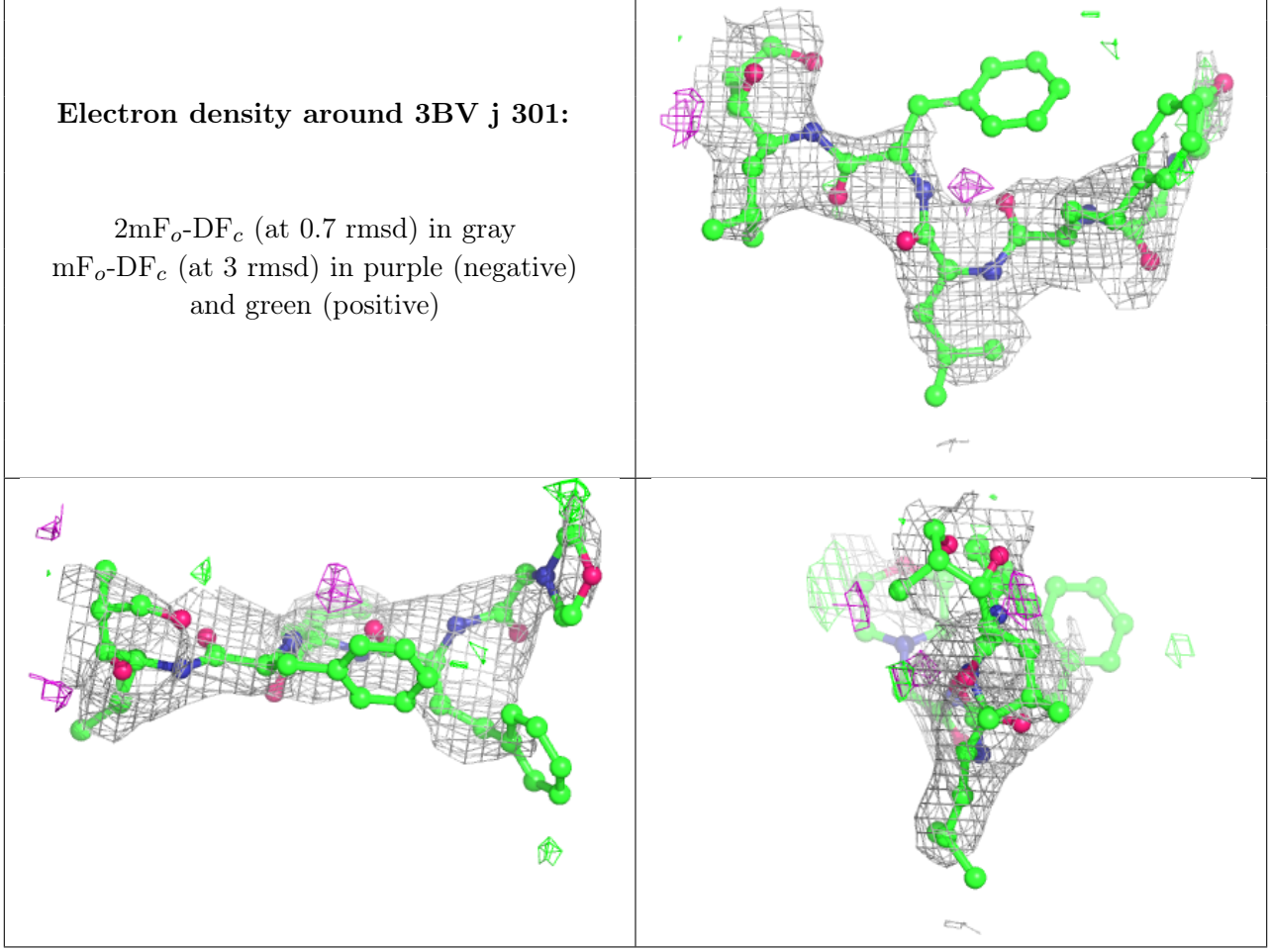
Electron density around 3BV V 301:

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



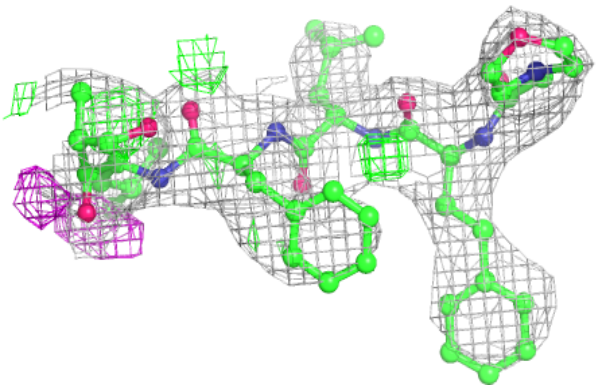
Electron density around 3BV j 301:

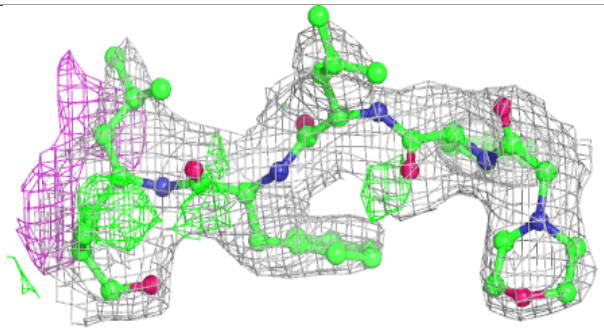
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

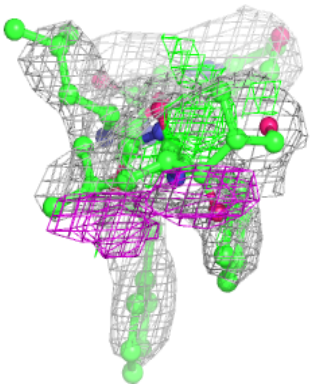


Electron density around 3BV 3 301:

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

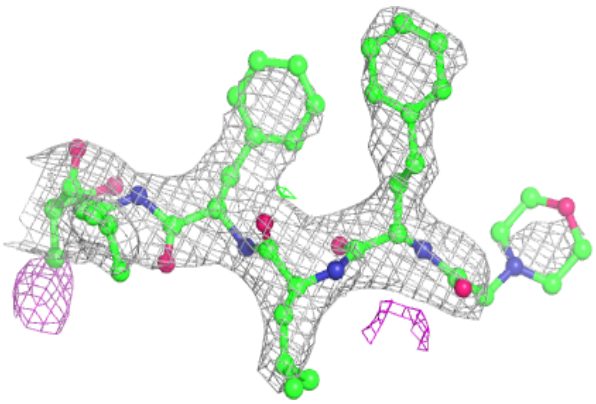


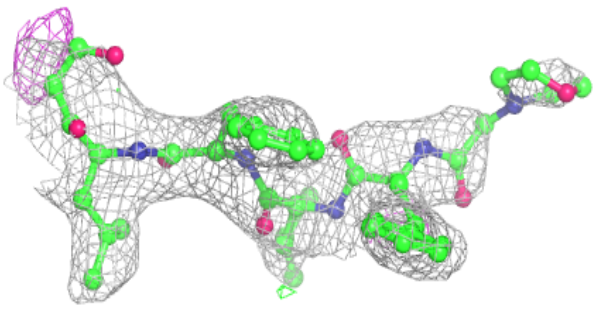


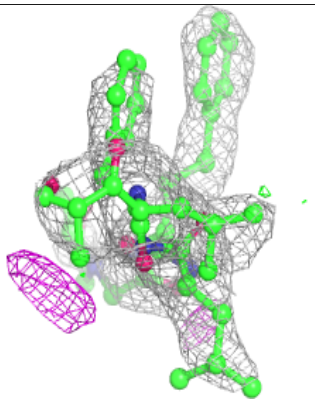


Electron density around 3BV y 301:

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

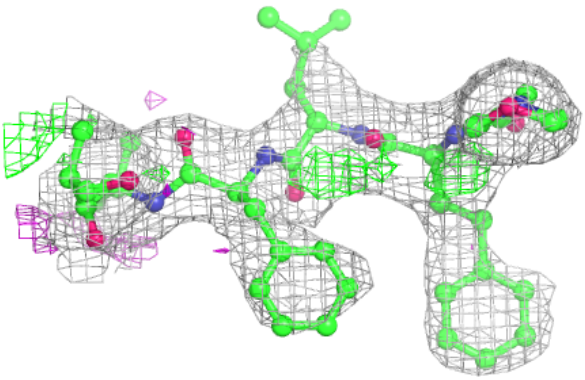


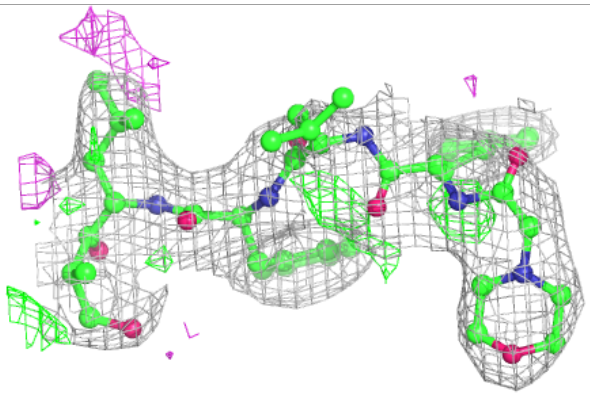


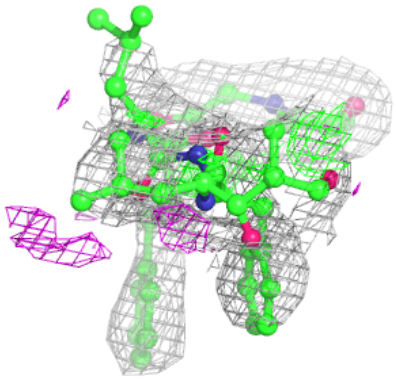


Electron density around 3BV n 301:

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

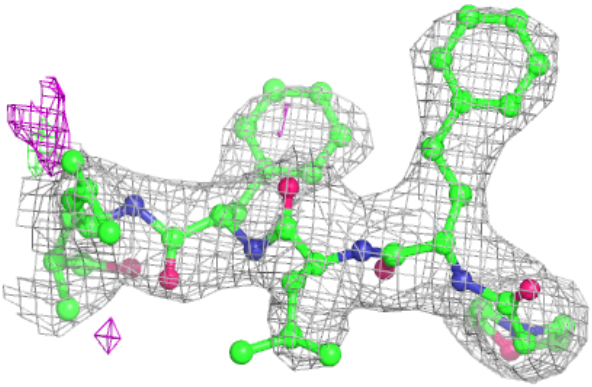


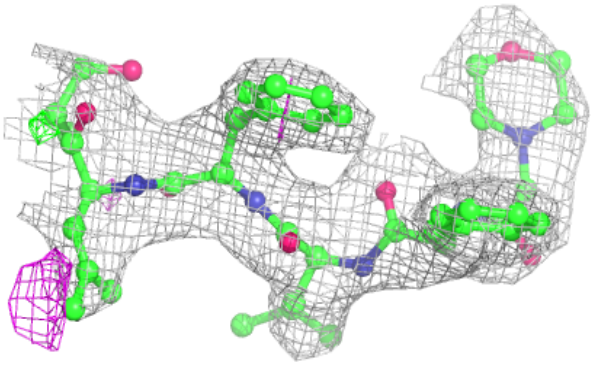


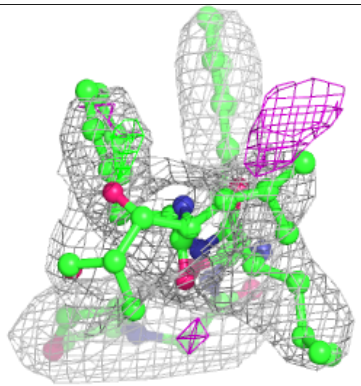


Electron density around 3BV Z 301:

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

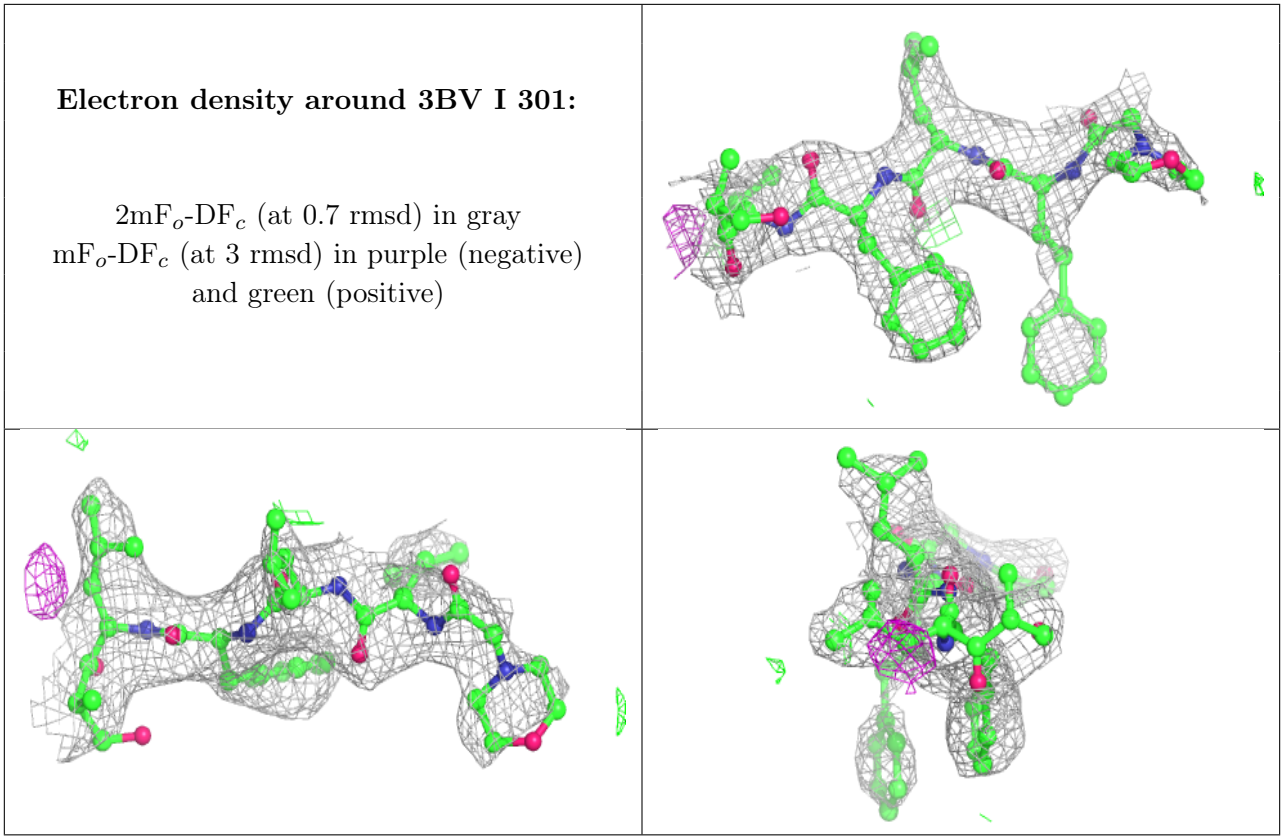






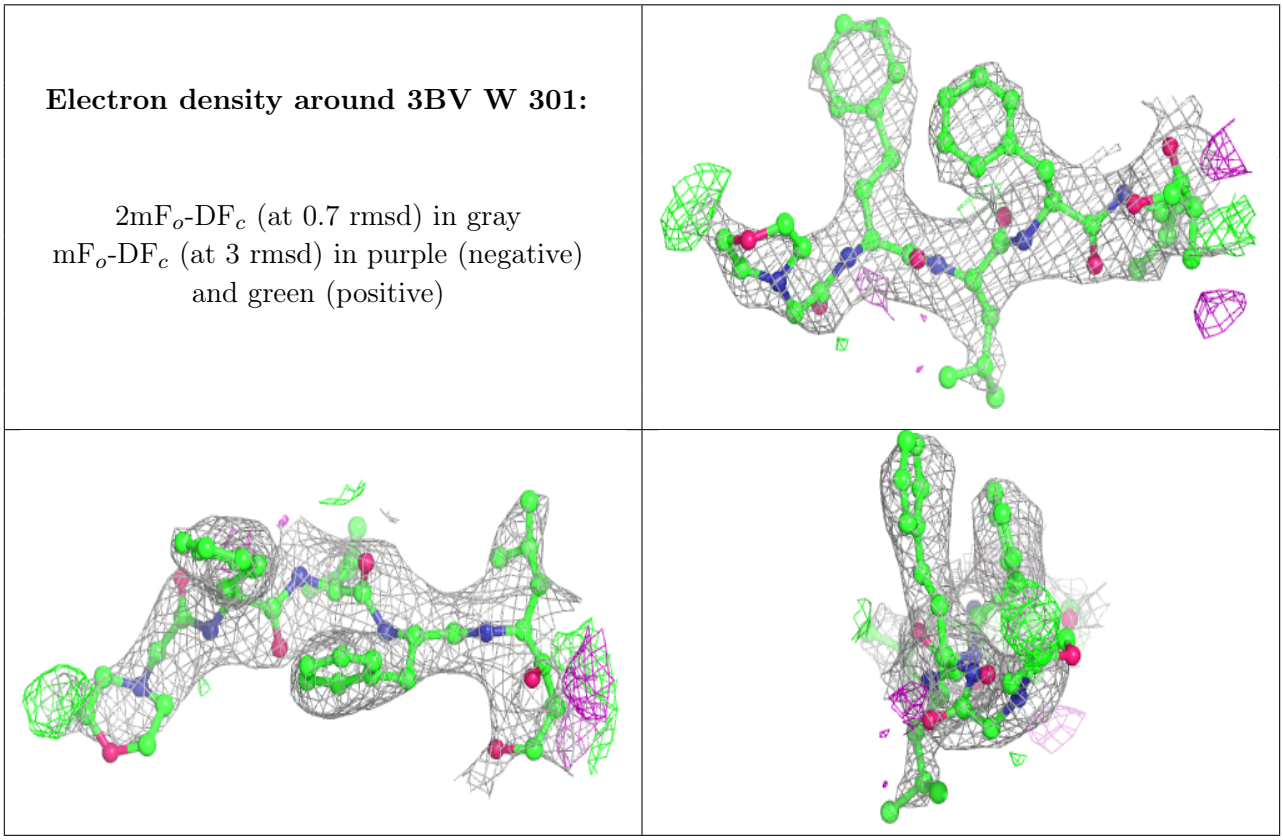
Electron density around 3BV I 301:

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



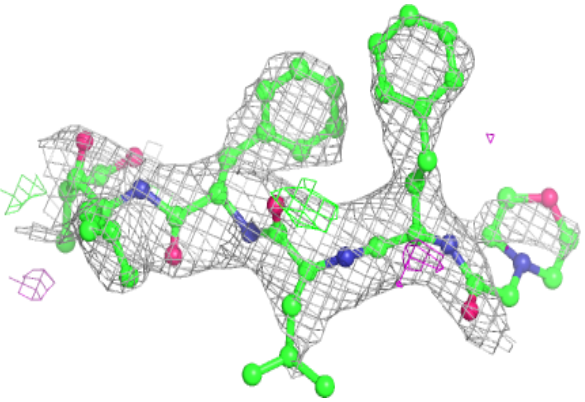
Electron density around 3BV W 301:

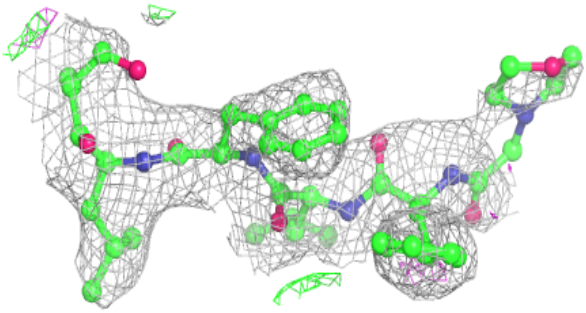
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

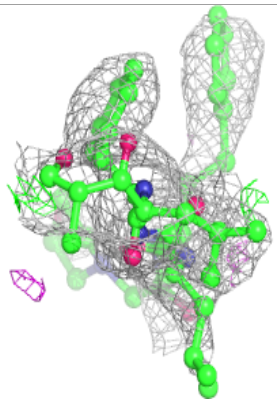


Electron density around 3BV k 301:

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

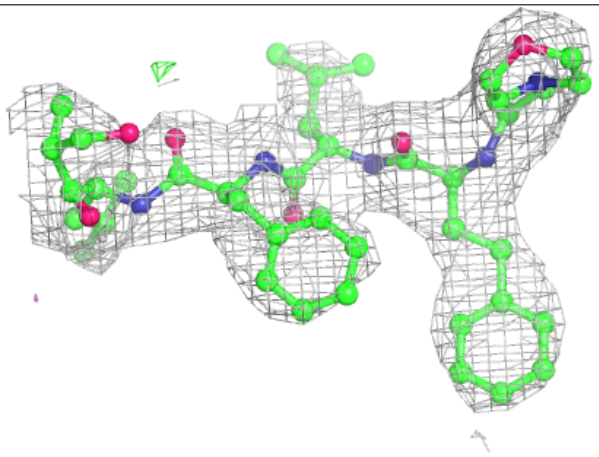


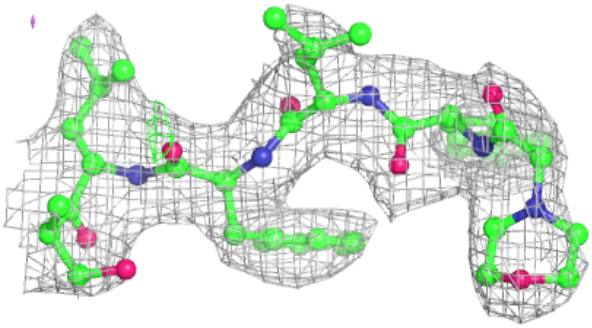


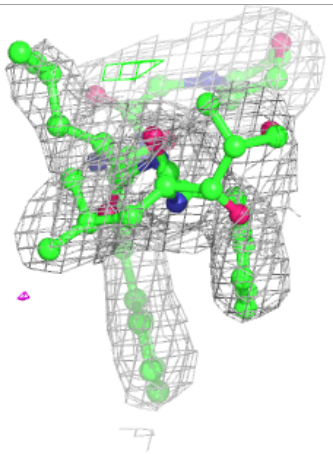


Electron density around 3BV L 301:

$2mF_o$-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.