Full wwPDB X-ray Structure Validation Report ⓘ

Jan 3, 2024 – 12:30 am GMT

PDB ID	:	5L65
Title	:	Yeast 20S proteasome with mouse beta5i (1-138) and mouse beta6 (97-111; 118-133) in complex with carfilzomib
Authors	:	Groll, M.; Huber, E.M.
Deposited on	:	2016-05-28
Resolution	:	2.90 Å(reported)

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

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

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

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

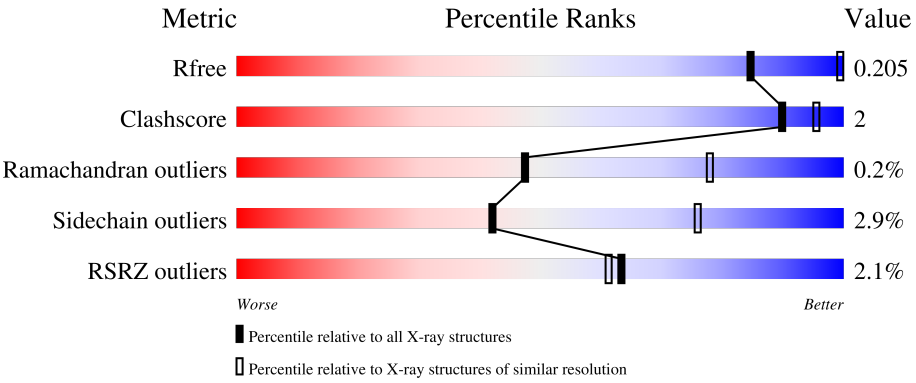
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	250	2% 98% ·
1	O	250	3% 98% ·
2	B	258	3% 88% 6% · 5%
2	P	258	3% 88% 6% 5%
3	C	254	6% 87% 6% · 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	6% 87% 6% 6%
4	D	260	85% 5% 10%
4	R	260	3% 86% 10%
5	E	234	3% 95%
5	S	234	2% 95%
6	F	288	2% 81% 16%
6	T	288	2% 81% 16%
7	G	252	2% 90% 6%
7	U	252	2% 90% 6%
8	H	232	2% 94%
8	V	232	2% 93%
9	I	205	92% 7%
9	W	205	93% 6%
10	J	198	2% 90% 6%
10	X	198	2% 89% 7%
11	K	211	88% 11%
11	Y	211	87% 12%
12	L	222	92% 7%
12	Z	222	2% 93% 7%
13	M	246	89% 5%
13	a	246	92% 5%
14	N	196	95%
14	b	196	98%

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 49939 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 11 is a protein called Proteasome subunit beta type-8,Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	211	Total	C	N	O	S	0	0	0
			1645	1039	281	313	12			
11	Y	211	Total	C	N	O	S	0	0	0
			1645	1039	281	313	12			

- Molecule 12 is a protein called Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1764	1119	305	336	4			
12	Z	222	Total	C	N	O	S	0	0	0
			1764	1119	305	336	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	1	0
			1832	1159	315	351	7			
13	a	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

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

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

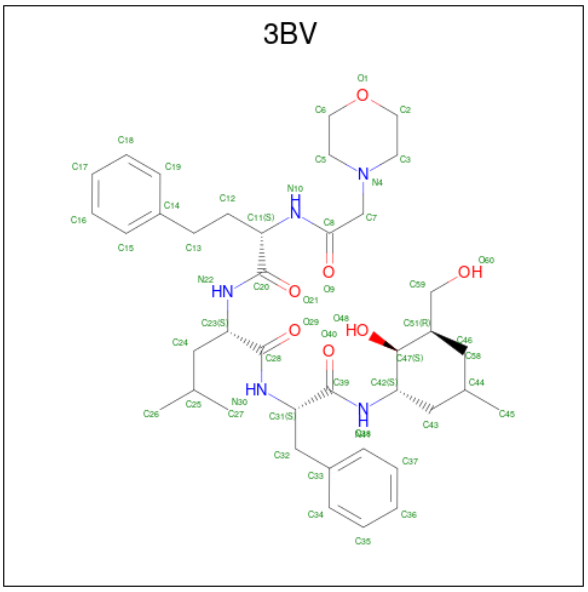
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

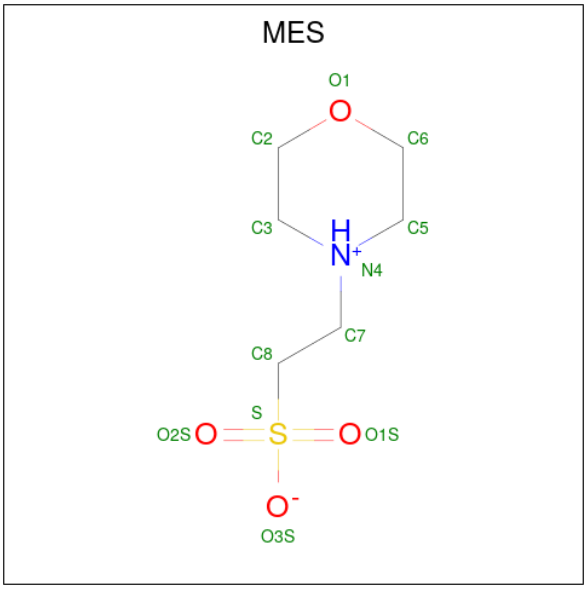
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total Cl 1 1	0	0
16	N	1	Total Cl 1 1	0	0
16	U	1	Total Cl 1 1	0	0
16	b	1	Total Cl 1 1	0	0

- Molecule 17 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
17	H	1	Total C N O 52 40 5 7	0	0
17	K	1	Total C N O 52 40 5 7	0	0
17	N	1	Total C N O 52 40 5 7	0	0
17	V	1	Total C N O 52 40 5 7	0	0
17	Y	1	Total C N O 52 40 5 7	0	0
17	b	1	Total C N O 52 40 5 7	0	0

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



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

- Molecule 19 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	6	Total O 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	B	12	Total O 12 12	0	0
19	C	6	Total O 6 6	0	0
19	D	3	Total O 3 3	0	0
19	E	3	Total O 3 3	0	0
19	F	11	Total O 11 11	0	0
19	G	7	Total O 7 7	0	0
19	H	7	Total O 7 7	0	0
19	I	5	Total O 5 5	0	0
19	J	7	Total O 7 7	0	0
19	K	6	Total O 6 6	0	0
19	L	9	Total O 9 9	0	0
19	M	11	Total O 11 11	0	0
19	N	10	Total O 10 10	0	0
19	O	6	Total O 6 6	0	0
19	P	1	Total O 1 1	0	0
19	Q	4	Total O 4 4	0	0
19	R	4	Total O 4 4	0	0
19	S	5	Total O 5 5	0	0
19	T	5	Total O 5 5	0	0
19	U	12	Total O 12 12	0	0
19	V	7	Total O 7 7	0	0

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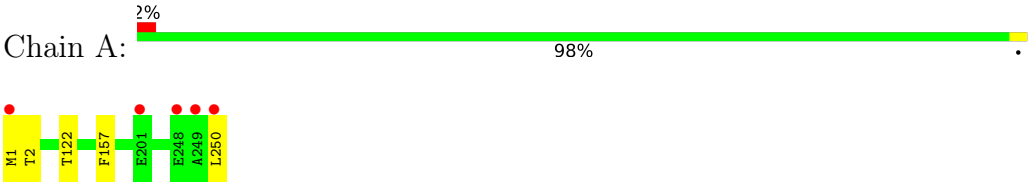
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	W	5	Total O 5 5	0	0
19	X	12	Total O 12 12	0	0
19	Y	7	Total O 7 7	0	0
19	Z	6	Total O 6 6	0	0
19	a	13	Total O 13 13	0	0
19	b	12	Total O 12 12	0	0

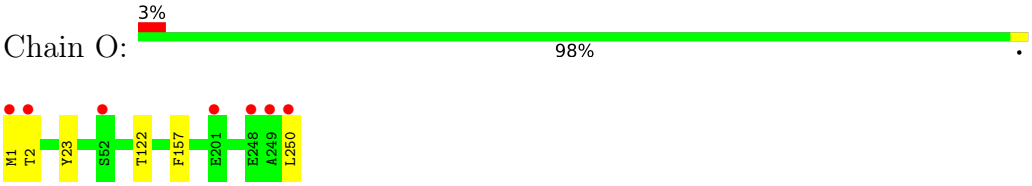
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

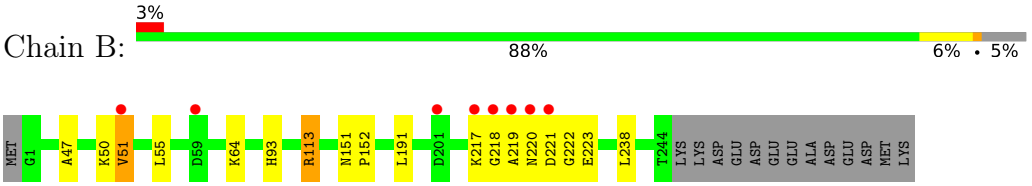
• Molecule 1: Proteasome subunit alpha type-2



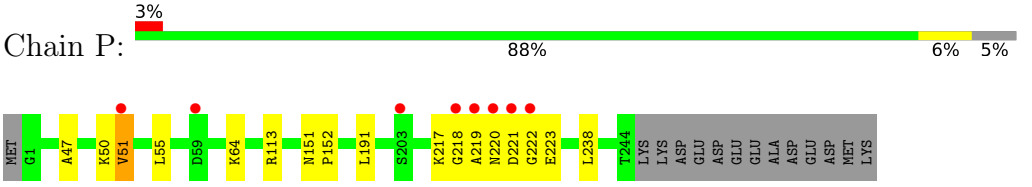
• Molecule 1: Proteasome subunit alpha type-2



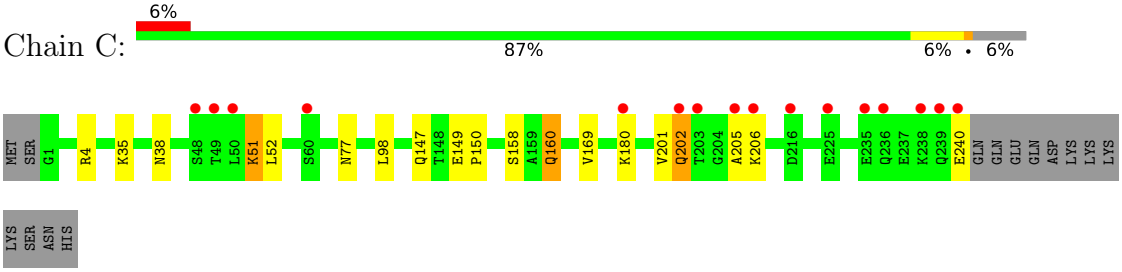
• Molecule 2: Proteasome subunit alpha type-3



• Molecule 2: Proteasome subunit alpha type-3

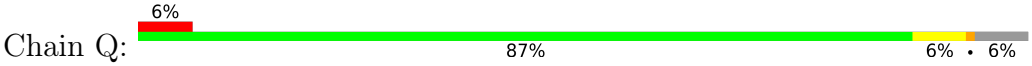


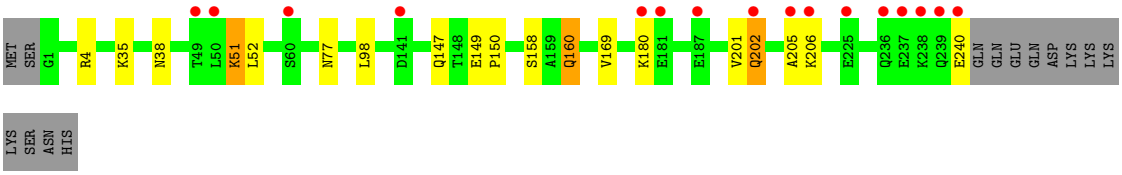
• Molecule 3: Proteasome subunit alpha type-4



• Molecule 3: Proteasome subunit alpha type-4

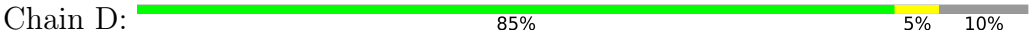
Chain Q:

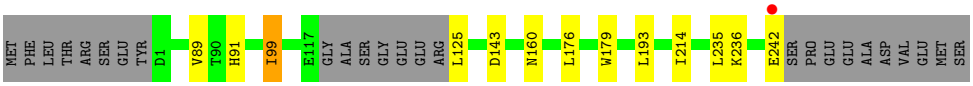




• Molecule 4: Proteasome subunit alpha type-5

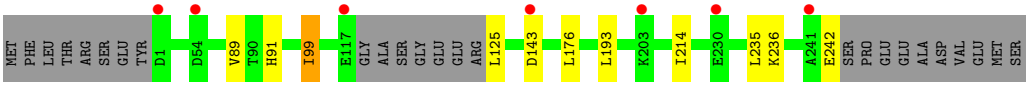
Chain D:





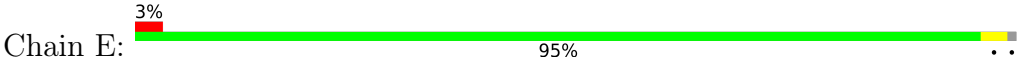
• Molecule 4: Proteasome subunit alpha type-5

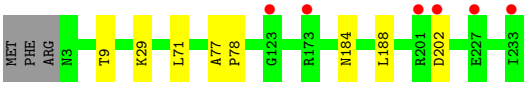
Chain R:



• Molecule 5: Proteasome subunit alpha type-6

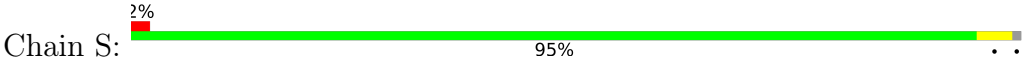
Chain E:

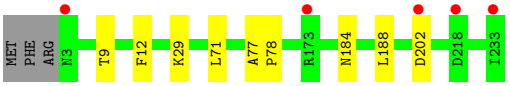




• Molecule 5: Proteasome subunit alpha type-6

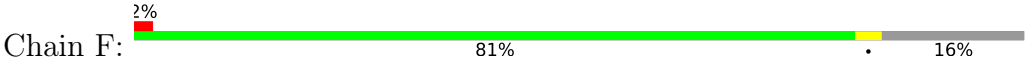
Chain S:

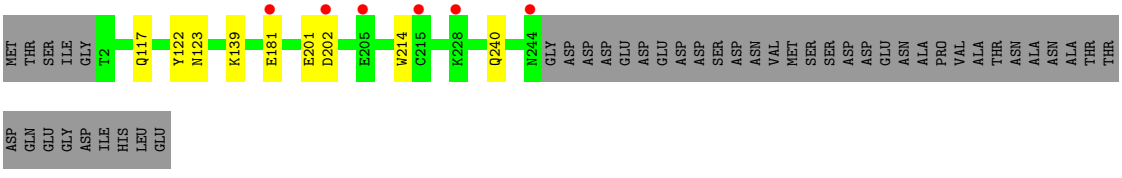




• Molecule 6: Probable proteasome subunit alpha type-7

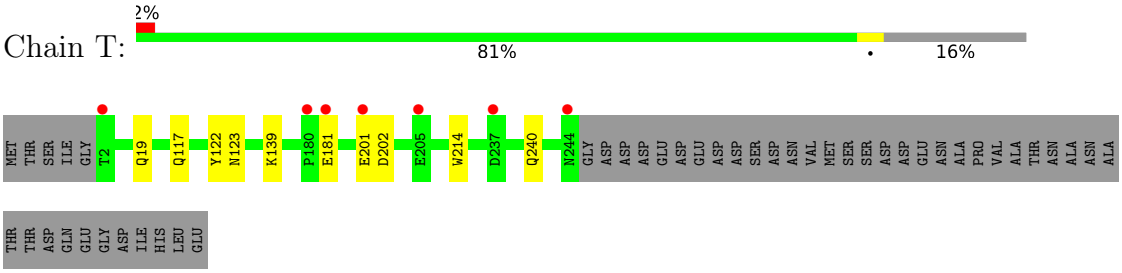
Chain F:





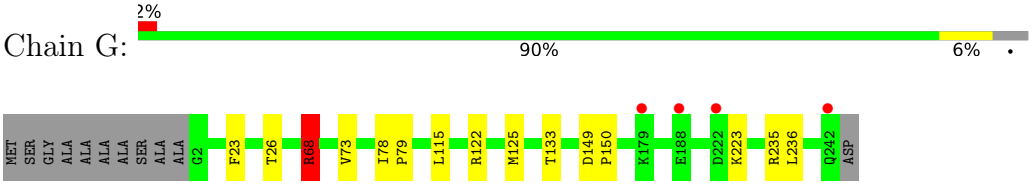
• Molecule 6: Probable proteasome subunit alpha type-7

Chain T:



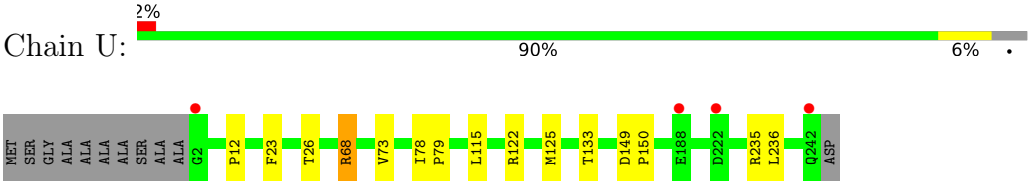
• Molecule 7: Proteasome subunit alpha type-1

Chain G:



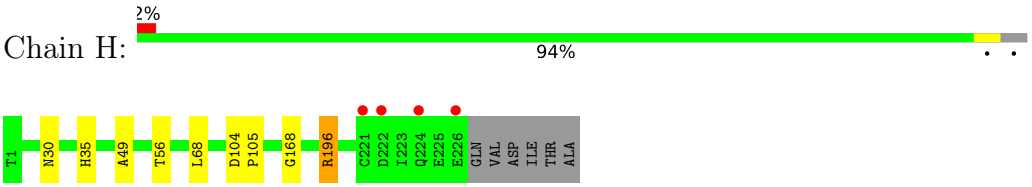
• Molecule 7: Proteasome subunit alpha type-1

Chain U:



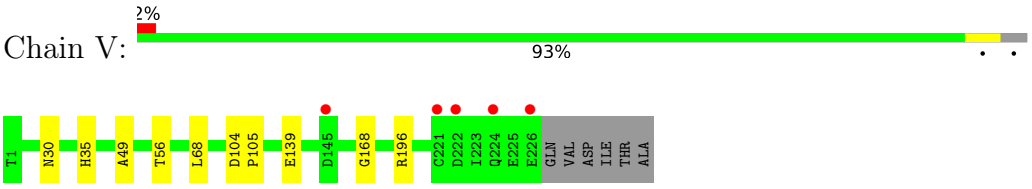
• Molecule 8: Proteasome subunit beta type-2

Chain H:



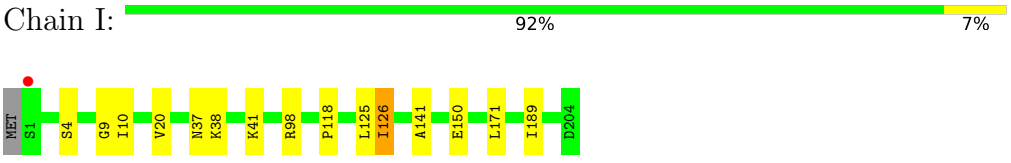
• Molecule 8: Proteasome subunit beta type-2

Chain V:



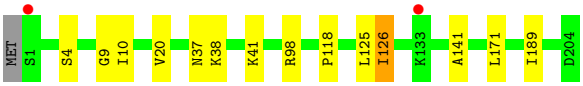
• Molecule 9: Proteasome subunit beta type-3

Chain I:

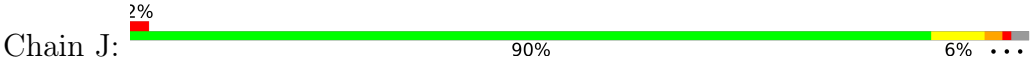


• Molecule 9: Proteasome subunit beta type-3

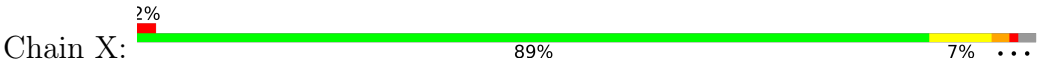
Chain W:

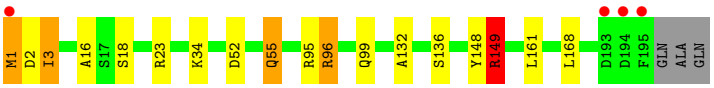


• Molecule 10: Proteasome subunit beta type-4

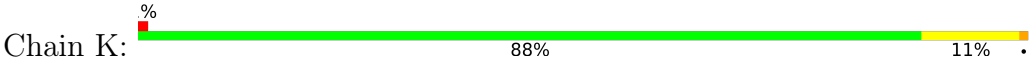


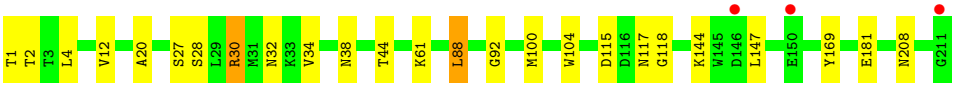
• Molecule 10: Proteasome subunit beta type-4



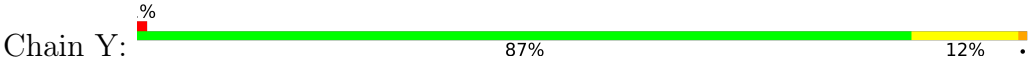


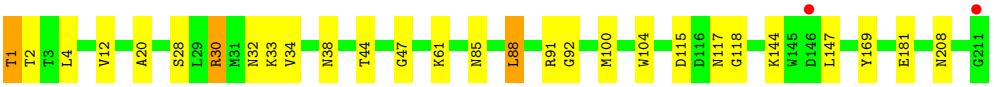
• Molecule 11: Proteasome subunit beta type-8,Proteasome subunit beta type-5



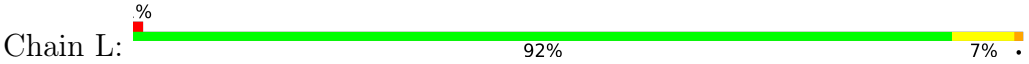


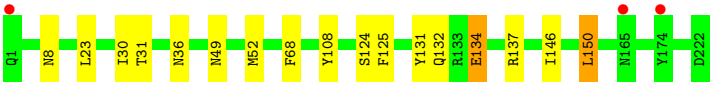
• Molecule 11: Proteasome subunit beta type-8,Proteasome subunit beta type-5



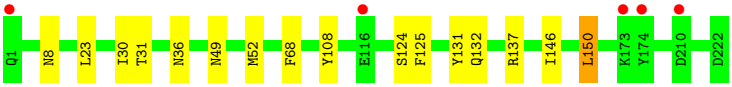


• Molecule 12: Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6



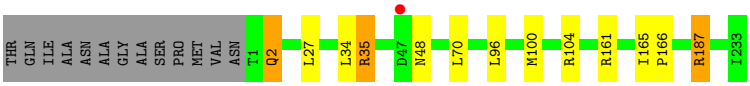


• Molecule 12: Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6



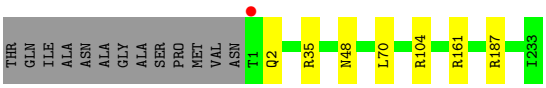
• Molecule 13: Proteasome subunit beta type-7

Chain M:



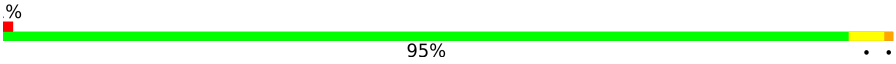
• Molecule 13: Proteasome subunit beta type-7

Chain a:



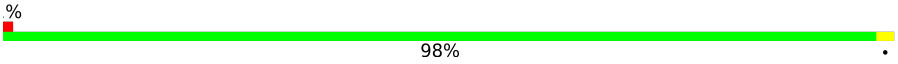
• Molecule 14: Proteasome subunit beta type-1

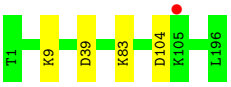
Chain N:



• Molecule 14: Proteasome subunit beta type-1

Chain b:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	135.50Å 300.39Å 145.49Å 90.00° 112.77° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 15.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.8 (15.00-2.90) 96.8 (15.00-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.89 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.176 , 0.201 0.182 , 0.205	Depositor DCC
R_{free} test set	11347 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	63.5	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 44.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	49939	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% 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, CL, MG, MES

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.27	0/1952	0.46	0/2642
1	O	0.27	0/1952	0.46	0/2642
2	B	0.27	0/1934	0.49	0/2618
2	P	0.27	0/1934	0.49	0/2618
3	C	0.27	0/1910	0.50	0/2586
3	Q	0.27	0/1910	0.50	0/2586
4	D	0.27	0/1837	0.47	0/2475
4	R	0.26	0/1837	0.47	0/2475
5	E	0.26	0/1800	0.47	0/2433
5	S	0.27	0/1800	0.47	0/2433
6	F	0.27	0/1932	0.45	0/2609
6	T	0.27	0/1932	0.45	0/2609
7	G	0.27	0/1945	0.72	4/2634 (0.2%)
7	U	0.28	0/1945	0.74	4/2634 (0.2%)
8	H	0.25	0/1750	0.49	0/2373
8	V	0.25	0/1750	0.49	0/2373
9	I	0.27	0/1611	0.50	0/2174
9	W	0.27	0/1611	0.50	0/2174
10	J	0.32	0/1589	1.04	7/2142 (0.3%)
10	X	0.30	0/1589	0.85	5/2142 (0.2%)
11	K	0.35	0/1681	0.76	4/2268 (0.2%)
11	Y	0.35	1/1681 (0.1%)	0.72	4/2268 (0.2%)
12	L	0.30	0/1802	0.50	0/2430
12	Z	0.28	0/1802	0.49	0/2430
13	M	0.43	2/1866 (0.1%)	0.68	3/2528 (0.1%)
13	a	0.42	2/1855 (0.1%)	0.68	3/2514 (0.1%)
14	N	0.26	0/1541	0.49	0/2087
14	b	0.26	0/1541	0.49	0/2087
All	All	0.29	5/50289 (0.0%)	0.58	34/67984 (0.1%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	G	0	1
7	U	0	1
10	J	0	2
10	X	0	1
11	K	0	1
11	Y	0	1
All	All	0	7

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	35	ARG	CZ-NH1	-10.66	1.19	1.33
13	a	35	ARG	CZ-NH2	-10.57	1.19	1.33
13	M	35	ARG	CZ-NH2	-9.51	1.20	1.33
13	a	35	ARG	CZ-NH1	-9.24	1.21	1.33
11	Y	85	ASN	CG-ND2	-5.34	1.19	1.32

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	J	95	ARG	NE-CZ-NH2	-25.72	107.44	120.30
7	U	68	ARG	NE-CZ-NH2	-22.29	109.16	120.30
10	X	149	ARG	NE-CZ-NH2	-20.41	110.09	120.30
10	J	149	ARG	NE-CZ-NH1	-20.14	110.23	120.30
7	G	68	ARG	NE-CZ-NH1	-19.75	110.42	120.30
11	K	30	ARG	NE-CZ-NH1	16.58	128.59	120.30
10	J	149	ARG	NE-CZ-NH2	16.41	128.50	120.30
7	G	68	ARG	NE-CZ-NH2	16.31	128.45	120.30
13	M	35	ARG	NE-CZ-NH2	16.14	128.37	120.30
11	K	30	ARG	NE-CZ-NH2	-15.99	112.31	120.30
13	a	35	ARG	NE-CZ-NH1	15.98	128.29	120.30
11	Y	30	ARG	NE-CZ-NH2	15.40	128.00	120.30
11	Y	30	ARG	NE-CZ-NH1	-15.21	112.69	120.30
10	X	149	ARG	NE-CZ-NH1	15.07	127.83	120.30
7	U	68	ARG	NE-CZ-NH1	14.99	127.79	120.30
10	J	95	ARG	CD-NE-CZ	12.67	141.34	123.60
13	M	35	ARG	NH1-CZ-NH2	-12.06	106.13	119.40
13	a	35	ARG	NH1-CZ-NH2	-11.93	106.28	119.40
10	J	95	ARG	NE-CZ-NH1	10.98	125.79	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	U	68	ARG	CD-NE-CZ	10.81	138.73	123.60
10	X	95	ARG	NE-CZ-NH1	-10.49	115.05	120.30
13	M	35	ARG	NE-CZ-NH1	10.30	125.45	120.30
13	a	35	ARG	NE-CZ-NH2	9.95	125.28	120.30
10	J	149	ARG	CD-NE-CZ	9.86	137.40	123.60
10	X	149	ARG	CD-NE-CZ	9.79	137.30	123.60
7	G	68	ARG	CD-NE-CZ	9.58	137.01	123.60
10	X	95	ARG	NE-CZ-NH2	8.29	124.44	120.30
11	Y	30	ARG	CD-NE-CZ	7.84	134.57	123.60
11	K	30	ARG	CD-NE-CZ	7.23	133.72	123.60
10	J	95	ARG	CG-CD-NE	6.14	124.70	111.80
7	U	68	ARG	CG-CD-NE	-6.09	99.01	111.80
11	K	30	ARG	CG-CD-NE	5.26	122.85	111.80
11	Y	1	THR	CB-CA-C	-5.21	97.52	111.60
7	G	68	ARG	CG-CD-NE	5.00	122.31	111.80

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	G	68	ARG	Sidechain
10	J	149	ARG	Sidechain
10	J	95	ARG	Sidechain
11	K	30	ARG	Sidechain
7	U	68	ARG	Sidechain
10	X	149	ARG	Sidechain
11	Y	30	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	1	0
1	O	1915	0	1929	2	0
2	B	1904	0	1904	8	0
2	P	1904	0	1904	7	0
3	C	1881	0	1895	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Q	1881	0	1895	6	0
4	D	1813	0	1797	3	0
4	R	1813	0	1797	2	0
5	E	1773	0	1775	1	0
5	S	1773	0	1775	2	0
6	F	1892	0	1883	2	0
6	T	1892	0	1883	3	0
7	G	1907	0	1901	6	0
7	U	1907	0	1901	5	0
8	H	1719	0	1716	6	0
8	V	1719	0	1716	6	0
9	I	1581	0	1574	8	0
9	W	1581	0	1574	7	0
10	J	1561	0	1569	16	0
10	X	1561	0	1569	17	0
11	K	1645	0	1589	22	0
11	Y	1645	0	1589	23	0
12	L	1764	0	1716	9	0
12	Z	1764	0	1716	7	0
13	M	1832	0	1845	6	0
13	a	1824	0	1832	0	0
14	N	1512	0	1478	5	0
14	b	1512	0	1478	0	0
15	G	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	K	1	0	0	0	0
15	N	1	0	0	0	0
15	Z	1	0	0	0	0
16	G	1	0	0	0	0
16	N	1	0	0	0	0
16	U	1	0	0	0	0
16	b	1	0	0	0	0
17	H	52	0	59	4	0
17	K	52	0	58	5	0
17	N	52	0	59	1	0
17	V	52	0	59	3	0
17	Y	52	0	59	12	0
17	b	52	0	59	0	0
18	H	12	0	13	0	0
18	V	12	0	13	0	0
19	A	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	B	12	0	0	2	0
19	C	6	0	0	0	0
19	D	3	0	0	0	0
19	E	3	0	0	0	0
19	F	11	0	0	0	0
19	G	7	0	0	0	0
19	H	7	0	0	0	0
19	I	5	0	0	0	0
19	J	7	0	0	0	0
19	K	6	0	0	0	0
19	L	9	0	0	0	0
19	M	11	0	0	1	0
19	N	10	0	0	0	0
19	O	6	0	0	0	0
19	P	1	0	0	0	0
19	Q	4	0	0	0	0
19	R	4	0	0	0	0
19	S	5	0	0	0	0
19	T	5	0	0	0	0
19	U	12	0	0	0	0
19	V	7	0	0	0	0
19	W	5	0	0	0	0
19	X	12	0	0	0	0
19	Y	7	0	0	0	0
19	Z	6	0	0	0	0
19	a	13	0	0	0	0
19	b	12	0	0	0	0
All	All	49939	0	49508	171	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (171) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:134:GLU:OE1	12:L:137:ARG:NH2	1.80	1.12
10:J:96:ARG:HH21	11:K:92:GLY:HA3	1.20	1.01
11:Y:169:TYR:O	17:Y:301:3BV:H57	1.61	1.00
11:Y:47:GLY:O	17:Y:301:3BV:C46	2.12	0.95
11:Y:47:GLY:O	17:Y:301:3BV:H51	1.67	0.94
10:J:96:ARG:NH2	11:K:92:GLY:HA3	1.95	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:K:301:3BV:O40	17:K:301:3BV:H49	1.80	0.81
11:Y:47:GLY:O	17:Y:301:3BV:H53	1.85	0.76
17:Y:301:3BV:H53	17:Y:301:3BV:N41	2.02	0.74
10:X:96:ARG:HH21	11:Y:92:GLY:HA3	1.54	0.73
10:X:23:ARG:NH2	11:Y:117:ASN:OD1	2.26	0.68
10:J:1:MET:HB3	10:J:34:LYS:HE3	1.76	0.67
10:J:1:MET:CB	10:J:34:LYS:HE3	2.26	0.66
10:X:1:MET:HB3	10:X:34:LYS:HE3	1.77	0.66
12:L:108:TYR:OH	12:L:137:ARG:HD2	1.95	0.65
11:K:169:TYR:O	17:K:301:3BV:H57	1.96	0.65
10:X:1:MET:CB	10:X:34:LYS:HE3	2.27	0.65
2:B:93:HIS:HB3	19:B:301:HOH:O	2.00	0.62
10:J:23:ARG:NH2	11:K:117:ASN:OD1	2.32	0.61
10:J:96:ARG:HH21	11:K:92:GLY:CA	2.07	0.56
10:J:23:ARG:NH2	11:K:115:ASP:OD2	2.39	0.55
10:J:55:GLN:CD	11:K:88:LEU:HG	2.27	0.55
10:J:23:ARG:HH21	11:K:115:ASP:CG	2.10	0.55
7:U:23:PHE:O	7:U:26:THR:HB	2.07	0.54
12:Z:52:MET:HE1	12:Z:68:PHE:HB3	1.89	0.54
12:L:52:MET:HE1	12:L:68:PHE:HB3	1.89	0.54
7:G:23:PHE:O	7:G:26:THR:HB	2.06	0.54
11:K:208:ASN:O	9:W:38:LYS:NZ	2.41	0.54
11:Y:32:ASN:OD1	11:Y:34:VAL:O	2.26	0.53
11:K:1:THR:HG22	11:K:2:THR:N	2.23	0.52
17:K:301:3BV:H49	17:K:301:3BV:C39	2.39	0.52
9:W:125:LEU:HG	9:W:126:ILE:HG22	1.90	0.52
9:I:125:LEU:HG	9:I:126:ILE:HG22	1.91	0.52
8:H:168:GLY:O	17:H:301:3BV:H57	2.10	0.51
10:X:1:MET:HB2	10:X:34:LYS:CE	2.41	0.51
12:Z:108:TYR:OH	12:Z:137:ARG:HD2	2.11	0.51
8:V:168:GLY:O	17:V:301:3BV:H57	2.11	0.51
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.94	0.50
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.59	0.50
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.93	0.50
3:C:201:VAL:O	3:C:202:GLN:CB	2.59	0.50
10:J:1:MET:HB2	10:J:34:LYS:CE	2.41	0.50
9:I:38:LYS:NZ	11:Y:208:ASN:O	2.45	0.50
10:X:23:ARG:NH2	11:Y:115:ASP:CG	2.65	0.50
11:Y:169:TYR:O	17:Y:301:3BV:C58	2.47	0.49
2:B:113:ARG:NE	19:B:301:HOH:O	2.32	0.49
11:K:27:SER:OG	17:K:301:3BV:H33	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:23:ARG:NH2	11:Y:115:ASP:OD2	2.46	0.49
10:X:23:ARG:HH21	11:Y:115:ASP:CG	2.16	0.49
12:L:124:SER:HB2	12:L:134:GLU:OE2	2.13	0.49
17:H:301:3BV:O9	17:H:301:3BV:H16	2.13	0.49
17:V:301:3BV:H16	17:V:301:3BV:O9	2.13	0.48
10:X:1:MET:HB2	10:X:34:LYS:HE3	1.95	0.48
11:Y:144:LYS:HB2	11:Y:147:LEU:HD13	1.96	0.48
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.95	0.48
8:V:49:ALA:HB2	17:V:301:3BV:H52	1.96	0.48
17:Y:301:3BV:C39	17:Y:301:3BV:H47	2.43	0.48
10:X:55:GLN:CD	11:Y:88:LEU:HG	2.34	0.48
17:Y:301:3BV:H59	17:Y:301:3BV:H44	1.71	0.48
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.95	0.48
11:K:1:THR:CG2	11:K:2:THR:N	2.77	0.48
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.95	0.48
17:Y:301:3BV:O60	17:Y:301:3BV:O48	2.21	0.48
4:D:89:VAL:HG12	11:K:61:LYS:HG3	1.96	0.47
11:K:144:LYS:HB2	11:K:147:LEU:HD13	1.96	0.47
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.95	0.47
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.13	0.47
3:C:51:LYS:O	3:C:52:LEU:HB2	2.14	0.47
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.79	0.47
8:H:49:ALA:HB2	17:H:301:3BV:H52	1.96	0.47
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.95	0.47
11:K:32:ASN:OD1	11:K:34:VAL:O	2.33	0.47
13:M:27:LEU:HD21	13:M:34:LEU:HD22	1.97	0.47
11:Y:104:TRP:CE2	11:Y:181:GLU:HB3	2.50	0.47
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.79	0.46
11:K:104:TRP:CE2	11:K:181:GLU:HB3	2.50	0.46
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.96	0.46
11:Y:33:LYS:HE2	17:Y:301:3BV:H45	1.98	0.46
10:J:3:ILE:HG22	10:J:18:SER:HB3	1.97	0.46
1:O:1:MET:HG3	6:T:122:TYR:CZ	2.51	0.46
8:H:35:HIS:CB	8:H:56:THR:HG21	2.45	0.46
2:B:50:LYS:O	2:B:51:VAL:C	2.54	0.46
2:P:50:LYS:O	2:P:51:VAL:C	2.54	0.46
8:V:35:HIS:CB	8:V:56:THR:HG21	2.46	0.46
10:X:3:ILE:HG22	10:X:18:SER:HB3	1.97	0.45
11:Y:88:LEU:CD1	11:Y:118:GLY:HA3	2.46	0.45
11:Y:1:THR:HG22	11:Y:2:THR:N	2.31	0.45
11:K:88:LEU:CD1	11:K:118:GLY:HA3	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:35:ARG:NH2	14:N:114:PRO:HB3	2.32	0.45
13:M:187:ARG:NH1	8:V:139:GLU:OE1	2.47	0.45
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.47	0.45
11:K:27:SER:OG	17:K:301:3BV:C27	2.65	0.45
8:H:104:ASP:HB2	8:H:105:PRO:HD2	2.00	0.44
4:R:89:VAL:HG12	11:Y:61:LYS:HG3	1.99	0.44
11:Y:20:ALA:HB3	11:Y:28:SER:HB3	1.99	0.44
17:Y:301:3BV:C39	17:Y:301:3BV:C44	2.96	0.44
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.53	0.44
10:J:132:ALA:HB1	10:J:136:SER:HB2	2.00	0.44
10:X:132:ALA:HB1	10:X:136:SER:HB2	2.00	0.44
10:X:148:TYR:O	10:X:149:ARG:HD3	2.17	0.44
3:C:35:LYS:HG2	3:C:158:SER:O	2.18	0.43
12:L:8:ASN:HA	12:L:30:ILE:O	2.18	0.43
2:B:217:LYS:C	2:B:219:ALA:H	2.22	0.43
2:P:221:ASP:O	2:P:223:GLU:N	2.52	0.43
8:V:104:ASP:HB2	8:V:105:PRO:HD2	2.00	0.43
13:M:96:LEU:O	13:M:100:MET:HG2	2.19	0.43
2:B:221:ASP:O	2:B:223:GLU:N	2.51	0.43
7:G:68:ARG:NH1	14:N:39:ASP:OD2	2.51	0.43
11:K:20:ALA:HB3	11:K:28:SER:HB3	2.00	0.43
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.53	0.43
3:Q:201:VAL:O	3:Q:202:GLN:HB3	2.19	0.43
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.19	0.43
7:G:78:ILE:N	7:G:79:PRO:CD	2.82	0.43
14:N:152:VAL:HA	14:N:175:MET:HE1	2.00	0.43
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.53	0.43
2:P:217:LYS:C	2:P:219:ALA:H	2.21	0.42
12:Z:124:SER:O	12:Z:131:TYR:HA	2.19	0.42
14:N:176:VAL:HG12	14:N:178:LEU:HD13	2.01	0.42
10:J:23:ARG:NH2	11:K:115:ASP:CG	2.71	0.42
2:P:50:LYS:HD3	2:P:50:LYS:HA	1.83	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.42
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.49	0.42
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.02	0.42
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.02	0.42
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.50	0.42
12:Z:146:ILE:HG22	12:Z:150:LEU:HD22	2.02	0.42
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.19	0.42
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.50	0.42
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:3:ILE:HG22	10:J:18:SER:CB	2.49	0.42
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.02	0.42
8:H:196:ARG:NH2	9:I:150:GLU:O	2.53	0.42
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.85	0.42
17:Y:301:3BV:H28	17:Y:301:3BV:H30	1.63	0.42
2:B:47:ALA:HB1	2:B:64:LYS:HD2	2.02	0.41
3:C:201:VAL:O	3:C:202:GLN:HB3	2.19	0.41
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.84	0.41
12:L:124:SER:O	12:L:131:TYR:HA	2.20	0.41
13:M:2:GLN:NE2	19:M:301:HOH:O	2.53	0.41
2:P:47:ALA:HB1	2:P:64:LYS:HD2	2.02	0.41
5:S:12:PHE:H	6:T:19:GLN:HE22	1.66	0.41
10:J:3:ILE:CD1	10:J:168:LEU:HD13	2.51	0.41
10:X:3:ILE:HG22	10:X:18:SER:CB	2.50	0.41
9:I:20:VAL:HG23	9:I:189:ILE:HB	2.01	0.41
9:W:20:VAL:HG23	9:W:189:ILE:HB	2.01	0.41
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.50	0.41
5:E:77:ALA:N	5:E:78:PRO:CD	2.84	0.41
12:L:146:ILE:HG22	12:L:150:LEU:HD22	2.01	0.41
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.50	0.41
10:X:3:ILE:CD1	10:X:168:LEU:HD13	2.51	0.41
1:A:1:MET:HG3	6:F:122:TYR:CZ	2.55	0.41
6:T:202:ASP:OD1	6:T:202:ASP:N	2.54	0.41
10:X:96:ARG:HD3	11:Y:91:ARG:NH2	2.36	0.41
6:F:202:ASP:OD1	6:F:202:ASP:N	2.54	0.41
17:H:301:3BV:H32	17:H:301:3BV:H29	1.96	0.41
9:I:98:ARG:CD	9:I:126:ILE:HD12	2.51	0.41
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.03	0.41
5:S:77:ALA:N	5:S:78:PRO:CD	2.84	0.41
7:U:73:VAL:HG12	7:U:133:THR:HB	2.03	0.41
9:W:98:ARG:CD	9:W:126:ILE:HD12	2.51	0.41
11:Y:88:LEU:HD11	11:Y:118:GLY:HA3	2.03	0.41
7:G:73:VAL:HG12	7:G:133:THR:HB	2.03	0.40
11:K:44:THR:HG21	11:K:100:MET:HE3	2.02	0.40
9:W:9:GLY:HA3	9:W:41:LYS:HE2	2.04	0.40
9:I:9:GLY:HA3	9:I:41:LYS:HE2	2.03	0.40
11:K:88:LEU:HD11	11:K:118:GLY:HA3	2.03	0.40
2:B:50:LYS:HD3	2:B:50:LYS:HA	1.83	0.40
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.57	0.40
7:G:68:ARG:O	7:G:223:LYS:HA	2.21	0.40
17:N:201:3BV:O60	17:N:201:3BV:O48	2.17	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:44:THR:HG21	11:Y:100:MET:HE3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	238 (96%)	9 (4%)	1 (0%)	34	66
1	O	248/250 (99%)	238 (96%)	9 (4%)	1 (0%)	34	66
2	B	242/258 (94%)	234 (97%)	4 (2%)	4 (2%)	9	31
2	P	242/258 (94%)	232 (96%)	6 (2%)	4 (2%)	9	31
3	C	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	19	51
3	Q	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	19	51
4	D	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
4	R	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
5	E	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
5	S	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
6	F	241/288 (84%)	239 (99%)	2 (1%)	0	100	100
6	T	241/288 (84%)	239 (99%)	2 (1%)	0	100	100
7	G	239/252 (95%)	238 (100%)	1 (0%)	0	100	100
7	U	239/252 (95%)	238 (100%)	1 (0%)	0	100	100
8	H	224/232 (97%)	220 (98%)	4 (2%)	0	100	100
8	V	224/232 (97%)	220 (98%)	4 (2%)	0	100	100
9	I	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
9	W	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
10	J	193/198 (98%)	191 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	X	193/198 (98%)	191 (99%)	2 (1%)	0	100	100
11	K	209/211 (99%)	200 (96%)	9 (4%)	0	100	100
11	Y	209/211 (99%)	200 (96%)	9 (4%)	0	100	100
12	L	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
12	Z	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
13	M	232/246 (94%)	223 (96%)	9 (4%)	0	100	100
13	a	231/246 (94%)	222 (96%)	9 (4%)	0	100	100
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	b	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
All	All	6283/6612 (95%)	6122 (97%)	147 (2%)	14 (0%)	47	78

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
2	B	222	GLY
3	C	202	GLN
2	P	51	VAL
2	P	222	GLY
3	Q	202	GLN
1	A	2	THR
2	B	218	GLY
1	O	2	THR
2	P	218	GLY
3	C	205	ALA
3	Q	205	ALA
2	B	220	ASN
2	P	220	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	206 (99%)	3 (1%)	67	89
1	O	209/209 (100%)	206 (99%)	3 (1%)	67	89
2	B	203/216 (94%)	199 (98%)	4 (2%)	55	82
2	P	203/216 (94%)	199 (98%)	4 (2%)	55	82
3	C	212/226 (94%)	201 (95%)	11 (5%)	23	55
3	Q	212/226 (94%)	201 (95%)	11 (5%)	23	55
4	D	194/215 (90%)	185 (95%)	9 (5%)	27	60
4	R	194/215 (90%)	185 (95%)	9 (5%)	27	60
5	E	190/193 (98%)	184 (97%)	6 (3%)	39	73
5	S	190/193 (98%)	184 (97%)	6 (3%)	39	73
6	F	201/239 (84%)	194 (96%)	7 (4%)	36	70
6	T	201/239 (84%)	194 (96%)	7 (4%)	36	70
7	G	206/210 (98%)	201 (98%)	5 (2%)	49	79
7	U	206/210 (98%)	201 (98%)	5 (2%)	49	79
8	H	185/190 (97%)	182 (98%)	3 (2%)	62	86
8	V	185/190 (97%)	182 (98%)	3 (2%)	62	86
9	I	172/173 (99%)	168 (98%)	4 (2%)	50	80
9	W	172/173 (99%)	168 (98%)	4 (2%)	50	80
10	J	173/175 (99%)	166 (96%)	7 (4%)	31	65
10	X	173/175 (99%)	166 (96%)	7 (4%)	31	65
11	K	172/172 (100%)	168 (98%)	4 (2%)	50	80
11	Y	172/172 (100%)	168 (98%)	4 (2%)	50	80
12	L	186/186 (100%)	181 (97%)	5 (3%)	44	77
12	Z	186/186 (100%)	182 (98%)	4 (2%)	52	81
13	M	200/208 (96%)	194 (97%)	6 (3%)	41	75
13	a	199/208 (96%)	193 (97%)	6 (3%)	41	75
14	N	162/162 (100%)	158 (98%)	4 (2%)	47	78
14	b	162/162 (100%)	158 (98%)	4 (2%)	47	78
All	All	5329/5548 (96%)	5174 (97%)	155 (3%)	42	76

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
2	B	55	LEU
2	B	113	ARG
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	51	LYS
3	C	77	ASN
3	C	98	LEU
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	206	LYS
3	C	240	GLU
4	D	99	ILE
4	D	125	LEU
4	D	143	ASP
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	29	LYS
5	E	71	LEU
5	E	184	ASN
5	E	188	LEU
5	E	202	ASP
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	181	GLU
6	F	201	GLU
6	F	214	TRP
6	F	240	GLN
7	G	115	LEU
7	G	122	ARG
7	G	125	MET

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Mol	Chain	Res	Type
7	G	235	ARG
7	G	236	LEU
8	H	30	ASN
8	H	68	LEU
8	H	196	ARG
9	I	4	SER
9	I	37	ASN
9	I	126	ILE
9	I	171	LEU
10	J	2	ASP
10	J	3	ILE
10	J	52	ASP
10	J	55	GLN
10	J	95	ARG
10	J	96	ARG
10	J	99	GLN
11	K	4	LEU
11	K	12	VAL
11	K	38	ASN
11	K	88	LEU
12	L	23	LEU
12	L	49	ASN
12	L	132	GLN
12	L	134	GLU
12	L	150	LEU
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
14	N	9	LYS
14	N	39	ASP
14	N	83	LYS
14	N	104	ASP
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	55	LEU
2	P	113	ARG
2	P	191	LEU
2	P	238	LEU

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Mol	Chain	Res	Type
3	Q	4	ARG
3	Q	38	ASN
3	Q	51	LYS
3	Q	77	ASN
3	Q	98	LEU
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	206	LYS
3	Q	240	GLU
4	R	99	ILE
4	R	125	LEU
4	R	143	ASP
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	71	LEU
5	S	184	ASN
5	S	188	LEU
5	S	202	ASP
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	181	GLU
6	T	201	GLU
6	T	214	TRP
6	T	240	GLN
7	U	115	LEU
7	U	122	ARG
7	U	125	MET
7	U	235	ARG
7	U	236	LEU
8	V	30	ASN
8	V	68	LEU
8	V	196	ARG
9	W	4	SER

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Mol	Chain	Res	Type
9	W	37	ASN
9	W	126	ILE
9	W	171	LEU
10	X	1	MET
10	X	2	ASP
10	X	3	ILE
10	X	52	ASP
10	X	55	GLN
10	X	96	ARG
10	X	99	GLN
11	Y	4	LEU
11	Y	12	VAL
11	Y	38	ASN
11	Y	88	LEU
12	Z	23	LEU
12	Z	49	ASN
12	Z	132	GLN
12	Z	150	LEU
13	a	2	GLN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
14	b	9	LYS
14	b	39	ASP
14	b	83	LYS
14	b	104	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	20	GLN
2	B	58	GLN
2	B	119	GLN
2	B	123	GLN
3	C	17	GLN
3	C	77	ASN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN

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Mol	Chain	Res	Type
4	D	15	GLN
4	D	91	HIS
4	D	146	GLN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	151	ASN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
8	H	66	HIS
9	I	37	ASN
11	K	10	HIS
11	K	175	ASN
11	K	207	ASN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
13	M	48	ASN
13	M	102	GLN
13	M	179	ASN
1	O	94	HIS
2	P	20	GLN
2	P	58	GLN
2	P	119	GLN
2	P	123	GLN
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN

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Mol	Chain	Res	Type
3	Q	160	GLN
4	R	15	GLN
4	R	91	HIS
4	R	146	GLN
4	R	225	ASN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	151	ASN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
9	W	37	ASN
11	Y	10	HIS
11	Y	32	ASN
11	Y	175	ASN
11	Y	207	ASN
12	Z	3	ASN
12	Z	70	ASN
12	Z	79	HIS
12	Z	158	ASN
13	a	48	ASN
13	a	102	GLN
13	a	179	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

Of 19 ligands modelled in this entry, 11 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	3BV	K	301	11	54,54,54	1.28	4 (7%)	68,71,71	1.43	10 (14%)
17	3BV	N	201	14	54,54,54	1.29	3 (5%)	68,71,71	1.54	10 (14%)
17	3BV	Y	301	11	54,54,54	1.23	3 (5%)	68,71,71	1.43	9 (13%)
17	3BV	b	201	14	54,54,54	1.31	4 (7%)	68,71,71	1.51	9 (13%)
18	MES	H	302	-	12,12,12	2.29	1 (8%)	14,16,16	1.26	2 (14%)
17	3BV	V	301	8	54,54,54	1.10	3 (5%)	68,71,71	1.49	8 (11%)
18	MES	V	302	-	12,12,12	2.15	1 (8%)	14,16,16	1.41	3 (21%)
17	3BV	H	301	8	54,54,54	1.09	3 (5%)	68,71,71	1.51	8 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	3BV	K	301	11	-	13/59/67/67	0/3/3/3
17	3BV	N	201	14	-	13/59/67/67	0/3/3/3
17	3BV	Y	301	11	-	22/59/67/67	0/3/3/3
17	3BV	b	201	14	-	13/59/67/67	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	MES	H	302	-	-	2/6/14/14	0/1/1/1
17	3BV	V	301	8	-	13/59/67/67	0/3/3/3
18	MES	V	302	-	-	5/6/14/14	0/1/1/1
17	3BV	H	301	8	-	12/59/67/67	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	H	302	MES	C8-S	-7.64	1.66	1.77
18	V	302	MES	C8-S	-7.11	1.67	1.77
17	K	301	3BV	C32-C33	-6.26	1.36	1.51
17	Y	301	3BV	C32-C33	-6.13	1.36	1.51
17	b	201	3BV	C51-C47	5.80	1.63	1.53
17	N	201	3BV	C51-C47	5.75	1.63	1.53
17	b	201	3BV	C32-C33	-4.73	1.39	1.51
17	N	201	3BV	C32-C33	-4.66	1.40	1.51
17	H	301	3BV	C32-C33	-4.44	1.40	1.51
17	V	301	3BV	C32-C33	-4.42	1.40	1.51
17	Y	301	3BV	C13-C14	-4.29	1.39	1.51
17	K	301	3BV	C13-C14	-4.18	1.39	1.51
17	b	201	3BV	C13-C14	-3.70	1.41	1.51
17	N	201	3BV	C13-C14	-3.68	1.41	1.51
17	H	301	3BV	C51-C47	3.51	1.59	1.53
17	V	301	3BV	C51-C47	3.40	1.59	1.53
17	H	301	3BV	C13-C14	-3.32	1.42	1.51
17	V	301	3BV	C13-C14	-3.24	1.42	1.51
17	K	301	3BV	O48-C47	-2.62	1.36	1.43
17	Y	301	3BV	C43-C42	2.60	1.56	1.52
17	b	201	3BV	C59-C51	2.34	1.55	1.52
17	K	301	3BV	C51-C47	2.31	1.57	1.53

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	H	301	3BV	C43-C42-N41	-6.47	101.81	110.18
17	K	301	3BV	C43-C42-N41	-6.39	101.92	110.18
17	V	301	3BV	C43-C42-N41	-6.34	101.98	110.18
17	Y	301	3BV	C7-N4-C3	-5.99	101.81	111.09
17	N	201	3BV	C43-C42-N41	-5.85	102.61	110.18
17	b	201	3BV	C43-C42-N41	-5.80	102.68	110.18
17	N	201	3BV	C58-C51-C59	-4.96	103.36	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	b	201	3BV	C58-C51-C59	-4.75	103.63	109.88
17	H	301	3BV	O1-C6-C5	-3.82	103.38	111.80
17	V	301	3BV	O1-C6-C5	-3.81	103.40	111.80
17	H	301	3BV	C59-C51-C47	-3.43	104.50	110.99
17	K	301	3BV	C20-C11-N10	-3.41	101.87	111.16
17	Y	301	3BV	C3-N4-C5	3.41	116.51	108.83
17	Y	301	3BV	C20-C11-N10	-3.35	102.03	111.16
17	b	201	3BV	C33-C32-C31	-3.32	104.22	113.39
17	N	201	3BV	O1-C6-C5	-3.31	104.51	111.80
17	N	201	3BV	C33-C32-C31	-3.19	104.58	113.39
17	K	301	3BV	C24-C23-C28	-3.19	102.98	110.57
17	V	301	3BV	C59-C51-C47	-3.17	104.98	110.99
17	K	301	3BV	C58-C51-C59	-3.11	105.79	109.88
18	V	302	MES	O3S-S-C8	3.05	110.71	105.77
17	H	301	3BV	C33-C32-C31	-3.05	104.96	113.39
17	H	301	3BV	C13-C12-C11	-3.05	107.20	113.21
17	Y	301	3BV	O1-C6-C5	-3.04	105.10	111.80
17	V	301	3BV	C33-C32-C31	-3.04	105.01	113.39
17	V	301	3BV	C13-C12-C11	-3.00	107.30	113.21
17	b	201	3BV	O1-C6-C5	-3.00	105.19	111.80
17	H	301	3BV	C25-C24-C23	-2.93	107.39	115.43
17	N	201	3BV	O1-C2-C3	-2.91	105.38	111.80
17	V	301	3BV	C25-C24-C23	-2.88	107.51	115.43
17	K	301	3BV	C33-C32-C31	-2.81	105.64	113.39
17	b	201	3BV	O1-C2-C3	-2.77	105.69	111.80
18	V	302	MES	O1S-S-C8	2.75	110.22	106.92
17	Y	301	3BV	C33-C32-C31	-2.69	105.95	113.39
17	Y	301	3BV	C39-C31-N30	-2.64	103.97	111.16
17	V	301	3BV	C58-C51-C59	-2.60	106.46	109.88
17	Y	301	3BV	O1-C2-C3	-2.58	106.12	111.80
17	b	201	3BV	C12-C13-C14	-2.53	104.39	113.18
17	N	201	3BV	C12-C13-C14	-2.51	104.45	113.18
18	H	302	MES	O2S-S-C8	2.50	109.92	106.92
18	H	302	MES	O1S-S-C8	2.47	109.89	106.92
17	K	301	3BV	C8-C7-N4	-2.35	107.90	113.36
17	K	301	3BV	C23-C28-N30	-2.31	111.64	116.70
17	K	301	3BV	O48-C47-C42	-2.26	103.58	108.98
17	K	301	3BV	C39-C31-N30	-2.26	105.01	111.16
17	H	301	3BV	O1-C2-C3	-2.24	106.86	111.80
17	K	301	3BV	O29-C28-N30	2.22	127.03	122.93
17	Y	301	3BV	C24-C23-C28	-2.21	105.30	110.57
17	V	301	3BV	O1-C2-C3	-2.21	106.93	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	b	201	3BV	C13-C12-C11	-2.20	108.87	113.21
17	N	201	3BV	C13-C12-C11	-2.19	108.88	113.21
17	N	201	3BV	C25-C24-C23	-2.19	109.42	115.43
17	b	201	3BV	C25-C24-C23	-2.14	109.55	115.43
17	Y	301	3BV	C42-N41-C39	-2.11	119.34	123.07
17	N	201	3BV	C3-N4-C5	2.11	113.58	108.83
17	b	201	3BV	C3-N4-C5	2.07	113.49	108.83
18	V	302	MES	O2S-S-C8	2.07	109.40	106.92
17	N	201	3BV	C12-C11-C20	-2.05	105.41	110.20
17	H	301	3BV	C58-C51-C59	-2.01	107.23	109.88

There are no chirality outliers.

All (93) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	H	301	3BV	C8-C7-N4-C3
17	H	301	3BV	C47-C42-C43-C44
17	K	301	3BV	N10-C11-C12-C13
17	K	301	3BV	C20-C11-C12-C13
17	K	301	3BV	O48-C47-C51-C58
17	N	201	3BV	C47-C42-C43-C44
17	N	201	3BV	C42-C47-C51-C58
17	N	201	3BV	C42-C47-C51-C59
17	V	301	3BV	C8-C7-N4-C3
17	V	301	3BV	C47-C42-C43-C44
17	Y	301	3BV	N22-C23-C24-C25
17	Y	301	3BV	N41-C42-C43-C44
17	Y	301	3BV	C47-C42-C43-C44
17	Y	301	3BV	N41-C42-C47-O48
17	Y	301	3BV	C43-C42-C47-C51
17	Y	301	3BV	C43-C42-C47-O48
17	Y	301	3BV	O48-C47-C51-C58
17	b	201	3BV	C47-C42-C43-C44
17	b	201	3BV	C42-C47-C51-C58
17	b	201	3BV	C42-C47-C51-C59
18	H	302	MES	C8-C7-N4-C3
18	H	302	MES	C8-C7-N4-C5
18	V	302	MES	C7-C8-S-O2S
17	H	301	3BV	N10-C11-C12-C13
17	V	301	3BV	N10-C11-C12-C13
17	H	301	3BV	C20-C11-C12-C13
17	V	301	3BV	C20-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
17	Y	301	3BV	C28-C23-C24-C25
17	Y	301	3BV	C23-C24-C25-C27
17	Y	301	3BV	C23-C24-C25-C26
18	V	302	MES	C7-C8-S-O3S
17	K	301	3BV	C23-C24-C25-C27
17	K	301	3BV	N22-C23-C24-C25
17	N	201	3BV	O48-C47-C51-C59
17	b	201	3BV	O48-C47-C51-C59
17	Y	301	3BV	C42-C47-C51-C58
17	Y	301	3BV	N30-C31-C32-C33
17	K	301	3BV	C23-C24-C25-C26
17	Y	301	3BV	C43-C42-N41-C39
17	Y	301	3BV	N10-C11-C12-C13
17	K	301	3BV	N30-C31-C32-C33
17	N	201	3BV	O48-C47-C51-C58
17	V	301	3BV	O48-C47-C51-C58
17	b	201	3BV	O48-C47-C51-C58
17	N	201	3BV	C8-C7-N4-C5
17	N	201	3BV	C8-C7-N4-C3
17	b	201	3BV	C8-C7-N4-C5
17	b	201	3BV	C8-C7-N4-C3
17	K	301	3BV	N30-C31-C39-O40
17	H	301	3BV	N41-C42-C43-C44
17	N	201	3BV	N41-C42-C43-C44
17	V	301	3BV	N41-C42-C43-C44
17	b	201	3BV	N41-C42-C43-C44
17	H	301	3BV	C42-C47-C51-C58
17	K	301	3BV	C42-C47-C51-C58
17	V	301	3BV	C42-C47-C51-C58
17	Y	301	3BV	N30-C31-C39-O40
17	K	301	3BV	C8-C7-N4-C5
17	K	301	3BV	C8-C7-N4-C3
17	K	301	3BV	C11-C12-C13-C14
17	Y	301	3BV	C11-C12-C13-C14
17	K	301	3BV	N30-C31-C39-N41
17	V	301	3BV	C58-C51-C59-O60
17	H	301	3BV	O48-C47-C51-C58
17	Y	301	3BV	N30-C31-C39-N41
17	Y	301	3BV	C32-C31-C39-O40
18	V	302	MES	C7-C8-S-O1S
17	Y	301	3BV	N41-C42-C47-C51
17	Y	301	3BV	C32-C31-C39-N41

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Mol	Chain	Res	Type	Atoms
17	b	201	3BV	N10-C11-C20-N22
17	N	201	3BV	N10-C11-C20-N22
17	H	301	3BV	N30-C31-C39-O40
17	b	201	3BV	N10-C11-C20-O21
18	V	302	MES	C8-C7-N4-C5
17	N	201	3BV	N10-C11-C20-O21
17	V	301	3BV	N30-C31-C39-O40
17	N	201	3BV	N30-C31-C39-O40
17	b	201	3BV	N30-C31-C39-O40
17	H	301	3BV	N30-C31-C39-N41
17	N	201	3BV	N30-C31-C39-N41
17	V	301	3BV	N30-C31-C39-N41
17	b	201	3BV	N30-C31-C39-N41
17	H	301	3BV	C58-C51-C59-O60
17	N	201	3BV	C11-C12-C13-C14
17	b	201	3BV	C11-C12-C13-C14
17	V	301	3BV	C47-C51-C59-O60
17	H	301	3BV	C12-C13-C14-C15
17	V	301	3BV	C12-C13-C14-C15
17	Y	301	3BV	C12-C13-C14-C19
17	V	301	3BV	C12-C13-C14-C19
17	H	301	3BV	C12-C13-C14-C19
18	V	302	MES	C8-C7-N4-C3
17	Y	301	3BV	C12-C13-C14-C15

There are no ring outliers.

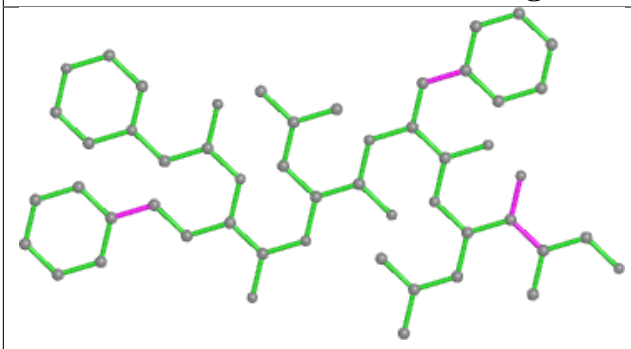
5 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	K	301	3BV	5	0
17	N	201	3BV	1	0
17	Y	301	3BV	12	0
17	V	301	3BV	3	0
17	H	301	3BV	4	0

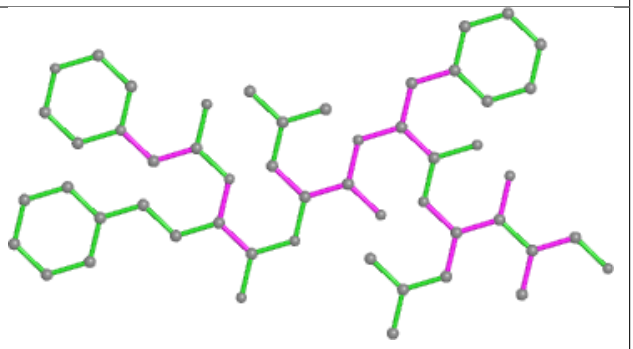
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

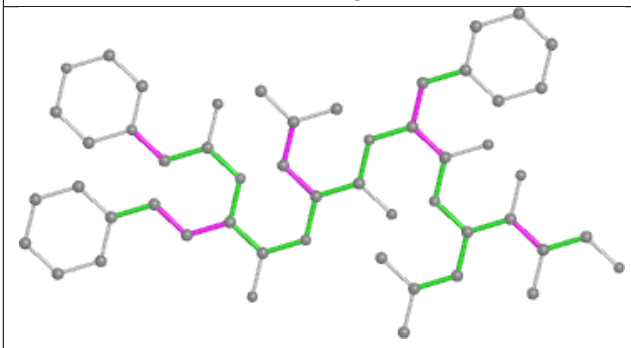
Ligand 3BV K 301



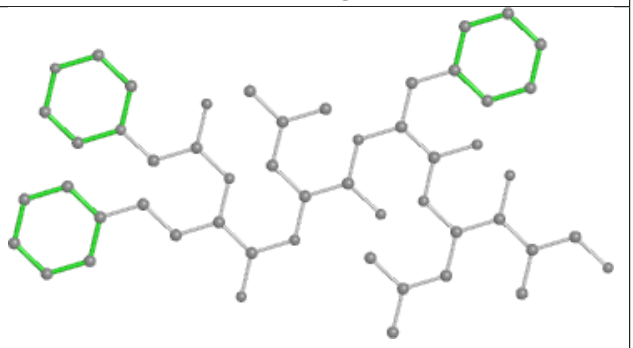
Bond lengths



Bond angles

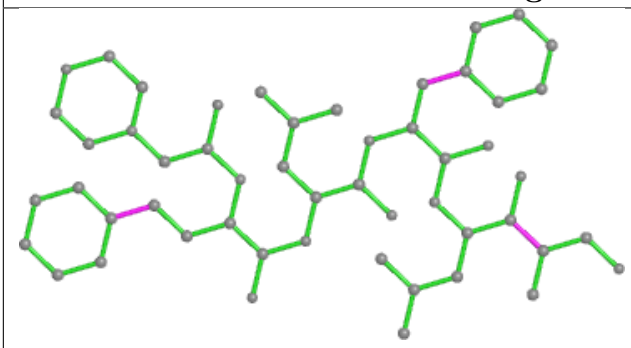


Torsions

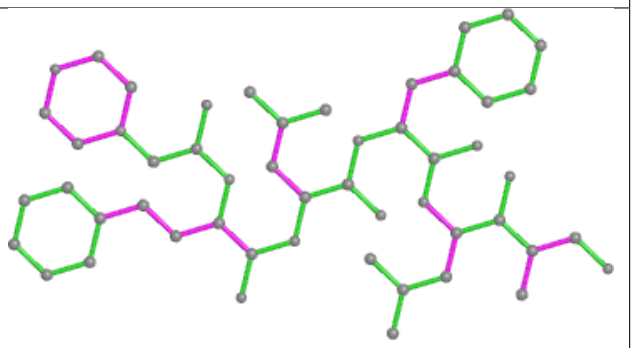


Rings

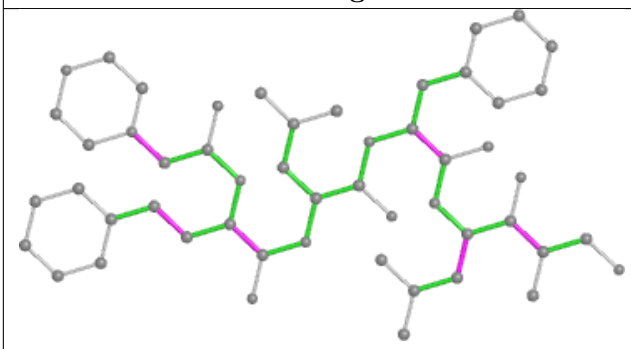
Ligand 3BV N 201



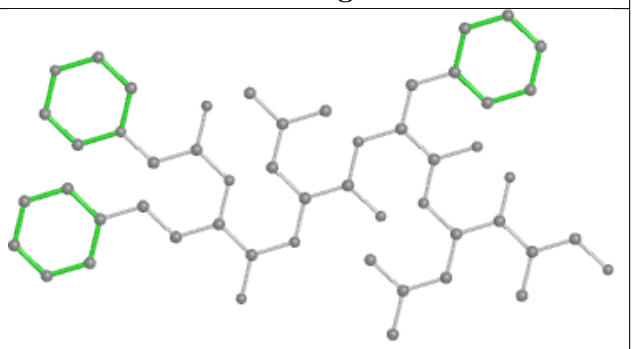
Bond lengths



Bond angles

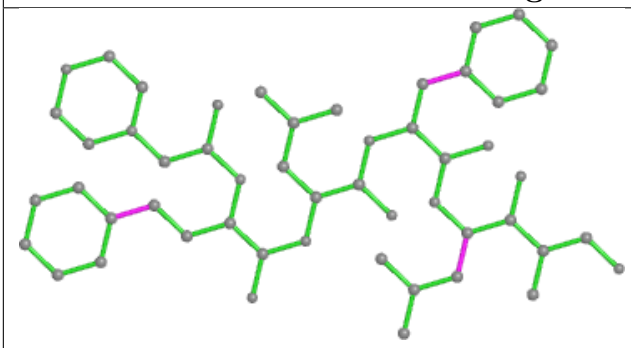


Torsions

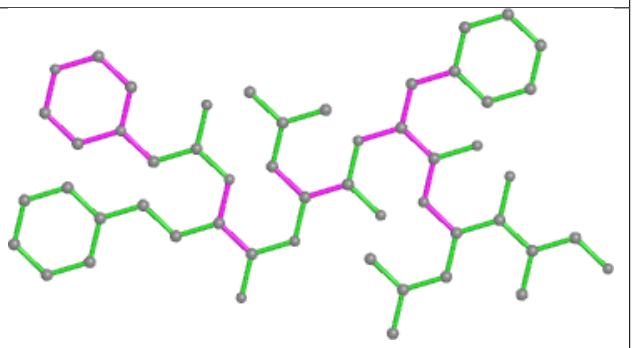


Rings

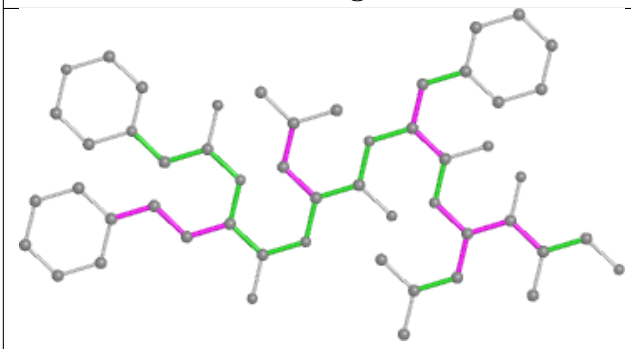
Ligand 3BV Y 301



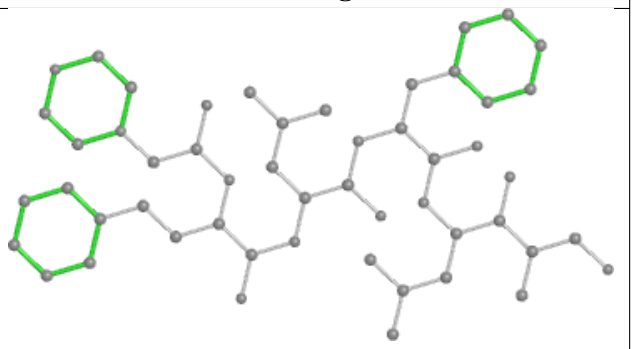
Bond lengths



Bond angles

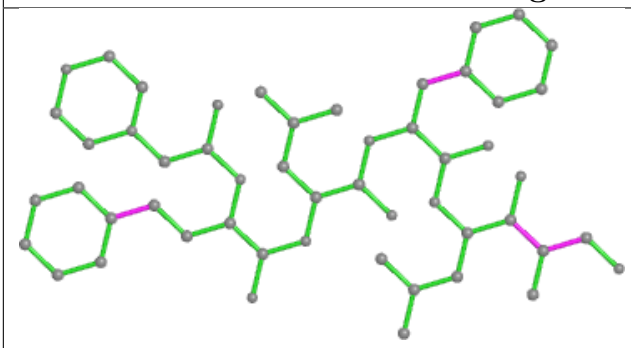


Torsions

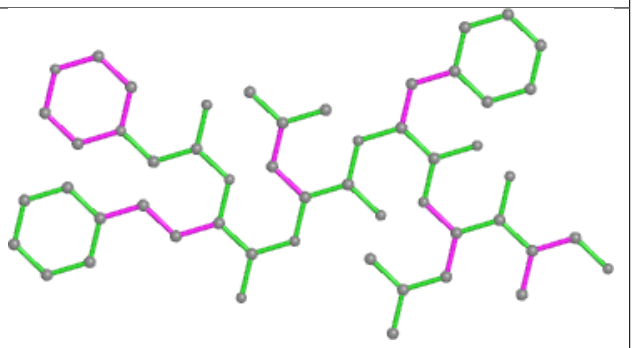


Rings

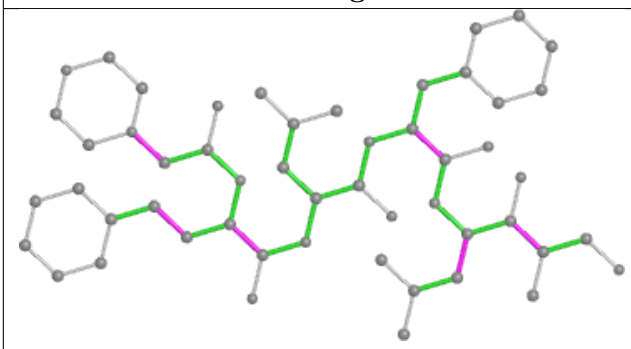
Ligand 3BV b 201



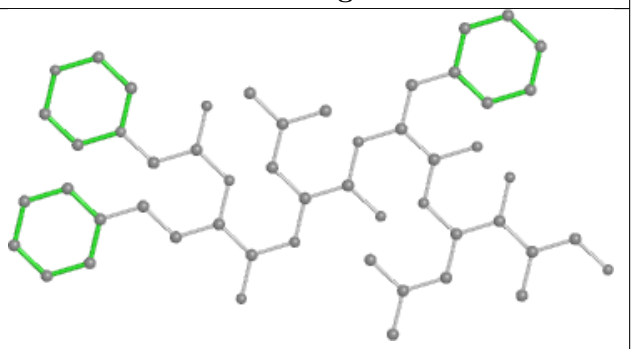
Bond lengths



Bond angles

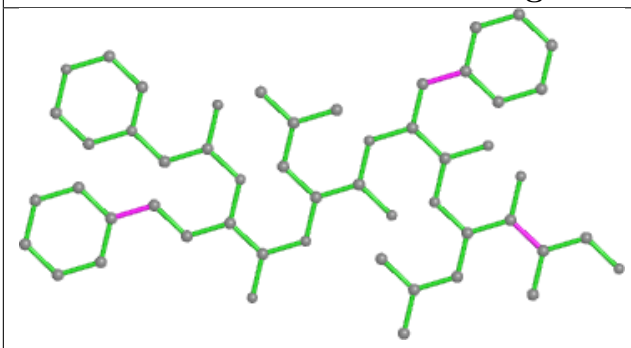


Torsions

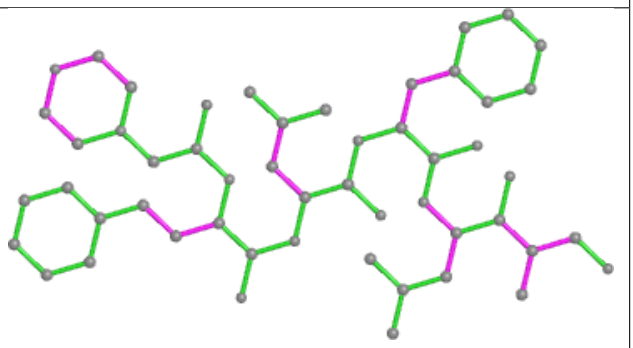


Rings

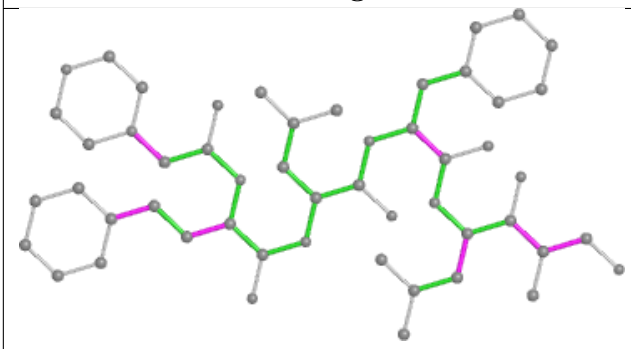
Ligand 3BV V 301



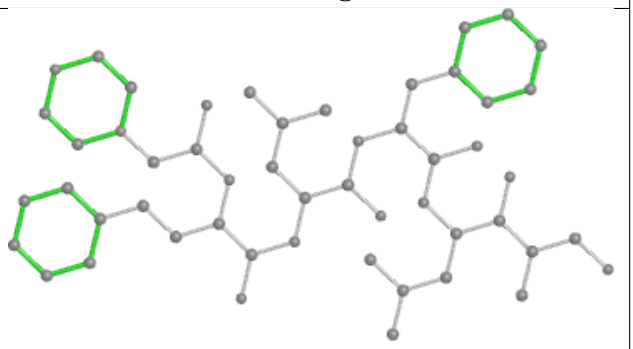
Bond lengths



Bond angles

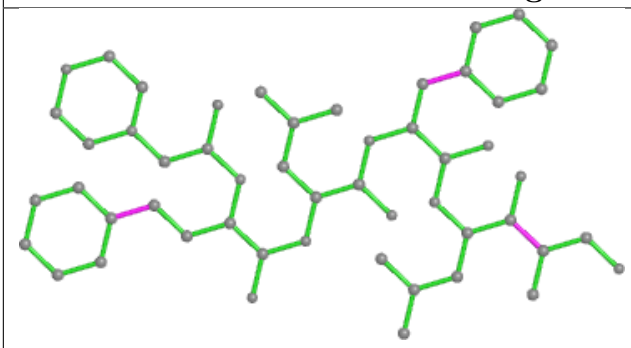


Torsions

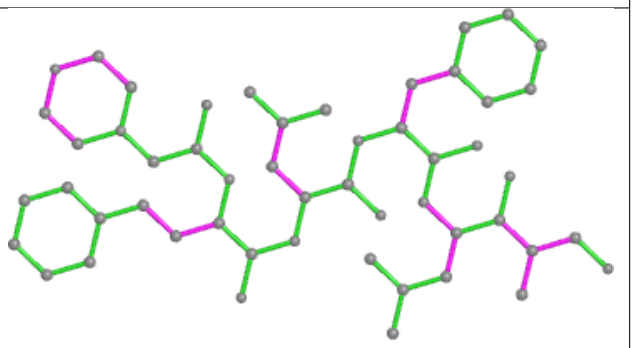


Rings

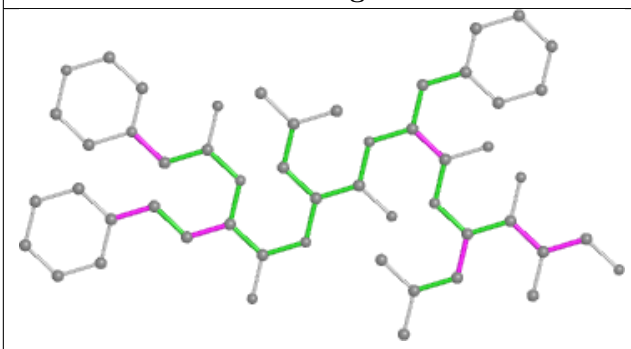
Ligand 3BV H 301



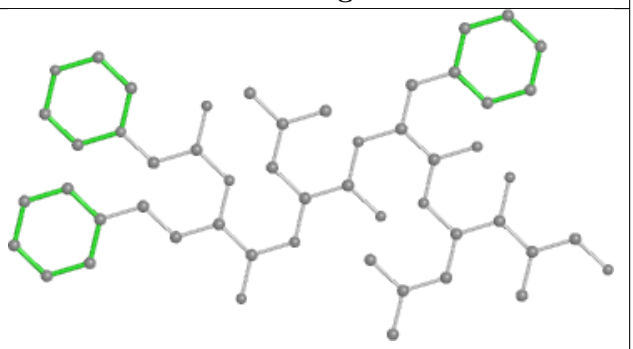
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	250/250 (100%)	-0.37	5 (2%)	65	63	36, 55, 92, 134	0
1	O	250/250 (100%)	-0.34	7 (2%)	53	49	40, 58, 102, 139	0
2	B	244/258 (94%)	-0.29	8 (3%)	46	41	41, 61, 106, 162	0
2	P	244/258 (94%)	-0.28	8 (3%)	46	41	44, 62, 105, 154	0
3	C	240/254 (94%)	-0.08	16 (6%)	17	13	40, 67, 135, 165	0
3	Q	240/254 (94%)	-0.02	16 (6%)	17	13	28, 74, 150, 182	0
4	D	235/260 (90%)	-0.35	1 (0%)	92	93	48, 65, 97, 130	0
4	R	235/260 (90%)	-0.21	7 (2%)	50	45	56, 76, 112, 139	0
5	E	231/234 (98%)	-0.25	6 (2%)	56	52	47, 68, 111, 156	0
5	S	231/234 (98%)	-0.26	5 (2%)	62	59	49, 71, 114, 147	0
6	F	243/288 (84%)	-0.43	6 (2%)	57	55	40, 60, 105, 139	0
6	T	243/288 (84%)	-0.35	7 (2%)	51	47	40, 67, 124, 149	0
7	G	241/252 (95%)	-0.45	4 (1%)	70	69	38, 56, 97, 154	0
7	U	241/252 (95%)	-0.43	4 (1%)	70	69	41, 56, 92, 132	0
8	H	226/232 (97%)	-0.47	4 (1%)	68	67	37, 52, 91, 147	0
8	V	226/232 (97%)	-0.40	5 (2%)	62	59	38, 52, 88, 156	0
9	I	204/205 (99%)	-0.58	1 (0%)	91	91	38, 54, 84, 106	0
9	W	204/205 (99%)	-0.58	2 (0%)	82	82	40, 54, 83, 111	0
10	J	195/198 (98%)	-0.41	3 (1%)	73	73	37, 55, 83, 127	0
10	X	195/198 (98%)	-0.41	4 (2%)	63	61	39, 58, 85, 141	0
11	K	211/211 (100%)	-0.34	3 (1%)	75	75	44, 62, 92, 120	0
11	Y	211/211 (100%)	-0.33	2 (0%)	84	84	45, 63, 92, 118	0
12	L	222/222 (100%)	-0.44	3 (1%)	75	75	44, 58, 101, 131	0
12	Z	222/222 (100%)	-0.40	5 (2%)	60	58	33, 61, 101, 137	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
13	M	233/246 (94%)	-0.57	1 (0%)	92 93	36, 52, 75, 93	0
13	a	233/246 (94%)	-0.55	1 (0%)	92 93	39, 54, 77, 93	0
14	N	196/196 (100%)	-0.60	1 (0%)	91 91	32, 49, 80, 108	0
14	b	196/196 (100%)	-0.58	1 (0%)	91 91	31, 49, 80, 112	0
All	All	6342/6612 (95%)	-0.38	136 (2%)	63 61	28, 60, 104, 182	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	221	ASP	5.5
3	C	206	LYS	5.2
3	Q	238	LYS	5.0
9	I	1	SER	5.0
9	W	1	SER	4.8
3	Q	206	LYS	4.8
12	L	174	TYR	4.7
3	C	238	LYS	4.6
8	V	226	GLU	4.5
10	X	1	MET	4.4
5	E	202	ASP	4.3
3	C	202	GLN	4.1
8	V	224	GLN	4.1
12	Z	174	TYR	4.1
2	P	51	VAL	4.0
3	Q	50	LEU	3.9
2	B	218	GLY	3.8
3	Q	239	GLN	3.8
8	V	222	ASP	3.8
2	P	218	GLY	3.7
3	Q	202	GLN	3.7
2	P	221	ASP	3.7
3	Q	240	GLU	3.7
10	J	194	ASP	3.7
2	P	59	ASP	3.7
10	J	1	MET	3.6
8	V	221	CYS	3.5
1	O	249	ALA	3.5
5	S	202	ASP	3.5
3	Q	49	THR	3.5
10	X	194	ASP	3.5
2	B	51	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
3	Q	225	GLU	3.3
1	O	2	THR	3.3
3	C	49	THR	3.3
3	Q	141	ASP	3.3
8	H	221	CYS	3.3
2	P	219	ALA	3.2
1	O	1	MET	3.2
8	H	226	GLU	3.2
1	O	201	GLU	3.1
3	C	236	GLN	3.1
2	B	220	ASN	3.1
3	C	225	GLU	3.1
11	K	211	GLY	3.1
3	C	60	SER	3.0
8	H	224	GLN	3.0
2	B	201	ASP	3.0
2	B	219	ALA	3.0
12	Z	173	LYS	3.0
3	C	203	THR	3.0
7	U	242	GLN	3.0
6	F	181	GLU	3.0
3	C	50	LEU	3.0
3	C	235	GLU	2.9
3	Q	236	GLN	2.9
6	F	244	ASN	2.9
2	P	220	ASN	2.9
7	G	188	GLU	2.9
1	A	1	MET	2.8
5	S	3	ASN	2.8
2	B	59	ASP	2.8
10	X	193	ASP	2.8
3	C	205	ALA	2.7
1	O	250	LEU	2.7
3	C	180	LYS	2.7
3	Q	180	LYS	2.7
4	R	230	GLU	2.7
6	T	244	ASN	2.7
7	U	188	GLU	2.6
4	R	54	ASP	2.6
6	T	181	GLU	2.6
3	C	239	GLN	2.6
12	Z	210	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
2	P	203	SER	2.6
5	E	173	ARG	2.5
3	Q	60	SER	2.5
12	L	165	ASN	2.5
8	H	222	ASP	2.5
11	Y	211	GLY	2.5
6	T	205	GLU	2.5
5	E	233	ILE	2.5
12	Z	116	GLU	2.5
6	T	180	PRO	2.5
3	Q	181	GLU	2.4
1	A	249	ALA	2.4
7	G	242	GLN	2.4
1	O	52	SER	2.4
11	K	150	GLU	2.4
4	R	241	ALA	2.4
5	S	218	ASP	2.3
1	A	201	GLU	2.3
3	C	240	GLU	2.3
4	R	1	ASP	2.3
2	P	222	GLY	2.3
5	S	173	ARG	2.3
14	N	195	GLN	2.3
7	U	222	ASP	2.3
9	W	133	LYS	2.3
3	Q	205	ALA	2.2
13	a	1	THR	2.2
13	M	47	ASP	2.2
7	U	2	GLY	2.2
2	B	217	LYS	2.2
8	V	145	ASP	2.2
11	Y	146	ASP	2.2
4	D	242	GLU	2.2
6	T	201	GLU	2.2
3	Q	187	GLU	2.2
3	C	48	SER	2.2
4	R	117	GLU	2.2
3	C	216	ASP	2.2
12	L	1	GLN	2.2
10	X	195	PHE	2.1
7	G	179	LYS	2.1
4	R	143	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
5	E	227	GLU	2.1
6	T	237	ASP	2.1
10	J	193	ASP	2.1
11	K	146	ASP	2.1
1	O	248	GLU	2.1
3	Q	237	GLU	2.1
6	F	202	ASP	2.1
6	F	215	CYS	2.1
5	E	123	GLY	2.1
5	E	201	ARG	2.1
6	T	2	THR	2.1
4	R	203	LYS	2.1
5	S	233	ILE	2.0
7	G	222	ASP	2.0
6	F	205	GLU	2.0
1	A	250	LEU	2.0
12	Z	1	GLN	2.0
6	F	228	LYS	2.0
1	A	248	GLU	2.0
14	b	105	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
17	3BV	Y	301	52/52	0.83	0.36	62,89,162,166	0
17	3BV	K	301	52/52	0.86	0.31	62,85,161,167	0
17	3BV	b	201	52/52	0.88	0.23	29,47,128,135	0

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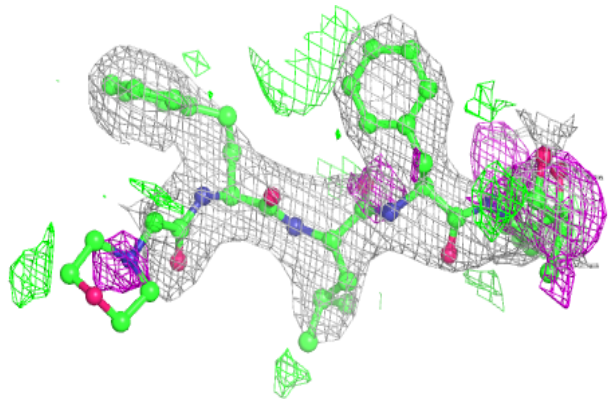
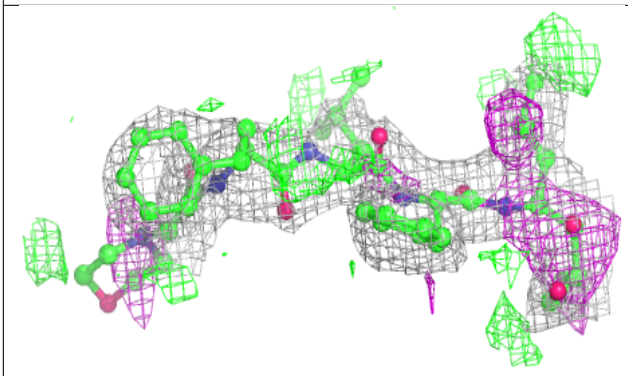
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
17	3BV	N	201	52/52	0.90	0.23	27,46,131,136	0
17	3BV	H	301	52/52	0.91	0.21	43,52,100,104	0
17	3BV	V	301	52/52	0.91	0.22	41,50,99,103	0
18	MES	H	302	12/12	0.91	0.33	68,72,91,101	0
18	MES	V	302	12/12	0.91	0.32	72,77,94,101	0
15	MG	J	201	1/1	0.94	0.23	52,52,52,52	0
15	MG	K	302	1/1	0.95	0.15	59,59,59,59	0
15	MG	Z	301	1/1	0.95	0.36	70,70,70,70	0
15	MG	I	301	1/1	0.96	0.12	57,57,57,57	0
16	CL	b	202	1/1	0.96	0.09	57,57,57,57	0
15	MG	G	301	1/1	0.98	0.11	57,57,57,57	0
15	MG	I	302	1/1	0.98	0.08	55,55,55,55	0
15	MG	N	202	1/1	0.99	0.08	51,51,51,51	0
16	CL	G	302	1/1	0.99	0.13	40,40,40,40	0
16	CL	N	203	1/1	0.99	0.09	60,60,60,60	0
16	CL	U	301	1/1	1.00	0.16	42,42,42,42	0

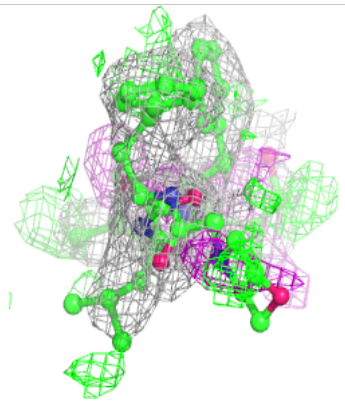
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 3BV 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)

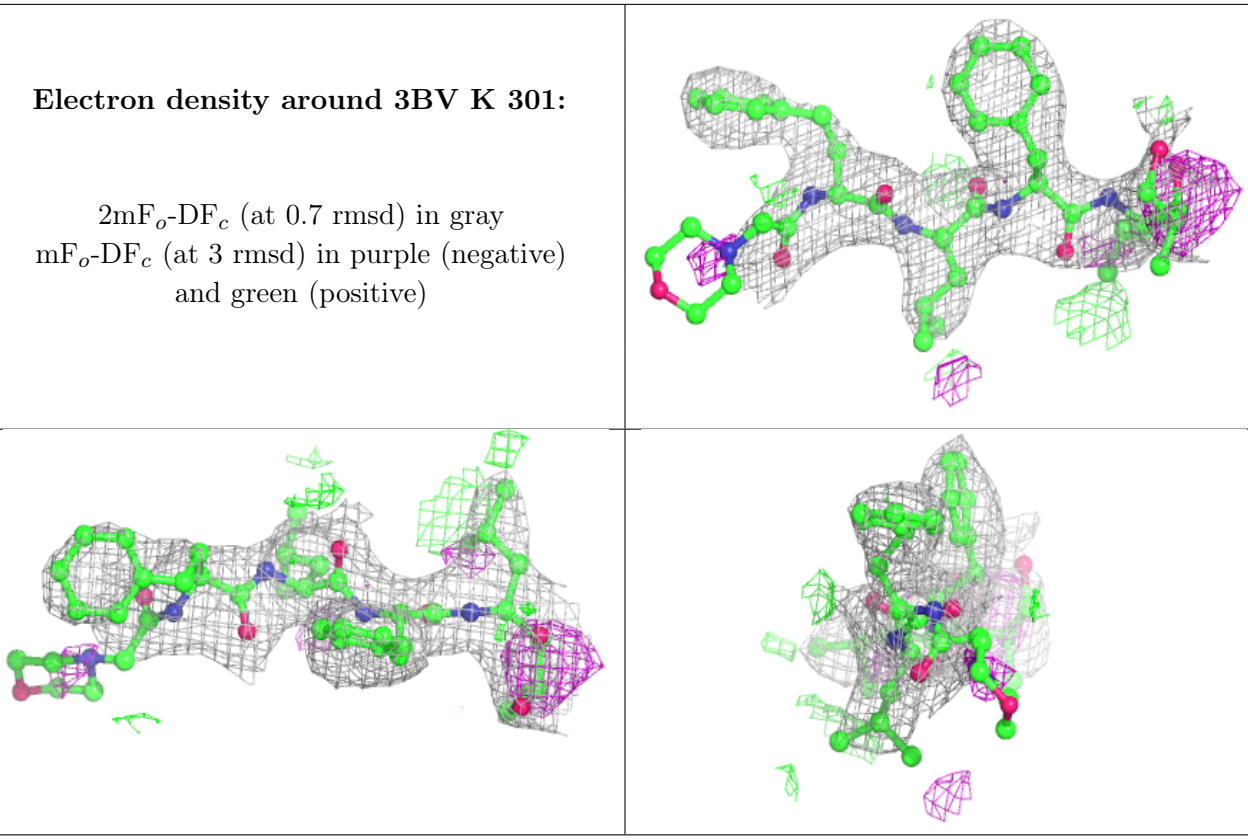






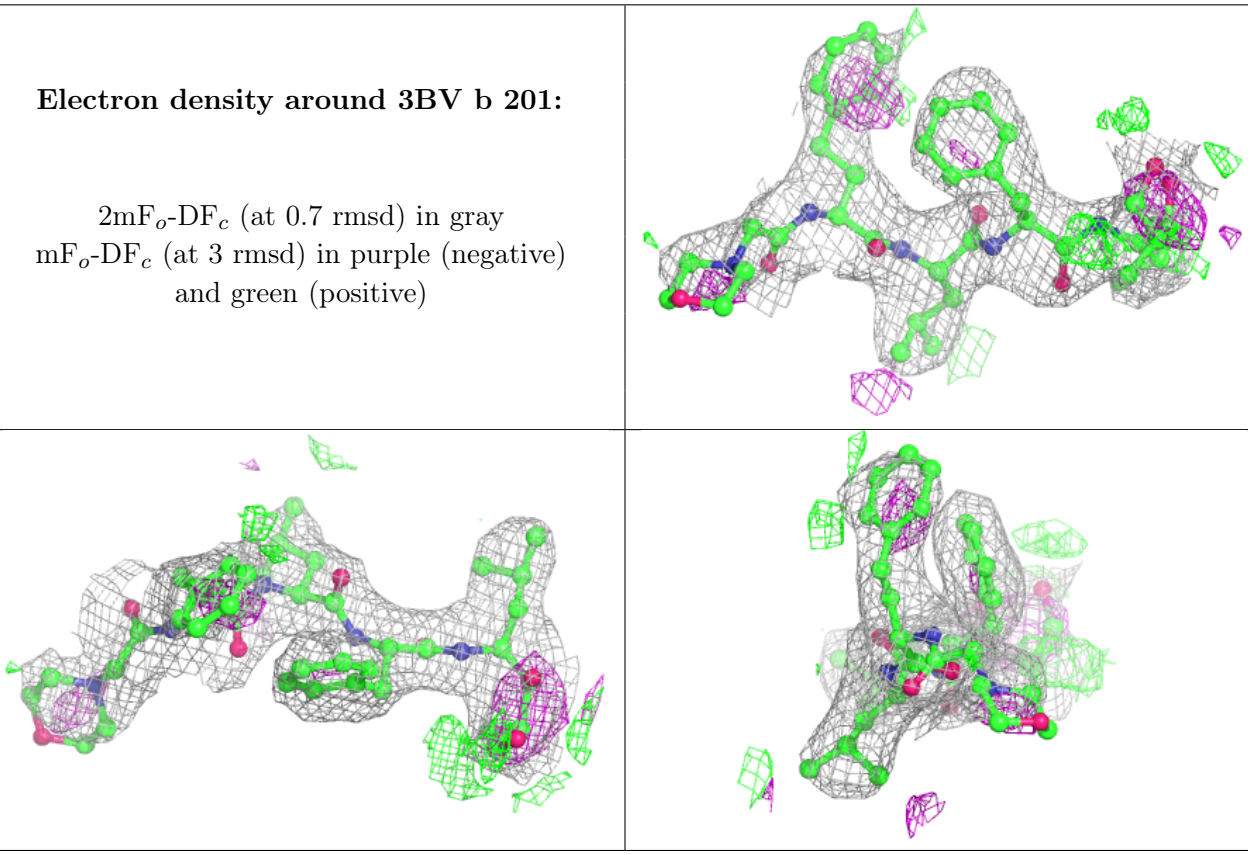
Electron density around 3BV K 301:

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



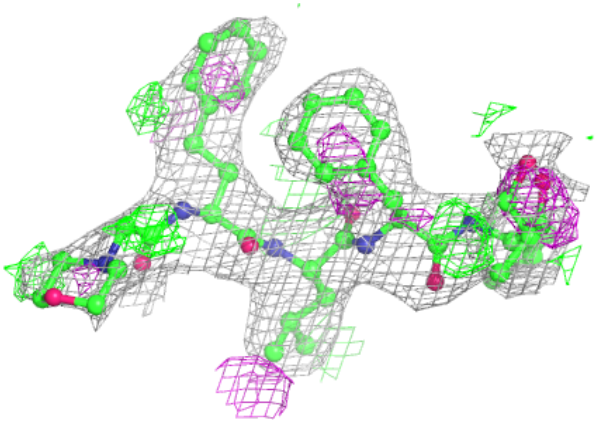
Electron density around 3BV b 201:

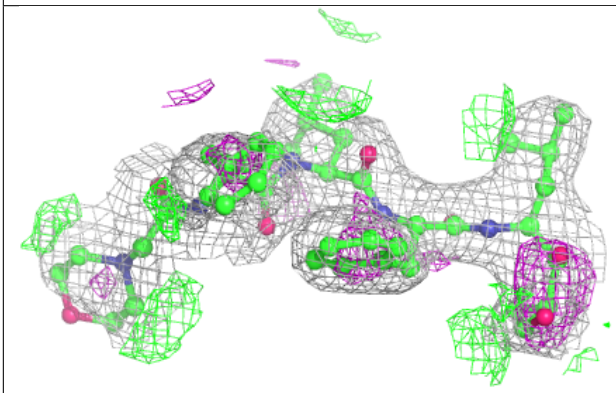
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

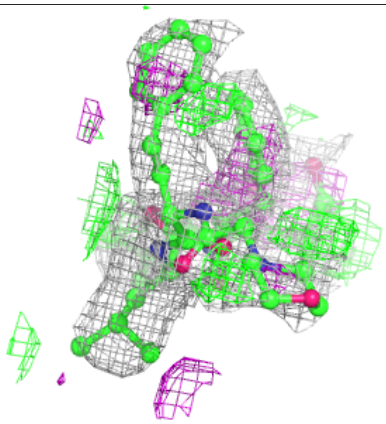


Electron density around 3BV N 201:

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

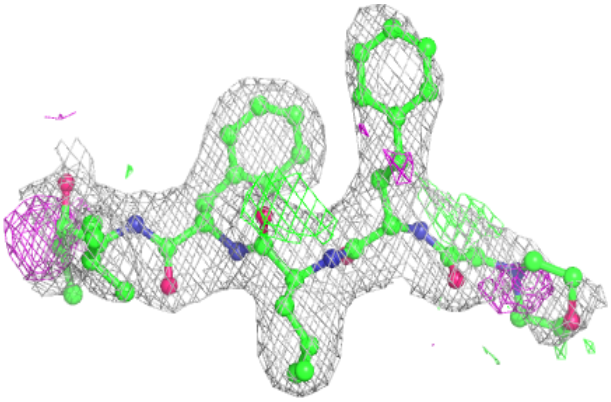


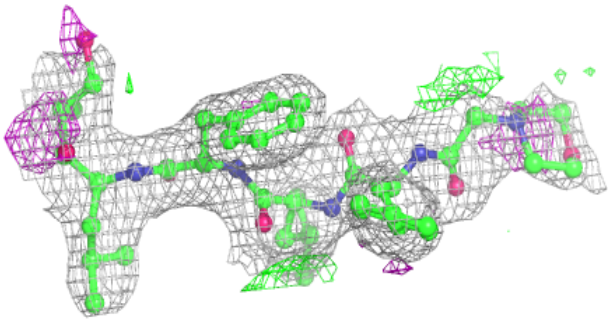


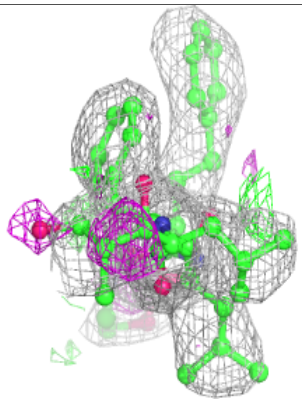


Electron density around 3BV H 301:

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

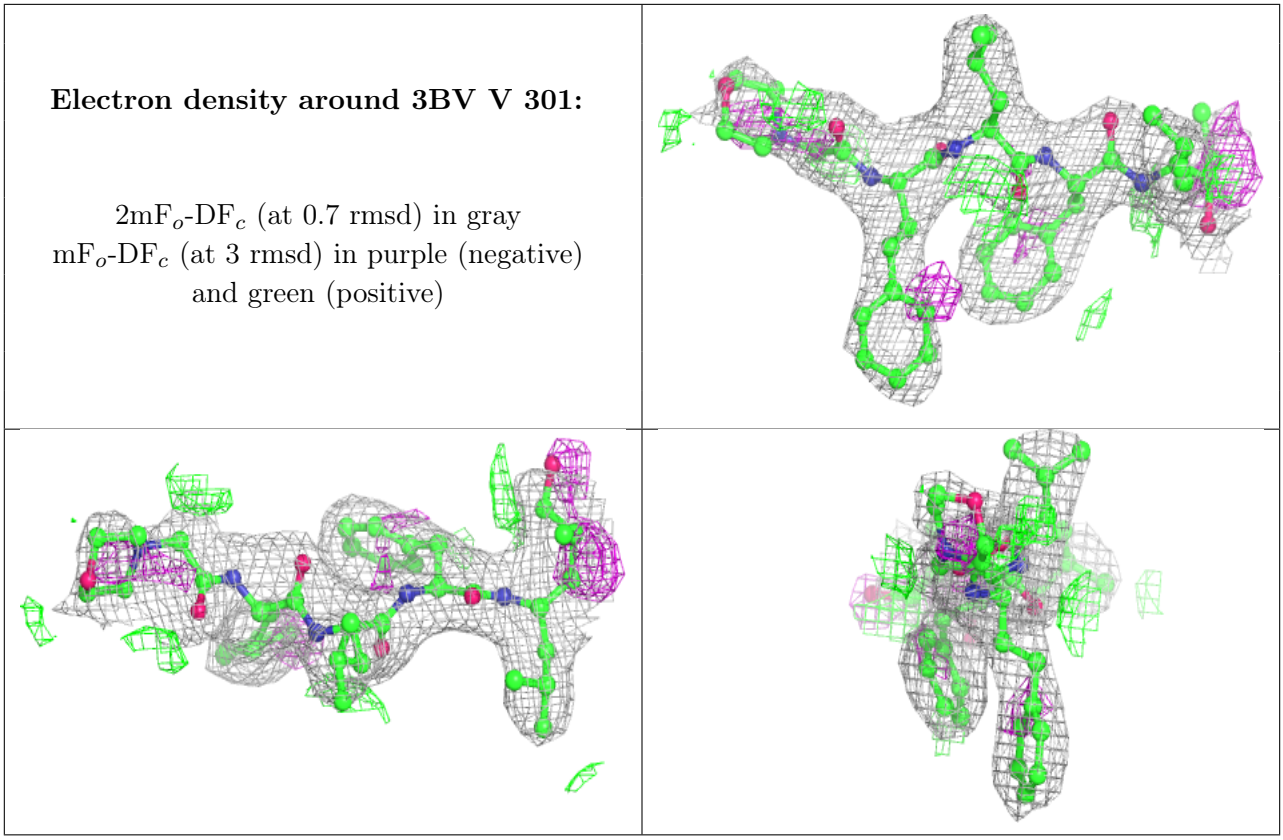






Electron density around 3BV V 301:

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



6.5 Other polymers (i)

There are no such residues in this entry.