



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 4, 2024 – 01:27 pm GMT

PDB ID : 5FGF
Title : Yeast 20S proteasome beta5-H(-2)A-T1A-K81R triple mutant in complex with Carfilzomib
Authors : Huber, E.M.; Groll, M.
Deposited on : 2015-12-20
Resolution : 2.60 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

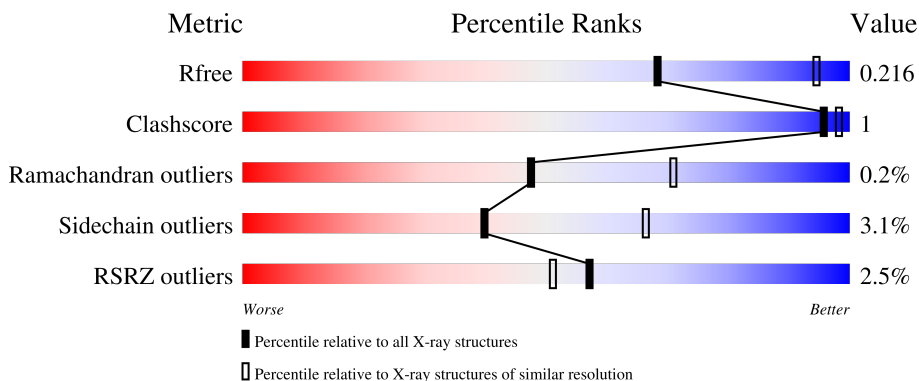
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	250	 2% 99%
1	O	250	 4% 98%
2	B	258	 5% 90% 5%
2	P	258	 5% 91% 5%
3	C	254	 7% 89% 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	7% 90% 6%
4	D	260	% 87% 10%
4	R	260	2% 87% 10%
5	E	234	2% 94% 5%
5	S	234	3% 94% 5%
6	F	288	2% 81% 16%
6	T	288	2% 81% 16%
7	G	252	3% 91% • •
7	U	252	2% 91% 5% •
8	H	232	% 92% • •
8	V	232	% 91% • •
9	I	205	93% 7%
9	W	205	% 93% 6%
10	J	198	2% 88% 8% • • •
10	X	198	2% 88% 9% • • •
11	K	214	% 92% 8%
11	Y	214	% 91% 8% •
12	L	222	2% 94% 6%
12	Z	222	2% 94% 6%
13	M	246	% 89% • • 5%
13	a	246	92% • 5%
14	N	196	% 96% •
14	b	196	99% •

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 50158 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
			Total	C	N	O	S			
1	A	250	Total 1915	C 1219	N 315	O 377	S 4	0	0	0
1	O	250	Total 1915	C 1219	N 315	O 377	S 4	0	0	0

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	241	Total 1907	C 1214	N 320	O 365	S 8	0	0	0
7	U	241	Total 1906	C 1214	N 320	O 364	S 8	0	0	0

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	214	1653	1049	284	313	7	0	0	0
11	Y	214	1653	1049	284	313	7	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-1	ALA	HIS	engineered mutation	UNP P30656
K	1	ALA	THR	engineered mutation	UNP P30656
K	81	ARG	LYS	engineered mutation	UNP P30656
Y	-1	ALA	HIS	engineered mutation	UNP P30656
Y	1	ALA	THR	engineered mutation	UNP P30656
Y	81	ARG	LYS	engineered mutation	UNP P30656

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

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

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

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

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

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

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

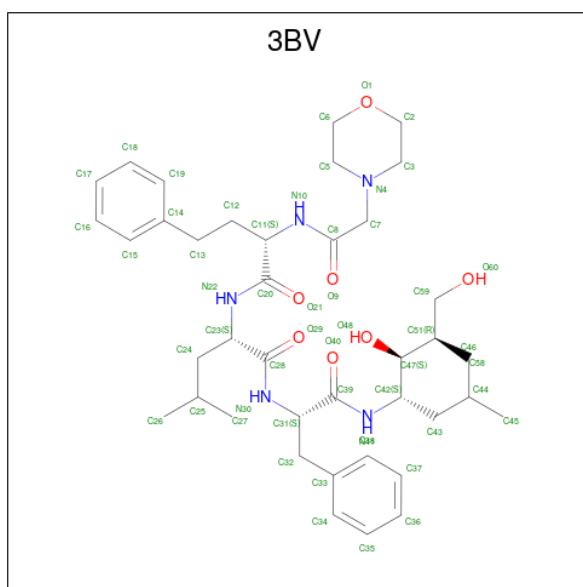
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

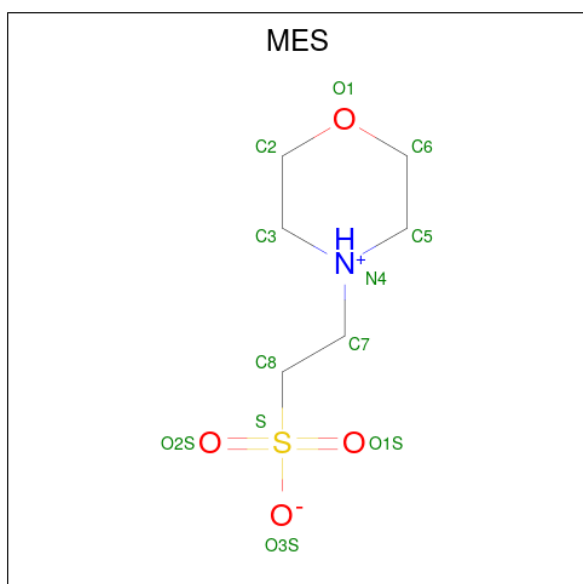
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	G	1	Total	Cl	0	0
			1	1		
16	N	1	Total	Cl	0	0
			1	1		
16	U	1	Total	Cl	0	0
			1	1		
16	b	1	Total	Cl	0	0
			1	1		

- 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: C₄₀H₆₁N₅O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
			Total	C	N			O	
17	H	1	Total	52	40	5	7	0	0
17	N	1	Total	52	40	5	7	0	0
17	V	1	Total	52	40	5	7	0	0
17	b	1	Total	52	40	5	7	0	0

- Molecule 18 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



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

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	23	Total	O	0	0
			23	23		
19	B	19	Total	O	0	0
			19	19		
19	C	20	Total	O	0	0
			20	20		
19	D	14	Total	O	0	0
			14	14		
19	E	9	Total	O	0	0
			9	9		
19	F	19	Total	O	0	0
			19	19		
19	G	31	Total	O	0	0
			31	31		
19	H	38	Total	O	0	0
			38	38		
19	I	18	Total	O	0	0
			18	18		
19	J	25	Total	O	0	0
			25	25		
19	K	25	Total	O	0	0
			25	25		
19	L	28	Total	O	0	0
			28	28		
19	M	32	Total	O	0	0
			32	32		
19	N	23	Total	O	0	0
			23	23		
19	O	16	Total	O	0	0
			16	16		
19	P	15	Total	O	0	0
			15	15		
19	Q	14	Total	O	0	0
			14	14		
19	R	16	Total	O	0	0
			16	16		

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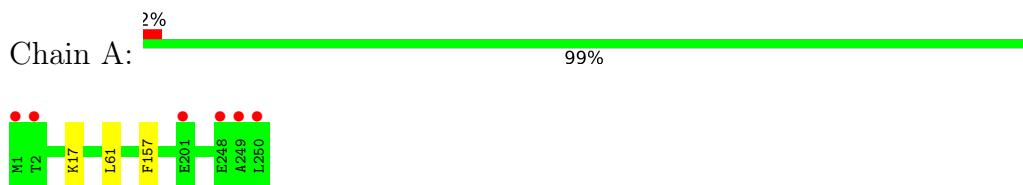
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	S	10	Total 10	O 10	0	0
19	T	11	Total 11	O 11	0	0
19	U	20	Total 20	O 20	0	0
19	V	26	Total 26	O 26	0	0
19	W	12	Total 12	O 12	0	0
19	X	21	Total 21	O 21	0	0
19	Y	19	Total 19	O 19	0	0
19	Z	30	Total 30	O 30	0	0
19	a	40	Total 40	O 40	0	0
19	b	26	Total 26	O 26	0	0

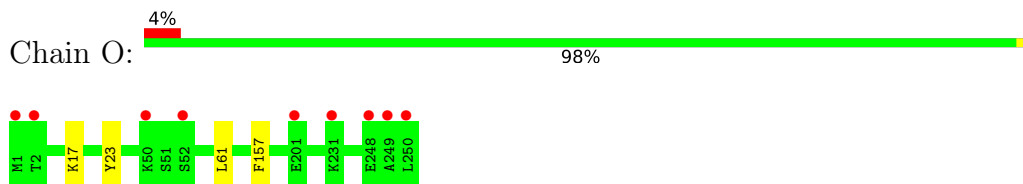
3 Residue-property plots i

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.

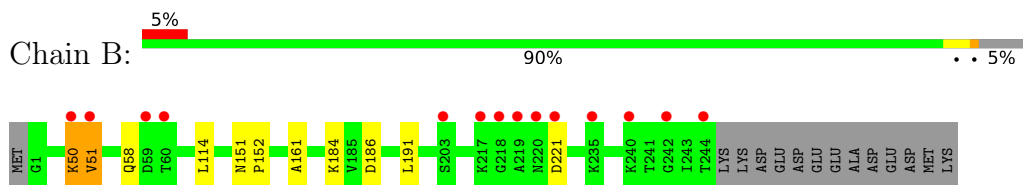
- Molecule 1: Proteasome subunit alpha type-2



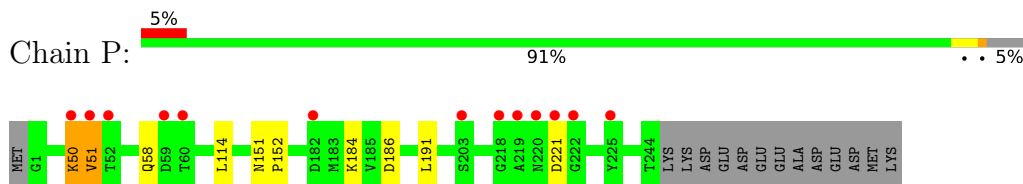
- Molecule 1: Proteasome subunit alpha type-2



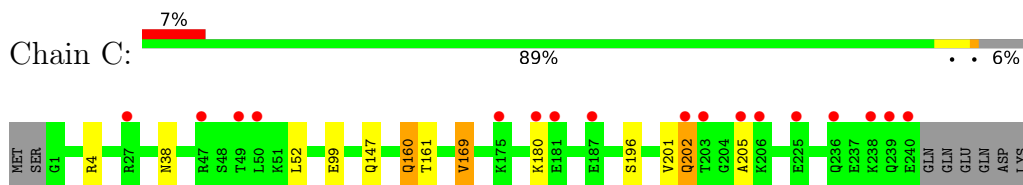
- Molecule 2: Proteasome subunit alpha type-3



- Molecule 2: Proteasome subunit alpha type-3

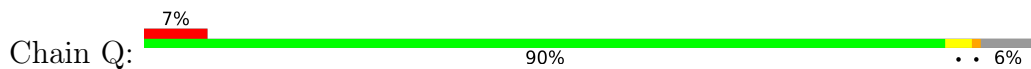


- Molecule 3: Proteasome subunit alpha type-4

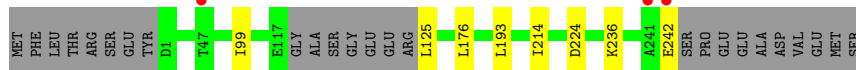
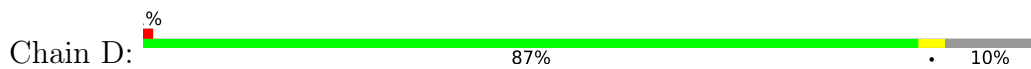


HIS

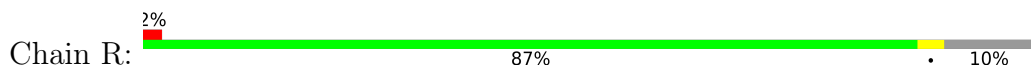
• Molecule 3: Proteasome subunit alpha type-4



• Molecule 4: Proteasome subunit alpha type-5



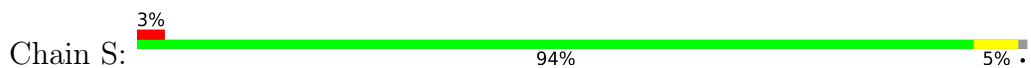
• Molecule 4: Proteasome subunit alpha type-5



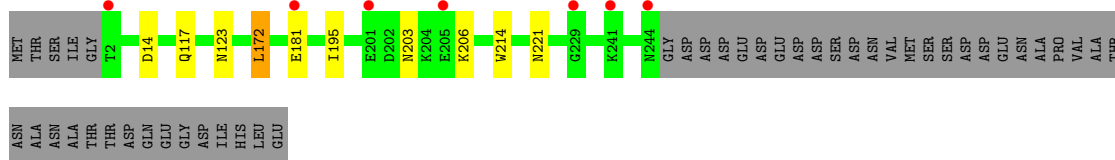
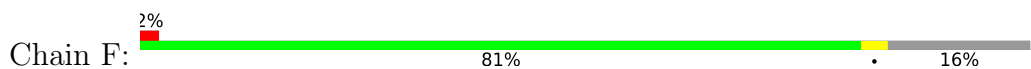
• Molecule 5: Proteasome subunit alpha type-6



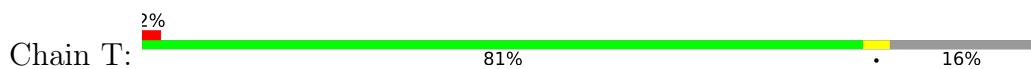
• Molecule 5: Proteasome subunit alpha type-6

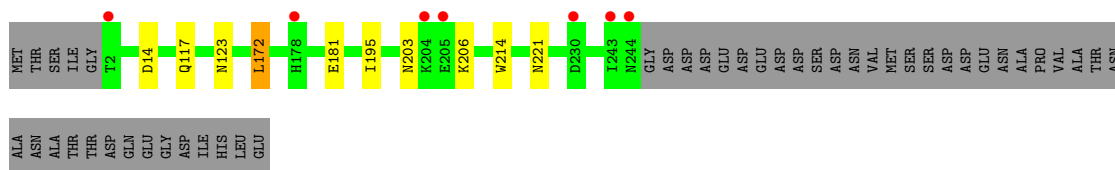


• Molecule 6: Probable proteasome subunit alpha type-7



• Molecule 6: Probable proteasome subunit alpha type-7

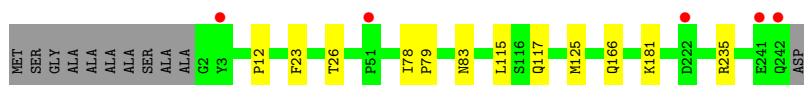




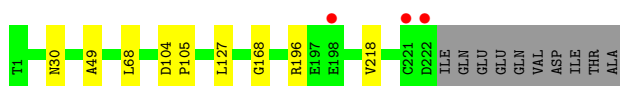
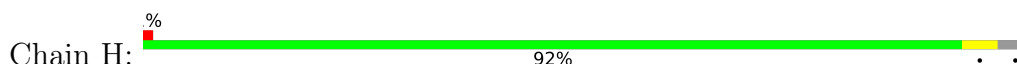
• Molecule 7: Proteasome subunit alpha type-1



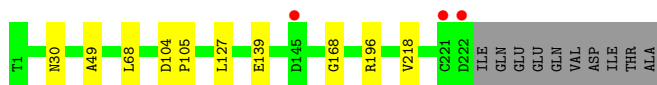
• Molecule 7: Proteasome subunit alpha type-1



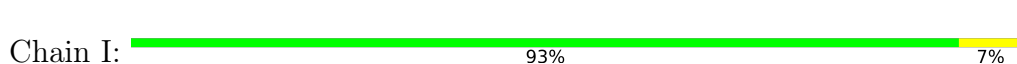
• Molecule 8: Proteasome subunit beta type-2



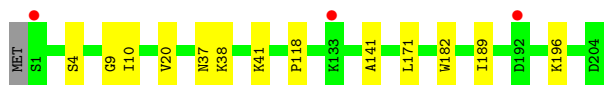
• Molecule 8: Proteasome subunit beta type-2



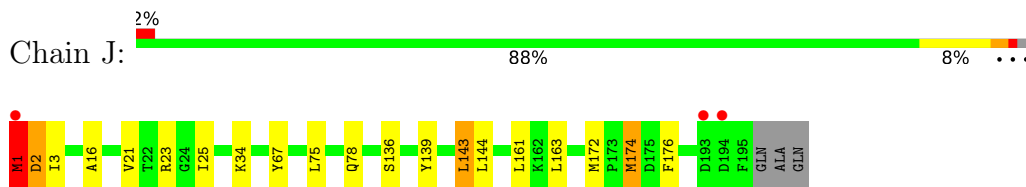
• Molecule 9: Proteasome subunit beta type-3



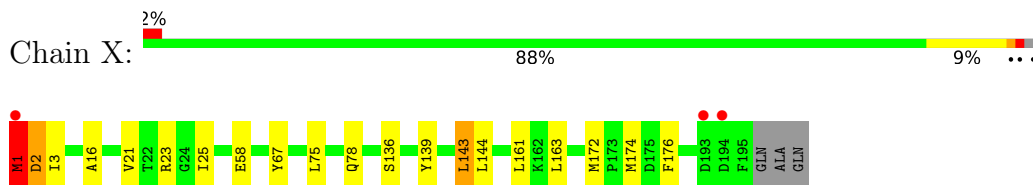
• Molecule 9: Proteasome subunit beta type-3



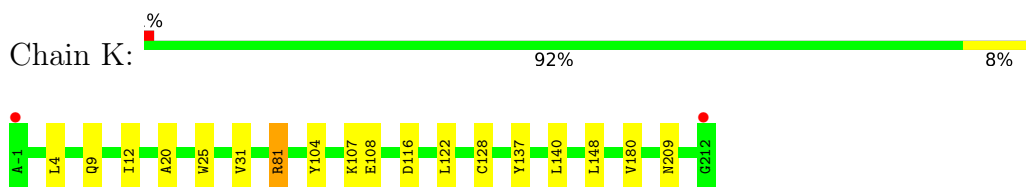
- Molecule 10: Proteasome subunit beta type-4



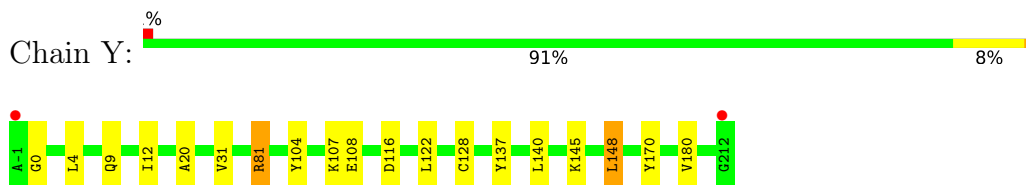
- Molecule 10: Proteasome subunit beta type-4



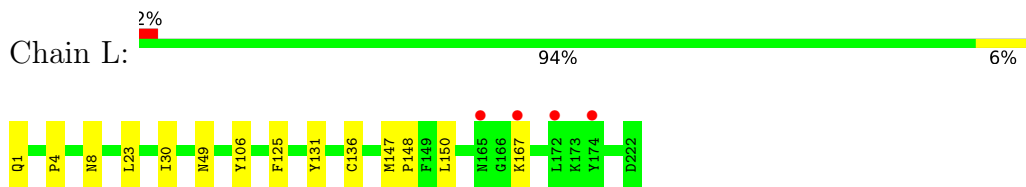
- Molecule 11: Proteasome subunit beta type-5



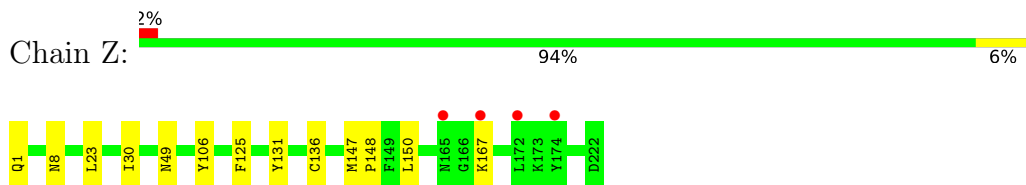
- Molecule 11: Proteasome subunit beta type-5



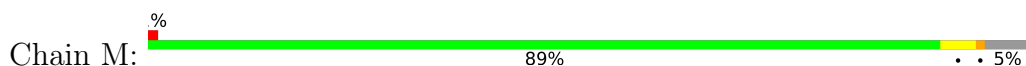
- Molecule 12: Proteasome subunit beta type-6



- Molecule 12: Proteasome subunit beta type-6



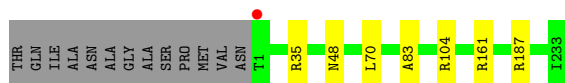
- Molecule 13: Proteasome subunit beta type-7





- Molecule 13: Proteasome subunit beta type-7

Chain a: 92% 5%



- Molecule 14: Proteasome subunit beta type-1

Chain N: 96%



- Molecule 14: Proteasome subunit beta type-1

Chain b: 99%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.08Å 300.97Å 144.89Å 90.00° 113.11° 90.00°	Depositor
Resolution (Å)	15.00 – 2.60 15.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.7 (15.00-2.60) 98.7 (15.00-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.192 , 0.214 0.196 , 0.216	Depositor DCC
R_{free} test set	16063 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	54.7	Xtrriage
Anisotropy	0.084	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 36.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	50158	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MES, CL, MG, 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	0.27	0/1952	0.46	0/2642
1	O	0.26	0/1952	0.46	0/2642
2	B	0.26	0/1934	0.47	0/2618
2	P	0.26	0/1934	0.47	0/2618
3	C	0.27	0/1910	0.50	0/2586
3	Q	0.27	0/1910	0.49	0/2586
4	D	0.26	0/1837	0.45	0/2475
4	R	0.26	0/1837	0.45	0/2475
5	E	0.26	0/1800	0.45	0/2433
5	S	0.26	0/1800	0.45	0/2433
6	F	0.27	0/1932	0.44	0/2609
6	T	0.26	0/1932	0.44	0/2609
7	G	0.27	0/1945	0.46	0/2634
7	U	0.27	0/1944	0.46	0/2632
8	H	0.25	0/1715	0.47	0/2326
8	V	0.25	0/1715	0.47	0/2326
9	I	0.27	0/1611	0.49	0/2174
9	W	0.26	0/1611	0.49	0/2174
10	J	0.35	0/1589	0.63	4/2142 (0.2%)
10	X	0.35	1/1589 (0.1%)	0.78	5/2142 (0.2%)
11	K	0.26	0/1690	0.75	3/2286 (0.1%)
11	Y	0.26	0/1690	0.81	3/2286 (0.1%)
12	L	0.29	0/1795	0.49	0/2420
12	Z	0.28	0/1795	0.48	0/2420
13	M	0.26	0/1855	0.52	0/2514
13	a	0.26	0/1855	0.52	0/2514
14	N	0.25	0/1541	0.47	0/2087
14	b	0.25	0/1541	0.48	0/2087
All	All	0.27	1/50211 (0.0%)	0.52	15/67890 (0.0%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
10	X	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	X	1	MET	CB-CG	-6.54	1.30	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Y	81	ARG	NE-CZ-NH1	-21.38	109.61	120.30
11	Y	81	ARG	NE-CZ-NH2	19.63	130.11	120.30
11	K	81	ARG	NE-CZ-NH2	-18.70	110.95	120.30
11	K	81	ARG	NE-CZ-NH1	17.26	128.93	120.30
10	X	1	MET	N-CA-C	-15.91	68.03	111.00
10	X	1	MET	CG-SD-CE	-14.77	76.57	100.20
10	J	1	MET	CG-SD-CE	-11.19	82.30	100.20
10	X	1	MET	N-CA-CB	-10.78	91.20	110.60
10	X	1	MET	CB-CA-C	9.25	128.90	110.40
11	K	81	ARG	CD-NE-CZ	8.74	135.84	123.60
11	Y	81	ARG	CD-NE-CZ	8.74	135.84	123.60
10	X	1	MET	CA-CB-CG	7.56	126.15	113.30
10	J	1	MET	N-CA-C	-6.33	93.92	111.00
10	J	1	MET	CA-CB-CG	-5.96	103.18	113.30
10	J	1	MET	CB-CA-C	5.78	121.96	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	X	1	MET	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	0	0
1	O	1915	0	1929	1	0
2	B	1904	0	1904	3	0
2	P	1904	0	1904	2	0
3	C	1881	0	1895	7	0
3	Q	1881	0	1895	5	0
4	D	1813	0	1797	0	0
4	R	1813	0	1797	0	0
5	E	1773	0	1775	2	0
5	S	1773	0	1775	2	0
6	F	1892	0	1883	1	0
6	T	1892	0	1883	1	0
7	G	1907	0	1901	2	0
7	U	1906	0	1901	3	0
8	H	1684	0	1685	4	0
8	V	1684	0	1685	5	0
9	I	1581	0	1574	6	0
9	W	1581	0	1574	6	0
10	J	1561	0	1569	13	0
10	X	1561	0	1567	12	0
11	K	1653	0	1601	9	0
11	Y	1653	0	1601	10	0
12	L	1757	0	1711	5	0
12	Z	1757	0	1711	3	0
13	M	1824	0	1832	6	0
13	a	1824	0	1832	0	0
14	N	1512	0	1478	4	0
14	b	1512	0	1478	0	0
15	G	1	0	0	0	0
15	I	2	0	0	0	0
15	K	1	0	0	0	0
15	L	1	0	0	0	0
15	N	1	0	0	0	0
15	Z	2	0	0	0	0
15	b	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	3	0
17	N	52	0	59	0	0
17	V	52	0	59	2	0
17	b	52	0	59	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	H	12	0	13	0	0
18	V	12	0	13	0	0
19	A	23	0	0	0	0
19	B	19	0	0	0	0
19	C	20	0	0	0	0
19	D	14	0	0	0	0
19	E	9	0	0	0	0
19	F	19	0	0	0	0
19	G	31	0	0	0	0
19	H	38	0	0	0	0
19	I	18	0	0	0	0
19	J	25	0	0	0	0
19	K	25	0	0	0	0
19	L	28	0	0	0	0
19	M	32	0	0	0	0
19	N	23	0	0	1	0
19	O	16	0	0	0	0
19	P	15	0	0	0	0
19	Q	14	0	0	0	0
19	R	16	0	0	0	0
19	S	10	0	0	0	0
19	T	11	0	0	0	0
19	U	20	0	0	0	0
19	V	26	0	0	0	0
19	W	12	0	0	0	0
19	X	21	0	0	0	0
19	Y	19	0	0	0	0
19	Z	30	0	0	0	0
19	a	40	0	0	0	0
19	b	26	0	0	0	0
All	All	50158	0	49328	96	0

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

All (96) 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)
10:J:25:ILE:O	10:X:139:TYR:OH	1.85	0.93
10:J:139:TYR:OH	10:X:25:ILE:O	1.89	0.90
10:J:1:MET:O	10:J:2:ASP:C	2.20	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:152:VAL:HA	14:N:175:MET:HE1	1.83	0.60
10:X:1:MET:O	10:X:2:ASP:O	2.21	0.59
14:N:35:THR:HG22	19:N:302:HOH:O	2.06	0.56
3:C:99:GLU:HG3	11:K:81:ARG:HE	1.70	0.56
10:X:67:TYR:CE1	10:X:75:LEU:HD13	2.42	0.55
11:K:128:CYS:HB2	11:K:137:TYR:CE2	2.41	0.55
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.42	0.54
11:Y:128:CYS:HB2	11:Y:137:TYR:CE2	2.43	0.53
3:C:201:VAL:O	3:C:202:GLN:CB	2.58	0.52
11:K:128:CYS:HB2	11:K:137:TYR:CZ	2.45	0.52
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.91	0.52
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.58	0.51
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.91	0.51
11:Y:128:CYS:HB2	11:Y:137:TYR:CZ	2.46	0.51
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.93	0.51
8:V:49:ALA:HA	17:V:301:3BV:H50	1.94	0.50
10:X:1:MET:O	10:X:2:ASP:C	2.49	0.50
12:L:4:PRO:O	13:M:104:ARG:NH1	2.42	0.49
8:V:168:GLY:O	17:V:301:3BV:H57	2.12	0.49
10:X:3:ILE:HD12	10:X:176:PHE:CG	2.47	0.49
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.93	0.49
10:J:3:ILE:HD12	10:J:176:PHE:CG	2.48	0.49
8:H:49:ALA:HA	17:H:301:3BV:H50	1.94	0.49
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.93	0.49
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.95	0.49
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.95	0.48
10:X:143:LEU:HD23	10:X:163:LEU:HD23	1.95	0.48
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.94	0.48
8:H:168:GLY:O	17:H:301:3BV:H57	2.13	0.48
7:G:23:PHE:O	7:G:26:THR:HB	2.14	0.48
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.96	0.47
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.96	0.47
10:J:143:LEU:HD23	10:J:163:LEU:HD23	1.96	0.47
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.96	0.47
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.96	0.47
10:J:1:MET:O	10:J:3:ILE:N	2.48	0.47
8:V:218:VAL:CG2	9:W:196:LYS:HB2	2.44	0.47
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.97	0.46
11:Y:107:LYS:HG3	11:Y:108:GLU:HG3	1.98	0.46
7:U:23:PHE:O	7:U:26:THR:HB	2.15	0.46
13:M:187:ARG:NH1	8:V:139:GLU:OE1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	1.98	0.46
10:J:2:ASP:OD1	10:J:34:LYS:CE	2.64	0.46
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.97	0.46
11:K:107:LYS:HG3	11:K:108:GLU:HG3	1.98	0.45
9:W:20:VAL:HG23	9:W:189:ILE:HB	1.98	0.45
10:J:2:ASP:OD1	10:J:34:LYS:HE2	2.17	0.45
6:T:172:LEU:CD1	6:T:195:ILE:HD13	2.46	0.45
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.97	0.45
9:I:20:VAL:HG23	9:I:189:ILE:HB	1.98	0.45
11:Y:0:GLY:HA3	11:Y:170:TYR:HB3	1.99	0.45
6:F:172:LEU:CD1	6:F:195:ILE:HD13	2.46	0.45
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.98	0.44
10:J:21:VAL:HG11	11:K:122:LEU:HD11	2.00	0.44
12:Z:147:MET:N	12:Z:148:PRO:HD2	2.33	0.44
10:X:58:GLU:CD	11:Y:81:ARG:HH12	2.22	0.43
14:N:176:VAL:HG12	14:N:178:LEU:HD13	2.01	0.43
12:L:147:MET:N	12:L:148:PRO:HD2	2.33	0.43
8:H:218:VAL:CG2	9:I:196:LYS:HB2	2.49	0.43
7:G:78:ILE:N	7:G:79:PRO:CD	2.83	0.42
11:K:209:ASN:O	9:W:38:LYS:NZ	2.53	0.42
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.55	0.42
12:L:8:ASN:HA	12:L:30:ILE:O	2.20	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.42
3:C:201:VAL:HG13	3:C:202:GLN:N	2.34	0.42
13:M:35:ARG:HH21	14:N:114:PRO:HG3	1.85	0.42
13:M:96:LEU:O	13:M:100:MET:HG2	2.20	0.42
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.55	0.42
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.85	0.41
17:H:301:3BV:H32	17:H:301:3BV:H29	1.96	0.41
10:J:1:MET:O	10:J:3:ILE:HG13	2.20	0.41
11:Y:12:ILE:HB	11:Y:180:VAL:HB	2.02	0.41
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.19	0.41
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.35	0.41
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.51	0.41
3:Q:161:THR:HG21	3:Q:169:VAL:HG13	2.03	0.41
13:M:27:LEU:HD21	13:M:34:LEU:HD22	2.02	0.41
2:P:50:LYS:O	2:P:51:VAL:C	2.59	0.41
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.86	0.41
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	2.03	0.41
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.50	0.41
3:C:161:THR:HG21	3:C:169:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:174:MET:HA	10:X:174:MET:HA	2.02	0.41
11:K:12:ILE:HB	11:K:180:VAL:HB	2.02	0.41
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.56	0.40
5:S:77:ALA:N	5:S:78:PRO:CD	2.84	0.40
2:B:50:LYS:O	2:B:51:VAL:C	2.60	0.40
11:K:25:TRP:HH2	12:L:147:MET:HB3	1.86	0.40
2:B:161:ALA:HB3	3:C:52:LEU:HD23	2.03	0.40
5:E:77:ALA:N	5:E:78:PRO:CD	2.85	0.40
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.04	0.40
9:I:14:MET:HB3	9:I:162:LEU:HD11	2.04	0.40
10:X:58:GLU:OE1	11:Y:81:ARG:NH1	2.55	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%)	241 (97%)	7 (3%)	0	100	100
1	O	248/250 (99%)	241 (97%)	7 (3%)	0	100	100
2	B	242/258 (94%)	234 (97%)	6 (2%)	2 (1%)	19	39
2	P	242/258 (94%)	234 (97%)	6 (2%)	2 (1%)	19	39
3	C	238/254 (94%)	230 (97%)	6 (2%)	2 (1%)	19	39
3	Q	238/254 (94%)	229 (96%)	7 (3%)	2 (1%)	19	39
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%)	224 (98%)	5 (2%)	0	100	100
5	S	229/234 (98%)	224 (98%)	5 (2%)	0	100	100
6	F	241/288 (84%)	236 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	T	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
7	G	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
7	U	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
8	H	220/232 (95%)	215 (98%)	5 (2%)	0	100	100
8	V	220/232 (95%)	215 (98%)	5 (2%)	0	100	100
9	I	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
9	W	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
10	J	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	29	52
10	X	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	29	52
11	K	212/214 (99%)	207 (98%)	5 (2%)	0	100	100
11	Y	212/214 (99%)	206 (97%)	6 (3%)	0	100	100
12	L	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
12	Z	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
13	M	231/246 (94%)	220 (95%)	10 (4%)	1 (0%)	34	57
13	a	231/246 (94%)	220 (95%)	10 (4%)	1 (0%)	34	57
14	N	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
14	b	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
All	All	6280/6618 (95%)	6112 (97%)	156 (2%)	12 (0%)	47	71

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN
2	P	51	VAL
3	Q	202	GLN
10	X	2	ASP
10	J	2	ASP
2	B	221	ASP
3	C	205	ALA
2	P	221	ASP
3	Q	205	ALA
13	M	83	ALA
13	a	83	ALA

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	85
1	O	209/209 (100%)	206 (99%)	3 (1%)	67	85
2	B	203/216 (94%)	197 (97%)	6 (3%)	41	67
2	P	203/216 (94%)	197 (97%)	6 (3%)	41	67
3	C	212/226 (94%)	206 (97%)	6 (3%)	43	69
3	Q	212/226 (94%)	206 (97%)	6 (3%)	43	69
4	D	194/215 (90%)	186 (96%)	8 (4%)	30	56
4	R	194/215 (90%)	186 (96%)	8 (4%)	30	56
5	E	190/193 (98%)	183 (96%)	7 (4%)	34	60
5	S	190/193 (98%)	183 (96%)	7 (4%)	34	60
6	F	201/239 (84%)	192 (96%)	9 (4%)	27	52
6	T	201/239 (84%)	192 (96%)	9 (4%)	27	52
7	G	206/210 (98%)	199 (97%)	7 (3%)	37	63
7	U	206/210 (98%)	199 (97%)	7 (3%)	37	63
8	H	181/190 (95%)	177 (98%)	4 (2%)	52	76
8	V	181/190 (95%)	177 (98%)	4 (2%)	52	76
9	I	172/173 (99%)	168 (98%)	4 (2%)	50	75
9	W	172/173 (99%)	168 (98%)	4 (2%)	50	75
10	J	173/175 (99%)	165 (95%)	8 (5%)	27	51
10	X	173/175 (99%)	166 (96%)	7 (4%)	31	57
11	K	168/168 (100%)	162 (96%)	6 (4%)	35	61
11	Y	168/168 (100%)	162 (96%)	6 (4%)	35	61
12	L	185/185 (100%)	178 (96%)	7 (4%)	33	59
12	Z	185/185 (100%)	178 (96%)	7 (4%)	33	59
13	M	199/208 (96%)	193 (97%)	6 (3%)	41	67
13	a	199/208 (96%)	193 (97%)	6 (3%)	41	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	162/162 (100%)	160 (99%)	2 (1%)	71	87
14	b	162/162 (100%)	160 (99%)	2 (1%)	71	87
All	All	5310/5538 (96%)	5145 (97%)	165 (3%)	40	66

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	61	LEU
1	A	157	PHE
2	B	50	LYS
2	B	58	GLN
2	B	114	LEU
2	B	184	LYS
2	B	186	ASP
2	B	191	LEU
3	C	4	ARG
3	C	38	ASN
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
4	D	99	ILE
4	D	125	LEU
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	224	ASP
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	29	LYS
5	E	54	GLU
5	E	71	LEU
5	E	184	ASN
5	E	188	LEU
5	E	202	ASP
6	F	14	ASP
6	F	117	GLN
6	F	123	ASN
6	F	172	LEU

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Mol	Chain	Res	Type
6	F	181	GLU
6	F	203	ASN
6	F	206	LYS
6	F	214	TRP
6	F	221	ASN
7	G	83	ASN
7	G	115	LEU
7	G	117	GLN
7	G	125	MET
7	G	166	GLN
7	G	181	LYS
7	G	235	ARG
8	H	30	ASN
8	H	68	LEU
8	H	127	LEU
8	H	196	ARG
9	I	4	SER
9	I	37	ASN
9	I	171	LEU
9	I	182	TRP
10	J	1	MET
10	J	23	ARG
10	J	78	GLN
10	J	136	SER
10	J	143	LEU
10	J	144	LEU
10	J	172	MET
10	J	174	MET
11	K	4	LEU
11	K	9	GLN
11	K	104	TYR
11	K	116	ASP
11	K	140	LEU
11	K	148	LEU
12	L	1	GLN
12	L	23	LEU
12	L	49	ASN
12	L	106	TYR
12	L	136	CYS
12	L	150	LEU
12	L	167	LYS
13	M	35	ARG

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Mol	Chain	Res	Type
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
14	N	22	THR
14	N	36	ARG
1	O	17	LYS
1	O	61	LEU
1	O	157	PHE
2	P	50	LYS
2	P	58	GLN
2	P	114	LEU
2	P	184	LYS
2	P	186	ASP
2	P	191	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
4	R	99	ILE
4	R	125	LEU
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	224	ASP
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	54	GLU
5	S	71	LEU
5	S	184	ASN
5	S	188	LEU
5	S	202	ASP
6	T	14	ASP
6	T	117	GLN
6	T	123	ASN
6	T	172	LEU
6	T	181	GLU

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Mol	Chain	Res	Type
6	T	203	ASN
6	T	206	LYS
6	T	214	TRP
6	T	221	ASN
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN
7	U	125	MET
7	U	166	GLN
7	U	181	LYS
7	U	235	ARG
8	V	30	ASN
8	V	68	LEU
8	V	127	LEU
8	V	196	ARG
9	W	4	SER
9	W	37	ASN
9	W	171	LEU
9	W	182	TRP
10	X	1	MET
10	X	23	ARG
10	X	78	GLN
10	X	136	SER
10	X	143	LEU
10	X	144	LEU
10	X	172	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	104	TYR
11	Y	116	ASP
11	Y	140	LEU
11	Y	148	LEU
12	Z	1	GLN
12	Z	23	LEU
12	Z	49	ASN
12	Z	106	TYR
12	Z	136	CYS
12	Z	150	LEU
12	Z	167	LYS
13	a	35	ARG
13	a	48	ASN
13	a	70	LEU

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Mol	Chain	Res	Type
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
14	b	22	THR
14	b	36	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
3	C	38	ASN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	91	HIS
4	D	210	GLN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	120	GLN
5	E	151	ASN
5	E	184	ASN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
7	G	83	ASN
7	G	117	GLN
7	G	121	GLN
8	H	86	HIS
9	I	203	GLN
10	J	55	GLN
10	J	146	HIS
11	K	85	ASN
11	K	176	ASN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN

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Mol	Chain	Res	Type
12	L	158	ASN
13	M	48	ASN
13	M	102	GLN
13	M	179	ASN
1	O	94	HIS
2	P	20	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
3	Q	38	ASN
3	Q	147	GLN
3	Q	160	GLN
4	R	91	HIS
4	R	100	ASN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	120	GLN
5	S	184	ASN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
7	U	83	ASN
7	U	117	GLN
7	U	121	GLN
8	V	86	HIS
10	X	55	GLN
10	X	146	HIS
10	X	147	HIS
11	Y	85	ASN
11	Y	176	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	158	ASN
13	a	48	ASN
13	a	102	GLN
13	a	179	ASN

5.3.3 RNA [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](#)

Of 19 ligands modelled in this entry, 13 are monoatomic - leaving 6 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
18	MES	V	302	-	12,12,12	2.22	1 (8%)	14,16,16	1.37	3 (21%)
17	3BV	H	301	8	54,54,54	1.09	3 (5%)	68,71,71	1.51	10 (14%)
17	3BV	V	301	8	54,54,54	1.06	3 (5%)	68,71,71	1.53	10 (14%)
17	3BV	N	201	14	54,54,54	1.25	3 (5%)	68,71,71	1.41	8 (11%)
17	3BV	b	201	14	54,54,54	1.23	3 (5%)	68,71,71	1.42	8 (11%)
18	MES	H	302	-	12,12,12	2.19	1 (8%)	14,16,16	1.39	2 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	MES	V	302	-	-	2/6/14/14	0/1/1/1
17	3BV	H	301	8	-	11/59/67/67	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	3BV	V	301	8	-	11/59/67/67	0/3/3/3
17	3BV	N	201	14	-	16/59/67/67	0/3/3/3
17	3BV	b	201	14	-	16/59/67/67	0/3/3/3
18	MES	H	302	-	-	5/6/14/14	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	V	302	MES	C8-S	-7.41	1.67	1.77
18	H	302	MES	C8-S	-7.28	1.67	1.77
17	N	201	3BV	C51-C47	6.08	1.64	1.53
17	b	201	3BV	C51-C47	5.69	1.63	1.53
17	H	301	3BV	C32-C33	-4.42	1.40	1.51
17	N	201	3BV	C32-C33	-4.37	1.40	1.51
17	b	201	3BV	C32-C33	-4.37	1.40	1.51
17	V	301	3BV	C32-C33	-4.24	1.41	1.51
17	H	301	3BV	C51-C47	3.84	1.60	1.53
17	V	301	3BV	C51-C47	3.70	1.60	1.53
17	b	201	3BV	C13-C14	-3.62	1.41	1.51
17	N	201	3BV	C13-C14	-3.60	1.41	1.51
17	H	301	3BV	C13-C14	-3.39	1.41	1.51
17	V	301	3BV	C13-C14	-3.34	1.42	1.51

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	V	301	3BV	C43-C42-N41	-5.88	102.57	110.18
17	H	301	3BV	C43-C42-N41	-5.74	102.76	110.18
17	b	201	3BV	C43-C42-N41	-5.64	102.89	110.18
17	N	201	3BV	C43-C42-N41	-5.49	103.08	110.18
17	N	201	3BV	C58-C51-C59	-4.89	103.45	109.88
17	b	201	3BV	C58-C51-C59	-4.76	103.62	109.88
17	V	301	3BV	C58-C51-C59	-4.31	104.21	109.88
17	H	301	3BV	C58-C51-C59	-4.12	104.47	109.88
17	H	301	3BV	O1-C6-C5	-3.79	103.46	111.80
17	V	301	3BV	O1-C6-C5	-3.74	103.56	111.80
18	H	302	MES	O2S-S-C8	3.41	111.03	106.92
17	H	301	3BV	C13-C12-C11	-3.38	106.55	113.21
17	V	301	3BV	C13-C12-C11	-3.36	106.59	113.21
17	H	301	3BV	C25-C24-C23	-3.26	106.47	115.43
17	V	301	3BV	C25-C24-C23	-3.18	106.68	115.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	N	201	3BV	O1-C2-C3	-3.08	105.01	111.80
17	V	301	3BV	C33-C32-C31	-2.97	105.19	113.39
17	H	301	3BV	C33-C32-C31	-2.96	105.22	113.39
17	N	201	3BV	O1-C6-C5	-2.95	105.29	111.80
17	b	201	3BV	O1-C2-C3	-2.94	105.31	111.80
17	V	301	3BV	O60-C59-C51	-2.93	105.33	111.33
17	b	201	3BV	O1-C6-C5	-2.86	105.50	111.80
18	V	302	MES	O1S-S-C8	2.80	110.29	106.92
17	H	301	3BV	O60-C59-C51	-2.78	105.65	111.33
17	b	201	3BV	C33-C32-C31	-2.63	106.14	113.39
17	N	201	3BV	C33-C32-C31	-2.55	106.35	113.39
18	V	302	MES	O3S-S-C8	2.52	109.84	105.77
18	V	302	MES	O2S-S-C8	2.41	109.82	106.92
17	V	301	3BV	C2-C3-N4	-2.35	106.55	110.10
17	b	201	3BV	C12-C13-C14	-2.34	105.05	113.18
17	b	201	3BV	O60-C59-C51	-2.32	106.59	111.33
17	N	201	3BV	C12-C13-C14	-2.29	105.20	113.18
17	N	201	3BV	O60-C59-C51	-2.26	106.72	111.33
18	H	302	MES	O1S-S-C8	2.25	109.63	106.92
17	H	301	3BV	O1-C2-C3	-2.21	106.92	111.80
17	N	201	3BV	C25-C24-C23	-2.21	109.36	115.43
17	b	201	3BV	C25-C24-C23	-2.20	109.38	115.43
17	H	301	3BV	C2-C3-N4	-2.20	106.77	110.10
17	V	301	3BV	O1-C2-C3	-2.15	107.06	111.80
17	H	301	3BV	C6-C5-N4	-2.15	106.85	110.10
17	V	301	3BV	C6-C5-N4	-2.13	106.87	110.10

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	H	301	3BV	C47-C42-C43-C44
17	H	301	3BV	O48-C47-C51-C58
17	H	301	3BV	C47-C51-C59-O60
17	N	201	3BV	N41-C42-C43-C44
17	N	201	3BV	C42-C47-C51-C58
17	N	201	3BV	C42-C47-C51-C59
17	N	201	3BV	O48-C47-C51-C58
17	V	301	3BV	C47-C42-C43-C44
17	V	301	3BV	O48-C47-C51-C58
17	V	301	3BV	C47-C51-C59-O60
17	b	201	3BV	N41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
17	b	201	3BV	C42-C47-C51-C58
17	b	201	3BV	C42-C47-C51-C59
17	b	201	3BV	O48-C47-C51-C58
18	H	302	MES	C7-C8-S-O1S
18	H	302	MES	C7-C8-S-O2S
18	H	302	MES	C7-C8-S-O3S
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
17	H	301	3BV	C42-C47-C51-C58
17	V	301	3BV	C42-C47-C51-C58
17	N	201	3BV	N4-C7-C8-N10
17	b	201	3BV	N4-C7-C8-N10
17	N	201	3BV	N4-C7-C8-O9
17	b	201	3BV	N4-C7-C8-O9
17	H	301	3BV	C42-C43-C44-C46
17	N	201	3BV	O48-C47-C51-C59
17	b	201	3BV	O48-C47-C51-C59
17	V	301	3BV	C42-C43-C44-C46
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
18	H	302	MES	C8-C7-N4-C5
18	V	302	MES	C8-C7-N4-C5
17	H	301	3BV	N41-C42-C43-C44
17	V	301	3BV	N41-C42-C43-C44
17	N	201	3BV	C42-C43-C44-C46
17	b	201	3BV	C42-C43-C44-C46
17	N	201	3BV	N10-C11-C12-C13
17	b	201	3BV	N10-C11-C12-C13
17	N	201	3BV	C47-C42-C43-C44
17	b	201	3BV	C47-C42-C43-C44
18	H	302	MES	C8-C7-N4-C3
18	V	302	MES	C8-C7-N4-C3
17	N	201	3BV	N10-C11-C20-O21
17	b	201	3BV	N10-C11-C20-O21
17	V	301	3BV	N30-C31-C39-O40
17	H	301	3BV	N30-C31-C39-O40
17	N	201	3BV	N10-C11-C20-N22
17	b	201	3BV	N10-C11-C20-N22

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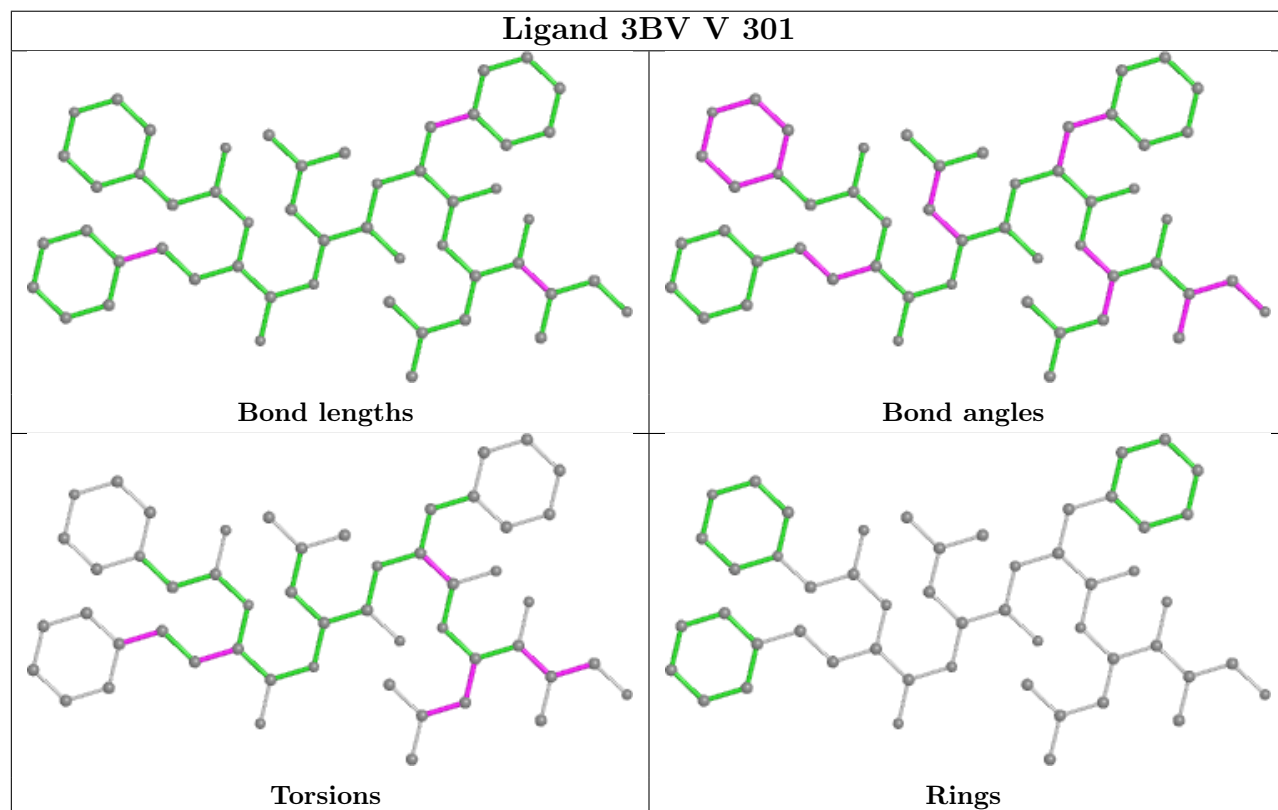
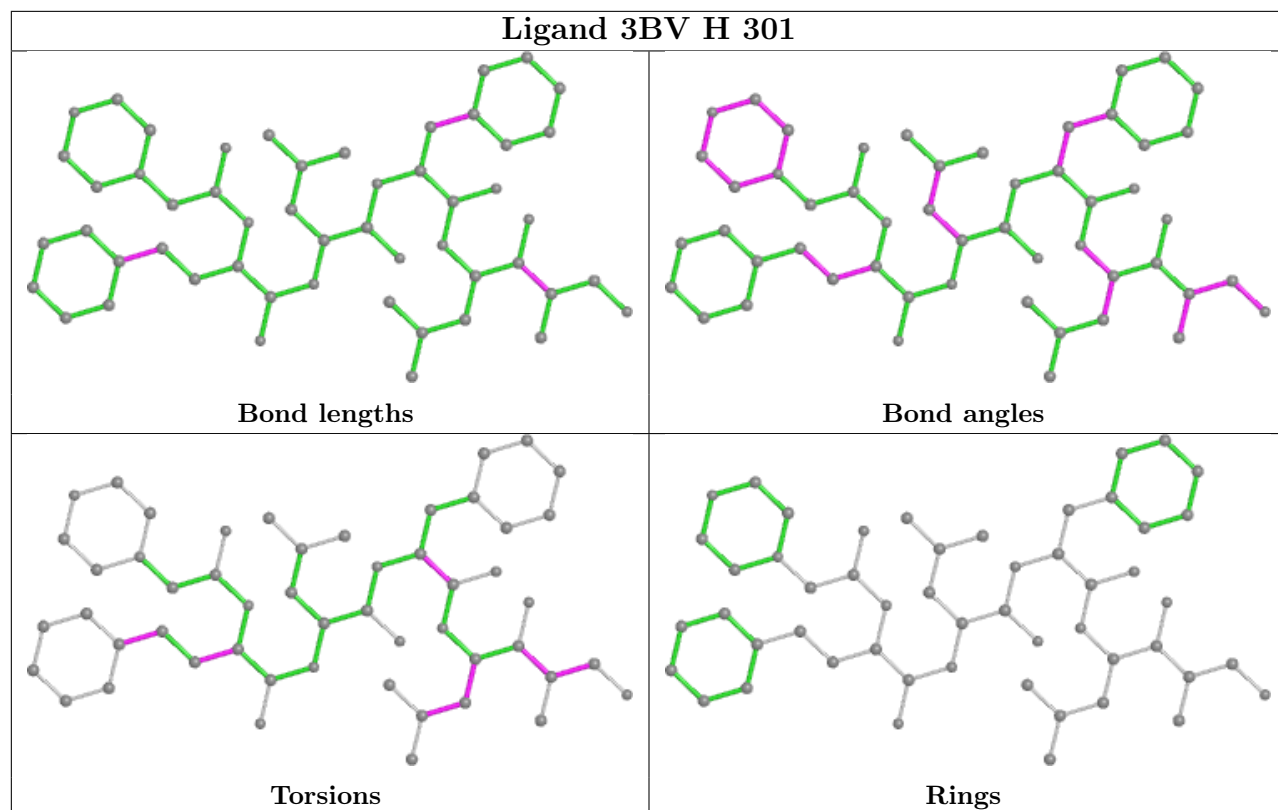
Mol	Chain	Res	Type	Atoms
17	N	201	3BV	C11-C12-C13-C14
17	b	201	3BV	C11-C12-C13-C14
17	H	301	3BV	C12-C13-C14-C15
17	V	301	3BV	C12-C13-C14-C15
17	N	201	3BV	N30-C31-C39-O40
17	b	201	3BV	N30-C31-C39-O40
17	H	301	3BV	C12-C13-C14-C19
17	V	301	3BV	C12-C13-C14-C19

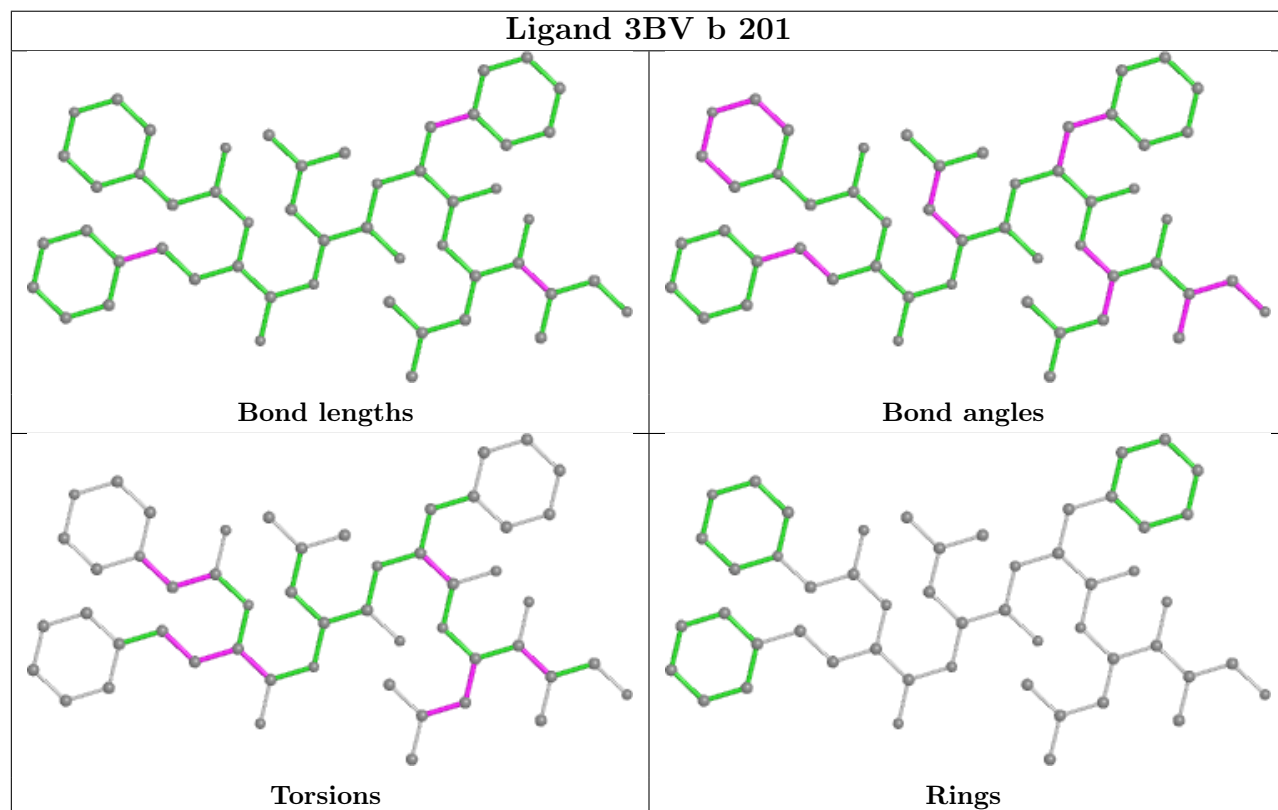
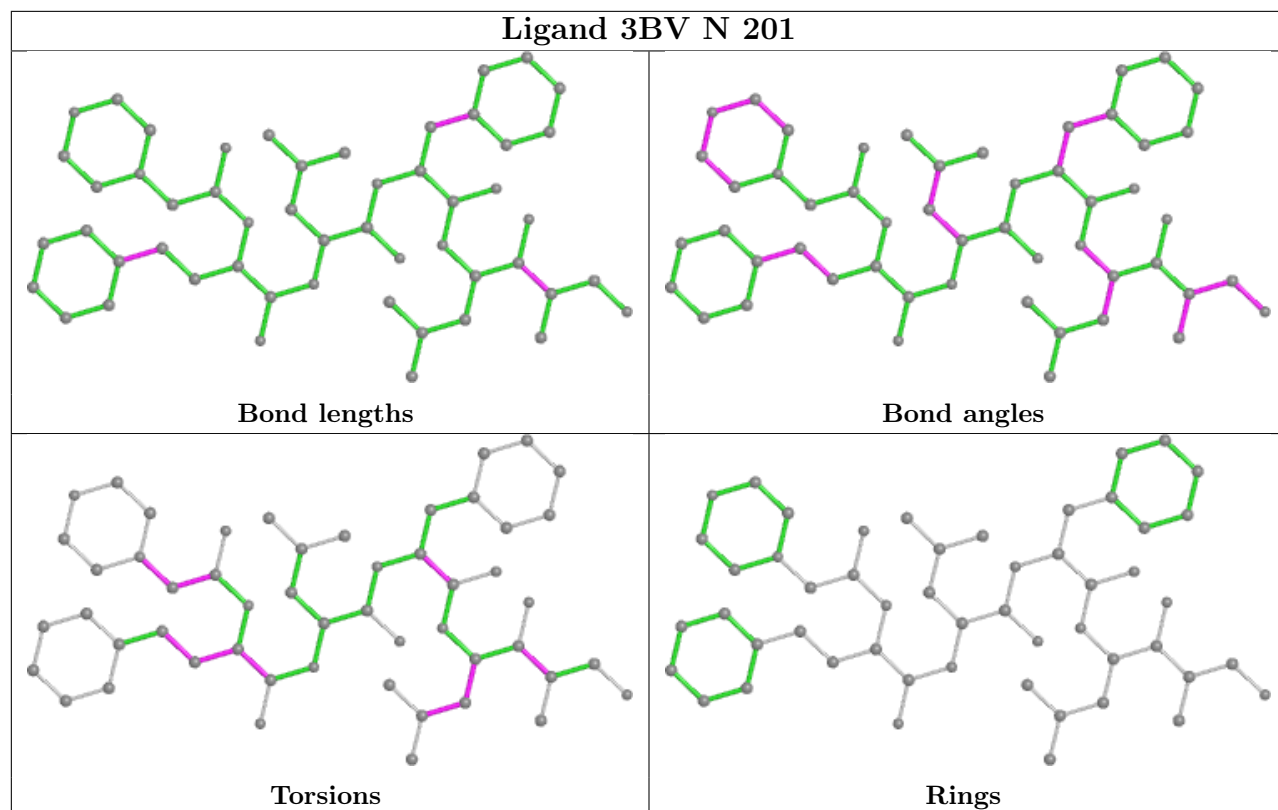
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	H	301	3BV	3	0
17	V	301	3BV	2	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/250 (100%)	-0.36	6 (2%) 59 53	36, 51, 88, 142	0
1	O	250/250 (100%)	-0.25	9 (3%) 42 35	42, 60, 106, 146	0
2	B	244/258 (94%)	-0.14	14 (5%) 23 18	39, 58, 106, 160	0
2	P	244/258 (94%)	-0.10	13 (5%) 26 20	43, 64, 109, 162	0
3	C	240/254 (94%)	0.01	17 (7%) 16 11	39, 64, 137, 174	0
3	Q	240/254 (94%)	0.13	18 (7%) 14 10	47, 73, 157, 188	0
4	D	235/260 (90%)	-0.32	3 (1%) 77 73	43, 65, 99, 145	0
4	R	235/260 (90%)	-0.19	5 (2%) 63 58	49, 68, 108, 151	0
5	E	231/234 (98%)	-0.15	5 (2%) 62 56	42, 65, 103, 143	0
5	S	231/234 (98%)	-0.07	8 (3%) 44 36	47, 74, 119, 156	0
6	F	243/288 (84%)	-0.34	7 (2%) 51 45	38, 59, 111, 136	0
6	T	243/288 (84%)	-0.23	7 (2%) 51 45	38, 69, 128, 169	0
7	G	241/252 (95%)	-0.40	8 (3%) 46 39	35, 52, 94, 142	0
7	U	241/252 (95%)	-0.37	5 (2%) 63 58	33, 57, 90, 137	0
8	H	222/232 (95%)	-0.52	3 (1%) 75 71	35, 48, 83, 118	0
8	V	222/232 (95%)	-0.45	3 (1%) 75 71	35, 52, 89, 131	0
9	I	204/205 (99%)	-0.70	1 (0%) 91 89	32, 47, 76, 98	0
9	W	204/205 (99%)	-0.60	3 (1%) 73 70	32, 51, 80, 109	0
10	J	195/198 (98%)	-0.38	3 (1%) 73 70	35, 54, 81, 119	0
10	X	195/198 (98%)	-0.39	3 (1%) 73 70	34, 56, 83, 136	0
11	K	214/214 (100%)	-0.46	2 (0%) 84 82	35, 52, 80, 102	1 (0%)
11	Y	214/214 (100%)	-0.45	2 (0%) 84 82	38, 53, 83, 106	1 (0%)
12	L	222/222 (100%)	-0.42	4 (1%) 68 64	33, 54, 103, 144	0
12	Z	222/222 (100%)	-0.38	4 (1%) 68 64	32, 54, 99, 130	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.62	2 (0%) 84 82	33, 50, 74, 84	0
13	a	233/246 (94%)	-0.59	1 (0%) 92 91	34, 49, 74, 82	0
14	N	196/196 (100%)	-0.61	1 (0%) 91 89	29, 46, 76, 102	0
14	b	196/196 (100%)	-0.63	0 100 100	35, 47, 80, 103	0
All	All	6340/6618 (95%)	-0.35	157 (2%) 57 51	29, 57, 105, 188	2 (0%)

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	206	LYS	8.9
1	A	1	MET	8.1
2	B	218	GLY	7.6
1	O	1	MET	7.3
2	P	218	GLY	7.0
3	Q	49	THR	6.5
3	Q	50	LEU	6.1
3	Q	206	LYS	6.0
5	S	202	ASP	5.9
10	X	194	ASP	5.8
2	B	220	ASN	5.5
9	W	1	SER	5.4
3	C	50	LEU	5.4
10	J	1	MET	5.3
2	P	219	ALA	5.3
3	C	49	THR	5.1
10	X	1	MET	5.1
2	P	59	ASP	5.1
2	B	51	VAL	4.9
2	P	51	VAL	4.8
2	B	219	ALA	4.7
5	E	202	ASP	4.6
3	Q	238	LYS	4.5
12	L	174	TYR	4.5
2	B	221	ASP	4.4
13	a	1	THR	4.4
3	C	238	LYS	4.3
3	Q	239	GLN	4.2
2	P	220	ASN	4.2
3	Q	205	ALA	4.1
5	S	233	ILE	4.0
4	R	241	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
12	Z	167	LYS	3.9
9	I	1	SER	3.9
2	P	221	ASP	3.8
3	C	202	GLN	3.8
10	J	194	ASP	3.7
8	V	221	CYS	3.7
2	B	59	ASP	3.7
3	Q	236	GLN	3.7
12	Z	174	TYR	3.6
3	C	239	GLN	3.6
3	Q	48	SER	3.6
2	B	242	GLY	3.6
7	U	242	GLN	3.6
6	T	243	ILE	3.6
11	K	-1	ALA	3.5
3	C	236	GLN	3.5
12	Z	172	LEU	3.5
2	P	203	SER	3.4
13	M	1	THR	3.3
2	P	222	GLY	3.3
5	E	201	ARG	3.2
4	R	242	GLU	3.2
6	F	244	ASN	3.2
2	P	182	ASP	3.2
4	D	242	GLU	3.2
11	Y	-1	ALA	3.2
12	L	172	LEU	3.1
8	V	222	ASP	3.1
6	T	2	THR	3.1
7	G	179	LYS	3.1
5	E	54	GLU	3.0
8	H	221	CYS	3.0
3	C	205	ALA	3.0
6	F	205	GLU	3.0
5	E	233	ILE	3.0
3	C	225	GLU	3.0
3	Q	240	GLU	3.0
1	O	201	GLU	3.0
4	R	125	LEU	3.0
14	N	195	GLN	3.0
10	X	193	ASP	3.0
2	P	52	THR	3.0

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Mol	Chain	Res	Type	RSRZ
13	M	47	ASP	2.9
1	A	249	ALA	2.9
5	S	180	LYS	2.8
3	C	47	ARG	2.8
6	F	2	THR	2.8
1	O	250	LEU	2.8
1	A	201	GLU	2.8
3	C	181	GLU	2.8
2	P	60	THR	2.8
1	A	250	LEU	2.8
11	K	212	GLY	2.8
7	U	222	ASP	2.8
2	B	235	LYS	2.8
9	W	133	LYS	2.8
11	Y	212	GLY	2.8
4	D	241	ALA	2.7
6	T	178	HIS	2.7
1	O	249	ALA	2.7
3	Q	51	LYS	2.7
7	G	181	LYS	2.7
1	A	2	THR	2.6
1	O	2	THR	2.6
2	B	60	THR	2.6
2	B	217	LYS	2.6
1	O	231	LYS	2.6
8	H	222	ASP	2.5
3	Q	202	GLN	2.5
3	Q	171	GLU	2.5
1	O	248	GLU	2.5
1	O	50	LYS	2.5
3	C	180	LYS	2.5
3	C	27	ARG	2.5
10	J	193	ASP	2.5
4	R	217	GLN	2.5
5	E	217	LYS	2.5
3	Q	225	GLU	2.4
2	P	50	LYS	2.4
7	G	240	ALA	2.4
6	F	181	GLU	2.4
1	O	52	SER	2.4
3	C	240	GLU	2.4
4	R	230	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
7	G	3	TYR	2.4
12	Z	165	ASN	2.4
3	C	175	LYS	2.4
2	B	240	LYS	2.3
2	P	225	TYR	2.3
12	L	165	ASN	2.3
7	U	241	GLU	2.3
9	W	192	ASP	2.3
7	G	242	GLN	2.3
4	D	47	THR	2.3
6	T	230	ASP	2.3
5	S	54	GLU	2.3
8	H	198	GLU	2.2
12	L	167	LYS	2.2
1	A	248	GLU	2.2
7	G	68	ARG	2.2
7	U	51	PRO	2.2
3	Q	201	VAL	2.2
2	B	244	THR	2.2
3	Q	141	ASP	2.2
6	F	201	GLU	2.2
6	T	205	GLU	2.2
7	U	3	TYR	2.2
5	S	225	ASP	2.2
2	B	203	SER	2.1
3	Q	60	SER	2.1
3	Q	223	SER	2.1
8	V	145	ASP	2.1
6	F	241	LYS	2.1
2	B	50	LYS	2.1
6	F	229	GLY	2.1
7	G	2	GLY	2.1
6	T	204	LYS	2.1
6	T	244	ASN	2.1
3	C	203	THR	2.1
3	Q	27	ARG	2.0
3	C	187	GLU	2.0
5	S	194	GLU	2.0
7	G	241	GLU	2.0
5	S	210	LEU	2.0
5	S	173	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

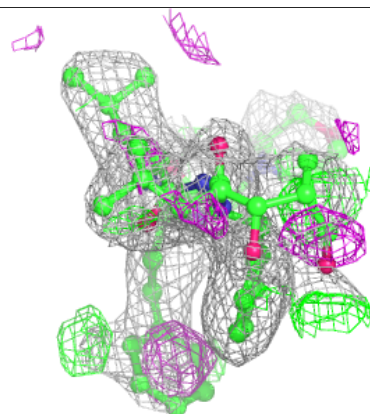
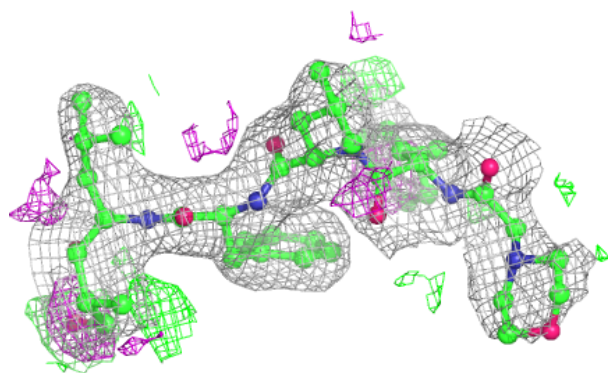
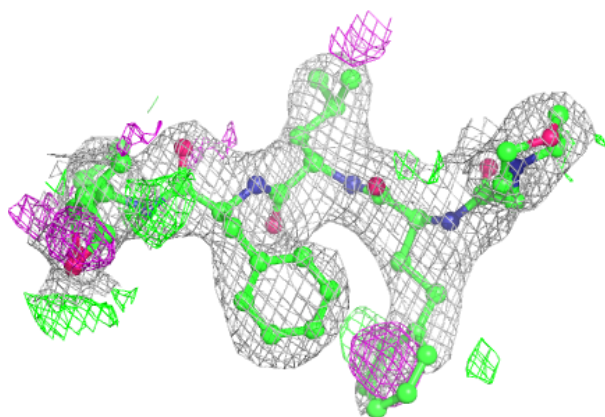
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
18	MES	V	302	12/12	0.86	0.35	73,75,88,99	0
17	3BV	b	201	52/52	0.87	0.22	38,51,129,132	0
17	3BV	N	201	52/52	0.87	0.23	35,50,129,133	0
17	3BV	V	301	52/52	0.89	0.20	43,52,102,106	0
17	3BV	H	301	52/52	0.90	0.19	40,50,98,102	0
18	MES	H	302	12/12	0.91	0.28	68,75,80,91	0
15	MG	G	301	1/1	0.93	0.07	52,52,52,52	0
15	MG	I	301	1/1	0.96	0.38	65,65,65,65	0
15	MG	Z	301	1/1	0.96	0.22	63,63,63,63	0
15	MG	I	302	1/1	0.97	0.07	65,65,65,65	0
15	MG	Z	302	1/1	0.97	0.14	41,41,41,41	0
16	CL	N	203	1/1	0.98	0.08	47,47,47,47	0
16	CL	b	203	1/1	0.98	0.04	50,50,50,50	0
15	MG	K	301	1/1	0.98	0.09	56,56,56,56	0
15	MG	N	202	1/1	0.98	0.14	54,54,54,54	0
15	MG	L	301	1/1	0.99	0.04	56,56,56,56	0
15	MG	b	202	1/1	0.99	0.07	42,42,42,42	0
16	CL	U	301	1/1	1.00	0.15	45,45,45,45	0
16	CL	G	302	1/1	1.00	0.07	44,44,44,44	0

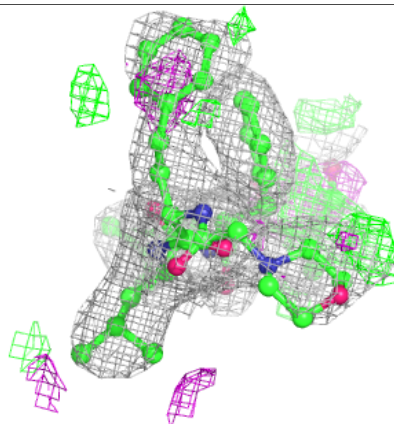
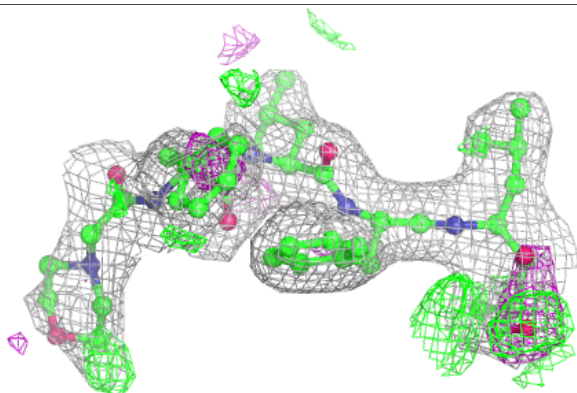
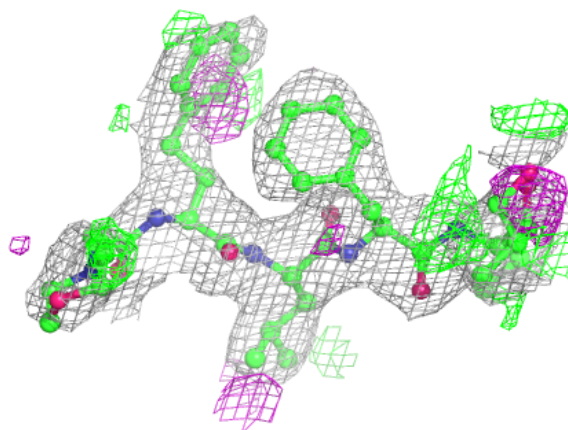
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 3BV 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)

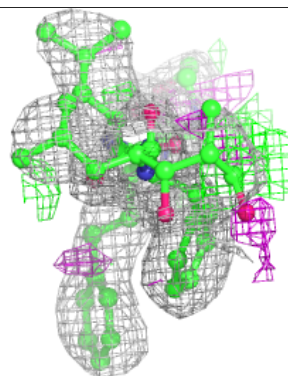
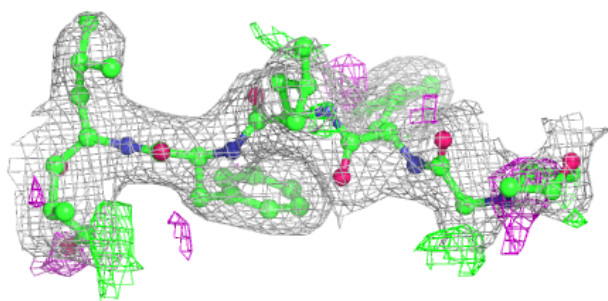
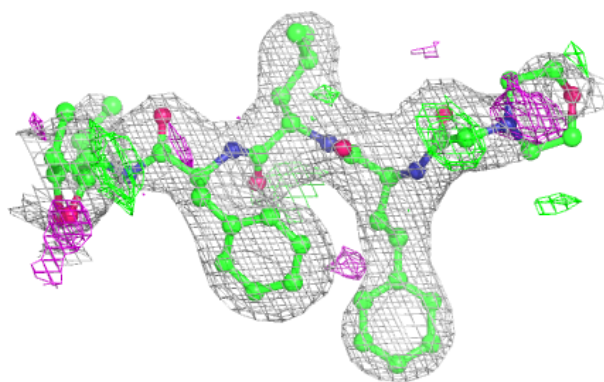
**Electron density around 3BV N 201:**

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

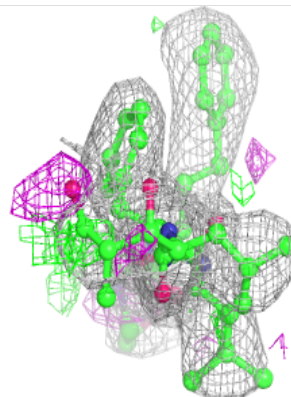
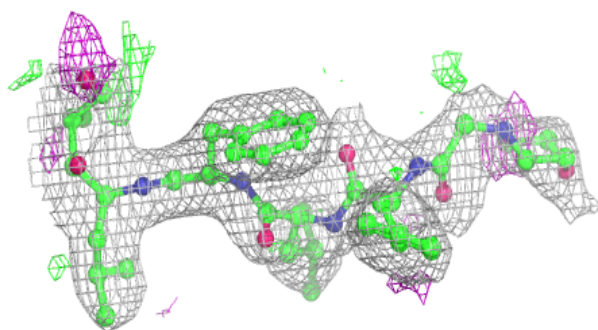
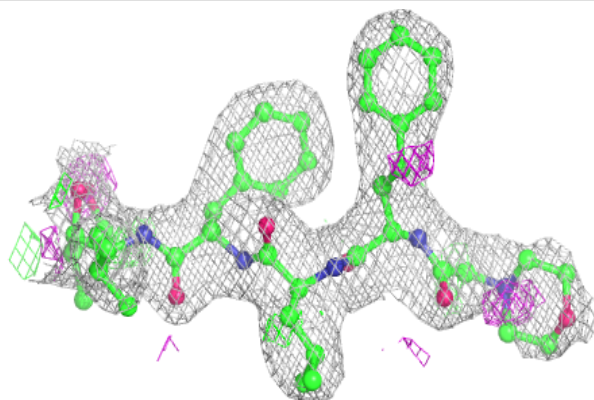


Electron density around 3BV V 301:

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

**Electron density around 3BV 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.