



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:29 AM UTC

PDB ID : 5DKJ / pdb_00005dkj
Title : Yeast 20S proteasome in complex with octreotide-PI
Authors : Beck, P.; Cui, H.; Groll, M.
Deposited on : 2015-09-03
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

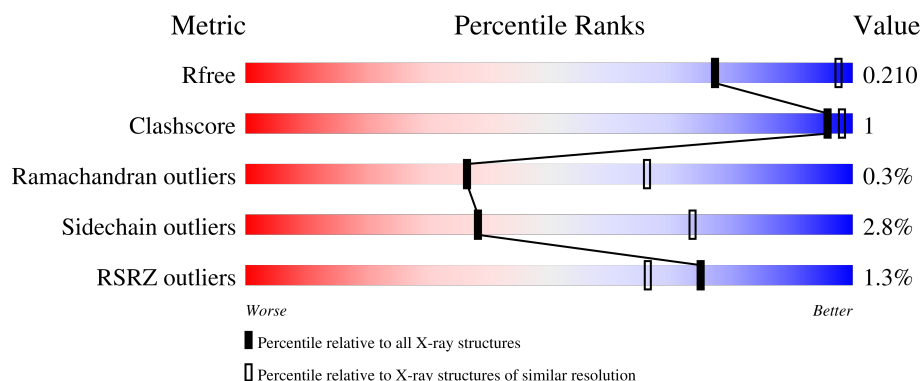
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

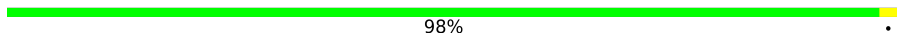
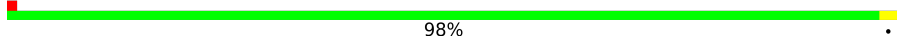
The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	 98% .
1	O	250	 98% .
2	B	258	 89% 5% 5%
2	P	258	 89% 5% 5%
3	C	254	 88% 5% . 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	 3% 88% 5% • 6%
4	D	260	 % 85% • • 10%
4	R	260	 % 85% 5% 10%
5	E	234	 % 96% • •
5	S	234	 % 96% • •
6	F	288	 % 83% • 16%
6	T	288	 2% 83% • 16%
7	G	252	 91% • • •
7	U	252	 90% 5% •
8	H	232	 93% • •
8	V	232	 92% 5% •
9	I	205	 94% 5%
9	W	205	 95% •
10	J	198	 2% 92% 5% • •
10	X	198	 2% 92% 5% • •
11	K	212	 3% 93% 7%
11	Y	212	 3% 92% 8%
12	L	222	 6% 95% •
12	Z	222	 6% 94% 5%
13	M	246	 % 89% 5% 5%
13	a	246	 89% 5% 5%
14	N	196	 95% • •
14	b	196	 95% • •

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 49867 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-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			

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

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

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

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

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

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

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	G	1	Total	Mg	0	0
			1	1		
15	I	1	Total	Mg	0	0
			1	1		

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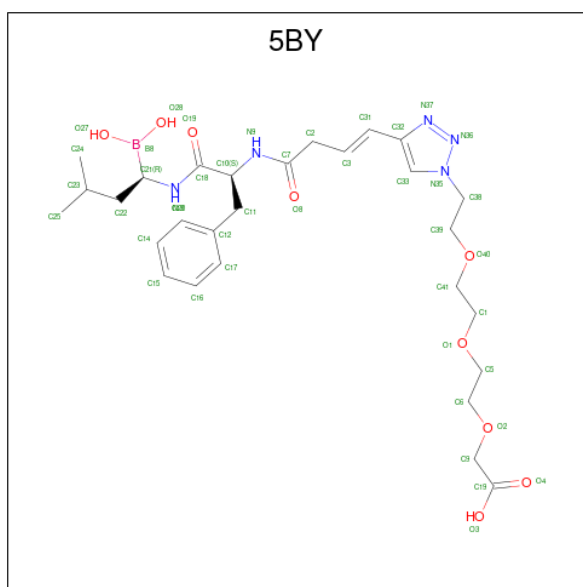
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	J	1	Total 1	Mg 1	0	0
15	K	1	Total 1	Mg 1	0	0
15	N	1	Total 1	Mg 1	0	0
15	V	1	Total 1	Mg 1	0	0
15	Y	1	Total 1	Mg 1	0	0
15	Z	1	Total 1	Mg 1	0	0

- Molecule 16 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 17 is {2-[2-(2-{4-[(1E)-4-{[(2S)-1-{[(1R)-1-(dihydroxyboranyl)-3-methylbutyl]amino}-1-oxo-3-phenylpropan-2-yl]amino}-4-oxobut-1-en-1-yl]-1H-1,2,3-triazol-1-yl}ethoxy)ethoxy]ethoxy}acetic acid (CCD ID: 5BY) (formula: C₂₈H₄₂BN₅O₉).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	H	1	Total	B	C	N	O	0	0
			34	1	23	5	5		
17	K	1	Total	B	C	N	O	0	0
			34	1	23	5	5		
17	N	1	Total	B	C	N	O	0	0
			34	1	23	5	5		
17	V	1	Total	B	C	N	O	0	0
			34	1	23	5	5		
17	Y	1	Total	B	C	N	O	0	0
			34	1	23	5	5		
17	b	1	Total	B	C	N	O	0	0
			34	1	23	5	5		

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	7	Total	O	0	0
			7	7		
18	B	14	Total	O	0	0
			14	14		
18	C	6	Total	O	0	0
			6	6		
18	D	6	Total	O	0	0
			6	6		
18	E	14	Total	O	0	0
			14	14		
18	F	8	Total	O	0	0
			8	8		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	G	10	Total O 10 10	0	0
18	H	10	Total O 10 10	0	0
18	I	14	Total O 14 14	0	0
18	J	8	Total O 8 8	0	0
18	K	10	Total O 10 10	0	0
18	L	14	Total O 14 14	0	0
18	M	17	Total O 17 17	0	0
18	N	7	Total O 7 7	0	0
18	O	5	Total O 5 5	0	0
18	P	8	Total O 8 8	0	0
18	Q	6	Total O 6 6	0	0
18	R	8	Total O 8 8	0	0
18	S	11	Total O 11 11	0	0
18	T	10	Total O 10 10	0	0
18	U	8	Total O 8 8	0	0
18	V	7	Total O 7 7	0	0
18	W	10	Total O 10 10	0	0
18	X	14	Total O 14 14	0	0
18	Y	13	Total O 13 13	0	0
18	Z	13	Total O 13 13	0	0
18	a	18	Total O 18 18	0	0

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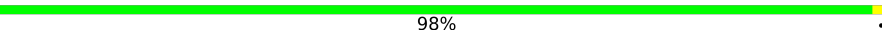
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	b	9	Total	O	0	0
			9	9		

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

Chain A:  98% .



- Molecule 1: Proteasome subunit alpha type-2

Chain O:  98% .



- Molecule 2: Proteasome subunit alpha type-3

Chain B:  89% 5% 5% .



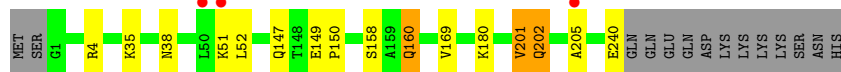
- Molecule 2: Proteasome subunit alpha type-3

Chain P:  89% 5% 5% .

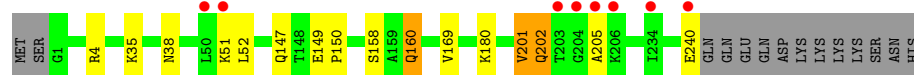
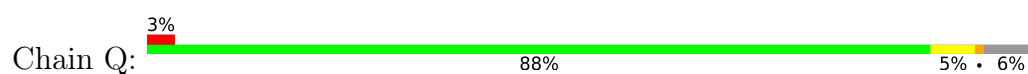


- Molecule 3: Proteasome subunit alpha type-4

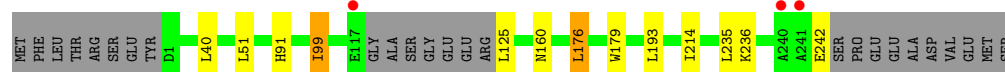
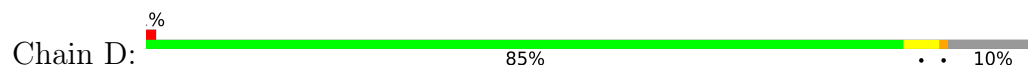
Chain C:  88% 5% 6% .



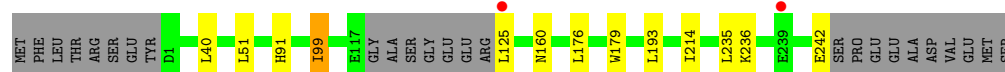
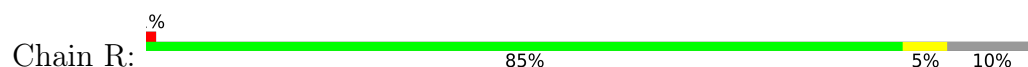
- Molecule 3: Proteasome subunit alpha type-4



- Molecule 4: Proteasome subunit alpha type-5



- Molecule 4: Proteasome subunit alpha type-5



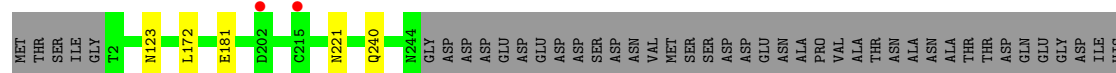
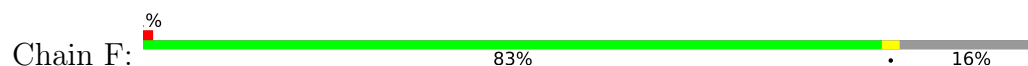
- Molecule 5: Proteasome subunit alpha type-6



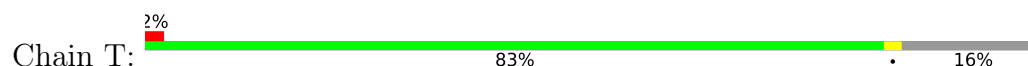
- Molecule 5: Proteasome subunit alpha type-6

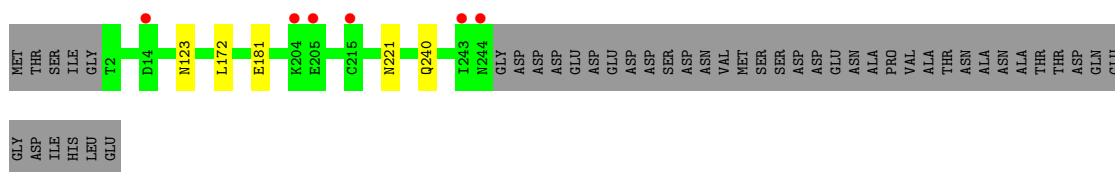


- Molecule 6: Probable proteasome subunit alpha type-7



- Molecule 6: Probable proteasome subunit alpha type-7





- Molecule 7: Proteasome subunit alpha type-1

Chain G: 91%



- Molecule 7: Proteasome subunit alpha type-1

Chain U: 90%



- Molecule 8: Proteasome subunit beta type-2

Chain H: 93%



- Molecule 8: Proteasome subunit beta type-2

Chain V: 92%



- Molecule 9: Proteasome subunit beta type-3

Chain I: 94%

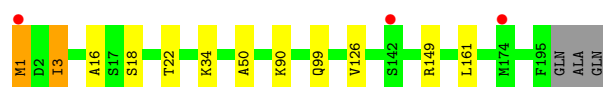
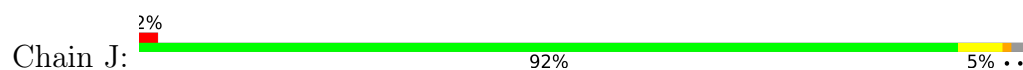


- Molecule 9: Proteasome subunit beta type-3

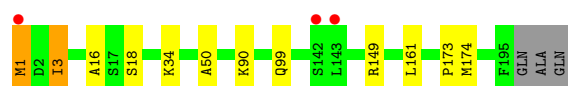
Chain W: 95%



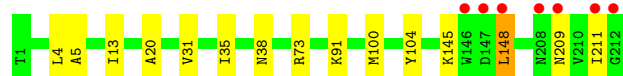
- Molecule 10: Proteasome subunit beta type-4



- Molecule 10: Proteasome subunit beta type-4



- Molecule 11: Proteasome subunit beta type-5



- Molecule 11: Proteasome subunit beta type-5



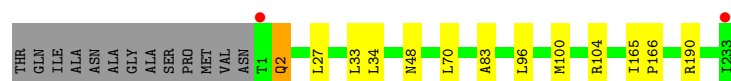
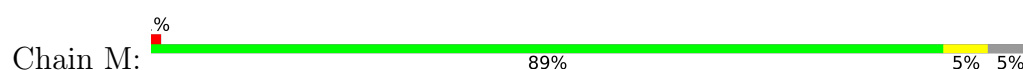
- Molecule 12: Proteasome subunit beta type-6



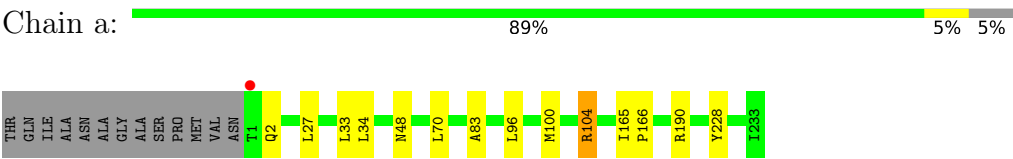
- Molecule 12: Proteasome subunit beta type-6



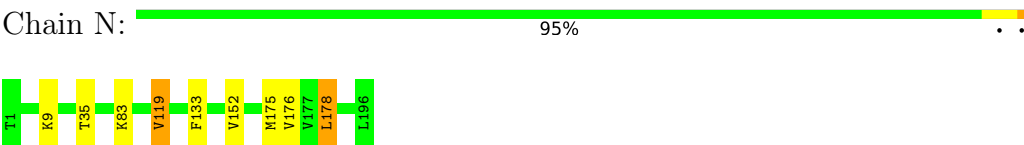
- Molecule 13: Proteasome subunit beta type-7



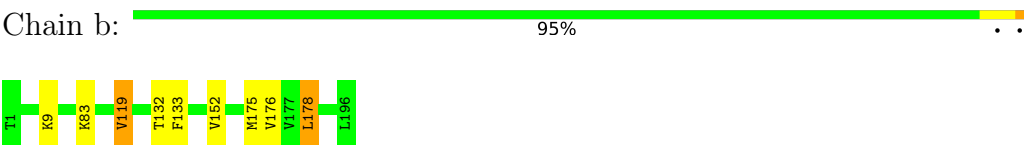
● Molecule 13: Proteasome subunit beta type-7



● Molecule 14: Proteasome subunit beta type-1



● Molecule 14: Proteasome subunit beta type-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.67Å 299.71Å 145.43Å 90.00° 113.16° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.0 (15.00-2.80) 97.4 (15.00-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.190 , 0.210 0.192 , 0.210	Depositor DCC
R_{free} test set	12808 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	59.3	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	49867	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CL, 5BY

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	0.39	0/1952	0.68	0/2642
1	O	0.39	0/1952	0.68	0/2642
2	B	0.40	0/1934	0.67	0/2618
2	P	0.39	0/1934	0.66	0/2618
3	C	0.39	0/1910	0.68	1/2586 (0.0%)
3	Q	0.39	0/1910	0.68	1/2586 (0.0%)
4	D	0.38	0/1837	0.65	0/2475
4	R	0.38	0/1837	0.66	0/2475
5	E	0.39	0/1800	0.65	0/2433
5	S	0.39	0/1800	0.65	0/2433
6	F	0.39	0/1932	0.67	0/2609
6	T	0.39	0/1932	0.68	0/2609
7	G	0.38	0/1945	0.67	0/2634
7	U	0.38	0/1945	0.67	0/2634
8	H	0.40	0/1750	0.70	0/2373
8	V	0.36	0/1750	0.67	0/2373
9	I	0.35	0/1611	0.69	0/2174
9	W	0.35	0/1611	0.69	0/2174
10	J	0.39	0/1589	0.67	0/2142
10	X	0.39	0/1589	0.67	0/2142
11	K	0.33	0/1681	0.67	0/2274
11	Y	0.34	0/1681	0.68	0/2274
12	L	0.38	0/1795	0.70	0/2420
12	Z	0.37	0/1795	0.70	0/2420
13	M	0.35	0/1855	0.69	0/2514
13	a	0.36	0/1855	0.69	0/2514
14	N	0.35	0/1541	0.68	0/2087
14	b	0.34	0/1541	0.68	0/2087
All	All	0.38	0/50264	0.68	2/67962 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	201	VAL	N-CA-C	6.28	116.44	110.42
3	C	201	VAL	N-CA-C	6.21	116.38	110.42

There are no chirality outliers.

There are no planarity outliers.

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	5	0
3	C	1881	0	1895	5	0
3	Q	1881	0	1895	5	0
4	D	1813	0	1797	3	0
4	R	1813	0	1797	2	0
5	E	1773	0	1775	2	0
5	S	1773	0	1775	1	0
6	F	1892	0	1883	0	0
6	T	1892	0	1883	0	0
7	G	1907	0	1901	4	0
7	U	1907	0	1901	4	0
8	H	1719	0	1718	8	0
8	V	1719	0	1718	8	0
9	I	1581	0	1574	7	0
9	W	1581	0	1574	5	0
10	J	1561	0	1569	6	0
10	X	1561	0	1569	6	0
11	K	1644	0	1594	7	0
11	Y	1644	0	1594	9	0
12	L	1757	0	1711	5	0
12	Z	1757	0	1711	7	0
13	M	1824	0	1832	5	0
13	a	1824	0	1832	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	N	1512	0	1480	6	0
14	b	1512	0	1480	5	0
15	G	1	0	0	0	0
15	I	1	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	V	1	0	0	0	0
15	Y	1	0	0	0	0
15	Z	1	0	0	0	0
16	G	1	0	0	0	0
16	N	1	0	0	0	0
16	U	1	0	0	0	0
16	b	1	0	0	0	0
17	H	34	0	31	1	0
17	K	34	0	31	0	0
17	N	34	0	31	0	0
17	V	34	0	31	1	0
17	Y	34	0	31	0	0
17	b	34	0	31	0	0
18	A	7	0	0	0	0
18	B	14	0	0	1	0
18	C	6	0	0	0	0
18	D	6	0	0	0	0
18	E	14	0	0	0	0
18	F	8	0	0	0	0
18	G	10	0	0	1	0
18	H	10	0	0	0	0
18	I	14	0	0	0	0
18	J	8	0	0	0	0
18	K	10	0	0	0	0
18	L	14	0	0	0	0
18	M	17	0	0	1	0
18	N	7	0	0	0	0
18	O	5	0	0	0	0
18	P	8	0	0	0	0
18	Q	6	0	0	0	0
18	R	8	0	0	0	0
18	S	11	0	0	0	0
18	T	10	0	0	0	0
18	U	8	0	0	0	0
18	V	7	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	W	10	0	0	0	0
18	X	14	0	0	1	0
18	Y	13	0	0	0	0
18	Z	13	0	0	0	0
18	a	18	0	0	0	0
18	b	9	0	0	0	0
All	All	49867	0	49310	108	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 (108) 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)
11:K:209:ASN:O	9:W:38:LYS:NZ	2.16	0.78
9:I:38:LYS:NZ	11:Y:209:ASN:O	2.17	0.78
11:K:73:ARG:NH2	11:K:104:TYR:O	2.30	0.64
11:Y:73:ARG:NH2	11:Y:104:TYR:O	2.31	0.62
17:V:302:5BY:C41	18:V:405:HOH:O	2.51	0.59
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.85	0.58
2:B:93:HIS:HB3	18:B:301:HOH:O	2.04	0.58
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.69	0.57
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.85	0.56
11:K:145:LYS:HB2	11:K:148:LEU:HD13	1.88	0.56
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	1.88	0.56
8:V:35:HIS:CB	8:V:56:THR:HG21	2.36	0.56
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.69	0.56
8:H:35:HIS:CB	8:H:56:THR:HG21	2.36	0.55
13:M:2:GLN:NE2	18:M:301:HOH:O	2.39	0.55
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.92	0.52
11:Y:1:THR:O	11:Y:130:GLY:HA3	2.09	0.52
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.92	0.51
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.58	0.51
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.92	0.51
3:C:201:VAL:O	3:C:202:GLN:CB	2.58	0.51
14:N:152:VAL:HA	14:N:175:MET:HE1	1.94	0.50
14:b:152:VAL:HA	14:b:175:MET:HE1	1.92	0.50
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.92	0.50
10:X:50:ALA:O	11:Y:91:LYS:NZ	2.44	0.50
2:B:50:LYS:O	2:B:51:VAL:C	2.56	0.49
7:G:23:PHE:O	7:G:26:THR:HB	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:50:LYS:O	2:P:51:VAL:C	2.55	0.49
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.94	0.48
7:U:23:PHE:O	7:U:26:THR:HB	2.13	0.48
8:H:196:ARG:NH2	9:I:150:GLU:O	2.47	0.48
10:J:50:ALA:O	11:K:91:LYS:NZ	2.47	0.47
10:J:1:MET:HG2	10:J:34:LYS:HE3	1.95	0.47
10:X:1:MET:HG2	10:X:34:LYS:HE3	1.95	0.47
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.97	0.46
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.98	0.45
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.98	0.45
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.96	0.45
13:M:96:LEU:O	13:M:100:MET:HG2	2.17	0.45
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.46	0.45
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.46	0.45
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.98	0.45
3:C:201:VAL:O	3:C:202:GLN:HB3	2.17	0.45
3:Q:201:VAL:O	3:Q:202:GLN:HB3	2.17	0.44
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.98	0.44
14:b:176:VAL:HG12	14:b:178:LEU:HD13	1.98	0.44
7:G:122:ARG:HD2	18:G:407:HOH:O	2.16	0.44
11:K:5:ALA:HA	11:K:13:ILE:O	2.18	0.44
13:a:96:LEU:O	13:a:100:MET:HG2	2.17	0.44
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.99	0.44
10:X:174:MET:HB2	18:X:209:HOH:O	2.18	0.44
13:a:27:LEU:HD21	13:a:34:LEU:HD22	2.00	0.44
8:H:196:ARG:NH2	9:I:150:GLU:HG3	2.33	0.44
12:Z:4:PRO:O	13:a:104:ARG:NH1	2.42	0.44
14:b:83:LYS:HG3	14:b:119:VAL:CG2	2.48	0.44
3:C:35:LYS:HG2	3:C:158:SER:O	2.17	0.43
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.48	0.43
11:Y:5:ALA:HA	11:Y:13:ILE:O	2.18	0.43
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.54	0.43
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.54	0.43
11:Y:38:ASN:OD1	11:Y:38:ASN:C	2.62	0.43
7:G:78:ILE:N	7:G:79:PRO:CD	2.82	0.43
14:N:133:PHE:HA	14:b:132:THR:O	2.19	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.42
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.19	0.42
10:J:3:ILE:HG23	10:J:18:SER:HB3	2.02	0.42
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.55	0.42
2:P:50:LYS:HD3	2:P:50:LYS:HA	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.49	0.42
13:M:27:LEU:HD21	13:M:34:LEU:HD22	2.01	0.42
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.49	0.42
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.50	0.42
8:H:49:ALA:HA	17:H:301:5BY:H8	2.02	0.42
8:V:196:ARG:NH2	9:W:150:GLU:O	2.53	0.42
11:K:38:ASN:OD1	11:K:38:ASN:C	2.62	0.42
12:Z:17:GLY:HA3	12:Z:20:PHE:CE1	2.55	0.42
12:L:17:GLY:HA3	12:L:20:PHE:CE1	2.55	0.42
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.50	0.42
10:X:3:ILE:HG23	10:X:18:SER:HB3	2.02	0.42
14:N:133:PHE:CE1	13:a:33:LEU:HD13	2.55	0.41
2:P:217:LYS:C	2:P:219:ALA:H	2.28	0.41
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.85	0.41
5:S:77:ALA:N	5:S:78:PRO:CD	2.84	0.41
10:J:22:THR:HG21	10:X:173:PRO:HB3	2.03	0.41
5:E:77:ALA:N	5:E:78:PRO:CD	2.84	0.41
12:Z:13:LEU:HD11	12:Z:150:LEU:HD21	2.02	0.41
8:H:84:LYS:HE2	8:H:119:THR:HG23	2.02	0.41
13:M:33:LEU:HD13	14:b:133:PHE:CE1	2.56	0.41
14:N:35:THR:HG21	13:a:228:TYR:HE2	1.85	0.41
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.85	0.41
8:V:84:LYS:HE2	8:V:119:THR:HG23	2.03	0.41
9:I:203:GLN:HG3	11:Y:197:PHE:CE2	2.56	0.41
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.55	0.41
13:a:165:ILE:HB	13:a:166:PRO:HD3	2.02	0.41
12:L:13:LEU:HD11	12:L:150:LEU:HD21	2.02	0.41
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.03	0.41
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.03	0.41
4:D:91:HIS:CD2	4:D:99:ILE:HG22	2.56	0.41
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.56	0.41
8:V:113:ILE:HG12	8:V:119:THR:HG22	2.03	0.41
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.20	0.41
8:H:113:ILE:HG12	8:H:119:THR:HG22	2.03	0.41
8:V:196:ARG:NH2	9:W:150:GLU:HG3	2.36	0.41
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.03	0.40
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.04	0.40
8:V:80:LEU:HD12	8:V:113:ILE:HD11	2.03	0.40
4:R:91:HIS:CD2	4:R:99:ILE:HG22	2.56	0.40
4:D:176:LEU:HD22	5:E:55:LEU:CD2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	239 (96%)	8 (3%)	1 (0%)	30	60
1	O	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	30	60
2	B	242/258 (94%)	233 (96%)	5 (2%)	4 (2%)	7	25
2	P	242/258 (94%)	232 (96%)	6 (2%)	4 (2%)	7	25
3	C	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	16	44
3	Q	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	16	44
4	D	231/260 (89%)	229 (99%)	2 (1%)	0	100	100
4	R	231/260 (89%)	229 (99%)	2 (1%)	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%)	237 (99%)	2 (1%)	0	100	100
7	U	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
8	H	224/232 (97%)	220 (98%)	4 (2%)	0	100	100
8	V	224/232 (97%)	219 (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%)	190 (98%)	3 (2%)	0	100	100
10	X	193/198 (98%)	190 (98%)	3 (2%)	0	100	100
11	K	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
11	Y	210/212 (99%)	205 (98%)	5 (2%)	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%)	221 (96%)	9 (4%)	1 (0%)	30	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	231/246 (94%)	221 (96%)	9 (4%)	1 (0%)	30	60
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	6284/6614 (95%)	6136 (98%)	132 (2%)	16 (0%)	36	66

All (16) 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
1	A	2	THR
2	B	218	GLY
2	B	222	GLY
1	O	2	THR
2	P	218	GLY
2	P	222	GLY
2	B	220	ASN
2	P	220	ASN
3	C	205	ALA
13	M	83	ALA
3	Q	205	ALA
13	a	83	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	205 (98%)	4 (2%)	50	81
1	O	209/209 (100%)	205 (98%)	4 (2%)	50	81
2	B	203/216 (94%)	197 (97%)	6 (3%)	36	72
2	P	203/216 (94%)	197 (97%)	6 (3%)	36	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	212/226 (94%)	203 (96%)	9 (4%)	26	61
3	Q	212/226 (94%)	203 (96%)	9 (4%)	26	61
4	D	194/215 (90%)	184 (95%)	10 (5%)	21	53
4	R	194/215 (90%)	184 (95%)	10 (5%)	21	53
5	E	190/193 (98%)	185 (97%)	5 (3%)	40	75
5	S	190/193 (98%)	185 (97%)	5 (3%)	40	75
6	F	201/239 (84%)	196 (98%)	5 (2%)	42	76
6	T	201/239 (84%)	196 (98%)	5 (2%)	42	76
7	G	206/210 (98%)	199 (97%)	7 (3%)	32	68
7	U	206/210 (98%)	199 (97%)	7 (3%)	32	68
8	H	185/190 (97%)	182 (98%)	3 (2%)	55	83
8	V	185/190 (97%)	181 (98%)	4 (2%)	45	78
9	I	172/173 (99%)	169 (98%)	3 (2%)	53	83
9	W	172/173 (99%)	169 (98%)	3 (2%)	53	83
10	J	173/175 (99%)	168 (97%)	5 (3%)	37	73
10	X	173/175 (99%)	168 (97%)	5 (3%)	37	73
11	K	169/169 (100%)	164 (97%)	5 (3%)	36	72
11	Y	169/169 (100%)	164 (97%)	5 (3%)	36	72
12	L	185/185 (100%)	182 (98%)	3 (2%)	55	83
12	Z	185/185 (100%)	182 (98%)	3 (2%)	55	83
13	M	199/208 (96%)	194 (98%)	5 (2%)	42	76
13	a	199/208 (96%)	194 (98%)	5 (2%)	42	76
14	N	162/162 (100%)	159 (98%)	3 (2%)	50	81
14	b	162/162 (100%)	159 (98%)	3 (2%)	50	81
All	All	5320/5540 (96%)	5173 (97%)	147 (3%)	38	73

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
2	B	55	LEU

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Mol	Chain	Res	Type
2	B	79	LEU
2	B	102	ASN
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	52	LEU
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	240	GLU
4	D	40	LEU
4	D	51	LEU
4	D	99	ILE
4	D	125	LEU
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	55	LEU
5	E	71	LEU
5	E	188	LEU
6	F	123	ASN
6	F	172	LEU
6	F	181	GLU
6	F	221	ASN
6	F	240	GLN
7	G	26	THR
7	G	75	ASN
7	G	115	LEU
7	G	122	ARG
7	G	125	MET
7	G	235	ARG
7	G	236	LEU
8	H	68	LEU

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Mol	Chain	Res	Type
8	H	144	GLN
8	H	196	ARG
9	I	37	ASN
9	I	126	ILE
9	I	171	LEU
10	J	1	MET
10	J	3	ILE
10	J	90	LYS
10	J	99	GLN
10	J	149	ARG
11	K	4	LEU
11	K	35	ILE
11	K	100	MET
11	K	148	LEU
11	K	211	ILE
12	L	23	LEU
12	L	49	ASN
12	L	150	LEU
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	190	ARG
14	N	9	LYS
14	N	119	VAL
14	N	178	LEU
1	O	1	MET
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	55	LEU
2	P	79	LEU
2	P	102	ASN
2	P	113	ARG
2	P	191	LEU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	51	LYS
3	Q	52	LEU
3	Q	147	GLN
3	Q	160	GLN

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Mol	Chain	Res	Type
3	Q	169	VAL
3	Q	180	LYS
3	Q	240	GLU
4	R	40	LEU
4	R	51	LEU
4	R	99	ILE
4	R	125	LEU
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	55	LEU
5	S	71	LEU
5	S	188	LEU
6	T	123	ASN
6	T	172	LEU
6	T	181	GLU
6	T	221	ASN
6	T	240	GLN
7	U	26	THR
7	U	75	ASN
7	U	115	LEU
7	U	122	ARG
7	U	125	MET
7	U	235	ARG
7	U	236	LEU
8	V	22	GLN
8	V	68	LEU
8	V	144	GLN
8	V	196	ARG
9	W	37	ASN
9	W	126	ILE
9	W	171	LEU
10	X	1	MET
10	X	3	ILE
10	X	90	LYS
10	X	99	GLN
10	X	149	ARG

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Mol	Chain	Res	Type
11	Y	4	LEU
11	Y	35	ILE
11	Y	100	MET
11	Y	148	LEU
11	Y	211	ILE
12	Z	23	LEU
12	Z	49	ASN
12	Z	150	LEU
13	a	2	GLN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	190	ARG
14	b	9	LYS
14	b	119	VAL
14	b	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (124) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	124	HIS
2	B	220	ASN
2	B	232	GLN
3	C	17	GLN
3	C	115	GLN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
4	D	91	HIS
4	D	225	ASN
5	E	68	HIS
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	58	GLN
6	F	86	ASN

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Mol	Chain	Res	Type
6	F	123	ASN
6	F	143	HIS
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	175	ASN
7	G	212	ASN
8	H	30	ASN
8	H	114	HIS
8	H	165	ASN
8	H	189	ASN
9	I	37	ASN
9	I	63	ASN
9	I	203	GLN
10	J	55	GLN
10	J	63	ASN
10	J	78	GLN
10	J	146	HIS
10	J	147	HIS
11	K	9	GLN
11	K	85	ASN
11	K	143	ASN
11	K	176	ASN
11	K	208	ASN
12	L	3	ASN
12	L	29	ASN
12	L	36	ASN
12	L	49	ASN
12	L	79	HIS
12	L	158	ASN
12	L	159	GLN
12	L	197	GLN
13	M	48	ASN
13	M	102	GLN
13	M	108	ASN
13	M	149	HIS
13	M	194	ASN
13	M	213	GLN
14	N	38	HIS
14	N	141	ASN
14	N	161	GLN
2	P	124	HIS

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Mol	Chain	Res	Type
2	P	220	ASN
2	P	232	GLN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
4	R	225	ASN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	120	GLN
5	S	151	ASN
5	S	184	ASN
6	T	19	GLN
6	T	58	GLN
6	T	86	ASN
6	T	123	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	172	ASN
8	V	30	ASN
8	V	189	ASN
9	W	37	ASN
9	W	63	ASN
9	W	172	ASN
9	W	203	GLN
10	X	55	GLN
10	X	63	ASN
10	X	78	GLN
10	X	146	HIS
10	X	147	HIS
11	Y	9	GLN
11	Y	85	ASN
11	Y	143	ASN
11	Y	176	ASN
11	Y	208	ASN
12	Z	3	ASN

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Mol	Chain	Res	Type
12	Z	29	ASN
12	Z	36	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	79	HIS
12	Z	80	ASN
12	Z	158	ASN
12	Z	159	GLN
12	Z	197	GLN
13	a	48	ASN
13	a	62	HIS
13	a	102	GLN
13	a	149	HIS
13	a	194	ASN
13	a	213	GLN
14	b	38	HIS
14	b	141	ASN
14	b	161	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 12 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	$\# Z > 2$
17	5BY	V	302	-	31,35,44	1.50	4 (12%)	38,45,55	3.39	9 (23%)
17	5BY	Y	302	-	31,35,44	1.55	5 (16%)	38,45,55	3.18	8 (21%)
17	5BY	b	201	-	31,35,44	1.47	6 (19%)	38,45,55	3.07	7 (18%)
17	5BY	H	301	-	31,35,44	1.59	5 (16%)	38,45,55	3.18	8 (21%)
17	5BY	K	301	-	31,35,44	1.46	2 (6%)	38,45,55	2.98	7 (18%)
17	5BY	N	201	-	31,35,44	1.40	5 (16%)	38,45,55	2.70	8 (21%)

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	5BY	V	302	-	-	5/29/34/43	0/2/2/2
17	5BY	Y	302	-	-	8/29/34/43	0/2/2/2
17	5BY	b	201	-	-	5/29/34/43	0/2/2/2
17	5BY	H	301	-	-	4/29/34/43	0/2/2/2
17	5BY	K	301	-	-	3/29/34/43	0/2/2/2
17	5BY	N	201	-	-	10/29/34/43	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	301	5BY	N37-N36	6.01	1.41	1.32
17	V	302	5BY	N37-N36	5.04	1.40	1.32
17	H	301	5BY	N37-N36	4.97	1.40	1.32
17	Y	302	5BY	N37-N36	4.74	1.39	1.32
17	b	201	5BY	N37-N36	4.38	1.39	1.32
17	K	301	5BY	N35-N36	4.29	1.41	1.34
17	N	201	5BY	N37-N36	4.04	1.38	1.32
17	H	301	5BY	N35-N36	3.58	1.40	1.34
17	V	302	5BY	N35-N36	3.53	1.40	1.34
17	b	201	5BY	N35-N36	3.18	1.39	1.34
17	Y	302	5BY	N35-N36	3.10	1.39	1.34
17	N	201	5BY	C32-N37	-3.09	1.34	1.37
17	Y	302	5BY	C32-N37	-3.06	1.34	1.37
17	V	302	5BY	C32-N37	-3.04	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	201	5BY	C32-N37	-2.58	1.34	1.37
17	H	301	5BY	C32-N37	-2.48	1.34	1.37
17	N	201	5BY	O19-C18	-2.46	1.18	1.23
17	H	301	5BY	O19-C18	-2.40	1.18	1.23
17	b	201	5BY	O19-C18	-2.34	1.18	1.23
17	N	201	5BY	O8-C7	-2.30	1.18	1.23
17	N	201	5BY	N35-N36	2.30	1.38	1.34
17	H	301	5BY	O8-C7	-2.30	1.18	1.23
17	b	201	5BY	C2-C7	-2.20	1.48	1.51
17	Y	302	5BY	O19-C18	-2.20	1.19	1.23
17	Y	302	5BY	O8-C7	-2.15	1.19	1.23
17	V	302	5BY	O19-C18	-2.06	1.19	1.23
17	b	201	5BY	O8-C7	-2.01	1.19	1.23

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	V	302	5BY	C33-C32-N37	14.30	115.83	107.88
17	Y	302	5BY	C33-C32-N37	13.27	115.26	107.88
17	H	301	5BY	C33-C32-N37	12.80	115.00	107.88
17	K	301	5BY	C33-C32-N37	12.54	114.86	107.88
17	V	302	5BY	C32-N37-N36	-12.52	103.31	109.25
17	b	201	5BY	C33-C32-N37	12.44	114.80	107.88
17	H	301	5BY	C32-N37-N36	-11.62	103.73	109.25
17	K	301	5BY	C32-N37-N36	-11.49	103.80	109.25
17	Y	302	5BY	C32-N37-N36	-11.41	103.83	109.25
17	b	201	5BY	C32-N37-N36	-11.11	103.98	109.25
17	N	201	5BY	C33-C32-N37	11.05	114.03	107.88
17	N	201	5BY	C32-N37-N36	-8.88	105.03	109.25
17	Y	302	5BY	C32-C33-N35	-4.38	102.36	106.70
17	V	302	5BY	C32-C33-N35	-4.29	102.45	106.70
17	N	201	5BY	C32-C33-N35	-4.02	102.72	106.70
17	b	201	5BY	C12-C11-C10	-3.98	102.76	113.36
17	Y	302	5BY	B8-C21-C22	-3.91	104.92	112.31
17	H	301	5BY	B8-C21-C22	-3.91	104.92	112.31
17	N	201	5BY	C38-N35-N36	-3.80	113.16	120.78
17	H	301	5BY	C32-C33-N35	-3.67	103.06	106.70
17	b	201	5BY	C33-C32-C31	-3.55	120.10	129.56
17	H	301	5BY	C12-C11-C10	-3.50	104.04	113.36
17	V	302	5BY	C33-C32-C31	-3.40	120.50	129.56
17	b	201	5BY	C32-C33-N35	-3.40	103.34	106.70
17	H	301	5BY	C33-C32-C31	-3.29	120.80	129.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	K	301	5BY	C32-C33-N35	-3.21	103.52	106.70
17	K	301	5BY	B8-C21-C22	-3.17	106.32	112.31
17	Y	302	5BY	C11-C10-N9	-3.02	104.58	110.83
17	N	201	5BY	C38-N35-C33	2.87	134.19	128.83
17	b	201	5BY	B8-C21-C22	-2.73	107.16	112.31
17	V	302	5BY	B8-C21-C22	-2.72	107.18	112.31
17	Y	302	5BY	C33-C32-C31	-2.68	122.43	129.56
17	b	201	5BY	C39-C38-N35	-2.62	106.16	111.61
17	V	302	5BY	C3-C2-C7	-2.53	106.37	112.40
17	N	201	5BY	B8-C21-C22	-2.49	107.62	112.31
17	Y	302	5BY	C38-N35-N36	-2.44	115.88	120.78
17	H	301	5BY	C3-C2-C7	-2.42	106.64	112.40
17	H	301	5BY	C21-C22-C23	-2.41	112.24	115.32
17	V	302	5BY	C21-C22-C23	-2.41	112.25	115.32
17	K	301	5BY	C38-N35-N36	-2.37	116.01	120.78
17	V	302	5BY	C38-N35-N36	-2.34	116.09	120.78
17	Y	302	5BY	C21-C22-C23	-2.30	112.38	115.32
17	K	301	5BY	C33-C32-C31	-2.29	123.48	129.56
17	N	201	5BY	C33-C32-C31	-2.24	123.60	129.56
17	K	301	5BY	C38-N35-C33	2.08	132.71	128.83
17	N	201	5BY	C2-C7-N9	2.06	119.63	115.92
17	V	302	5BY	C12-C11-C10	-2.02	107.97	113.36

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	K	301	5BY	N35-C38-C39-O40
17	N	201	5BY	C3-C31-C32-C33
17	N	201	5BY	C3-C31-C32-N37
17	V	302	5BY	N35-C38-C39-O40
17	Y	302	5BY	N35-C38-C39-O40
17	b	201	5BY	C3-C31-C32-C33
17	b	201	5BY	C3-C31-C32-N37
17	Y	302	5BY	C38-C39-O40-C41
17	Y	302	5BY	N20-C21-C22-C23
17	b	201	5BY	C2-C7-N9-C10
17	b	201	5BY	C38-C39-O40-C41
17	H	301	5BY	C38-C39-O40-C41
17	N	201	5BY	N20-C21-C22-C23
17	N	201	5BY	C38-C39-O40-C41
17	V	302	5BY	C38-C39-O40-C41

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Mol	Chain	Res	Type	Atoms
17	b	201	5BY	O8-C7-N9-C10
17	V	302	5BY	C3-C31-C32-N37
17	Y	302	5BY	C3-C31-C32-N37
17	V	302	5BY	C3-C31-C32-C33
17	Y	302	5BY	C3-C31-C32-C33
17	K	301	5BY	C39-C38-N35-C33
17	N	201	5BY	C39-C38-N35-C33
17	K	301	5BY	C39-C38-N35-N36
17	N	201	5BY	C39-C38-N35-N36
17	Y	302	5BY	C39-C38-N35-N36
17	Y	302	5BY	C39-C38-N35-C33
17	N	201	5BY	O8-C7-N9-C10
17	H	301	5BY	C21-C22-C23-C25
17	N	201	5BY	C21-C22-C23-C25
17	H	301	5BY	C7-C2-C3-C31
17	N	201	5BY	C7-C2-C3-C31
17	V	302	5BY	C7-C2-C3-C31
17	Y	302	5BY	C7-C2-C3-C31
17	H	301	5BY	N20-C21-C22-C23
17	N	201	5BY	C2-C7-N9-C10

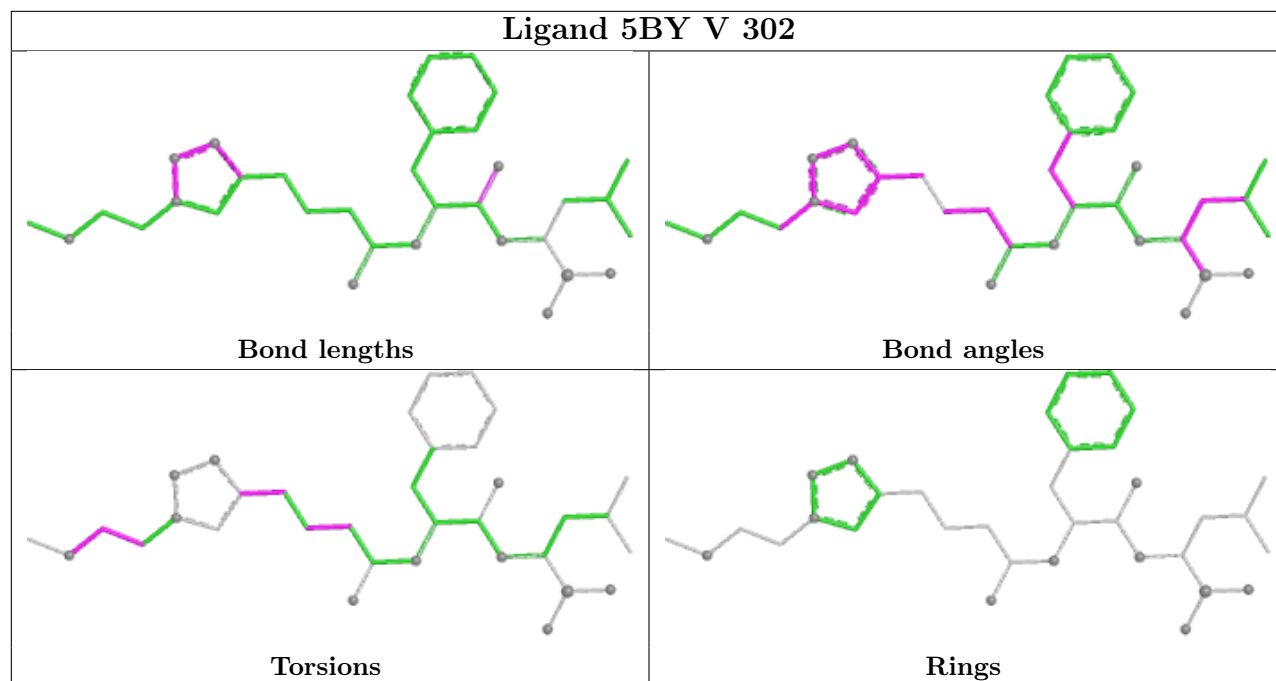
There are no ring outliers.

2 monomers are involved in 2 short contacts:

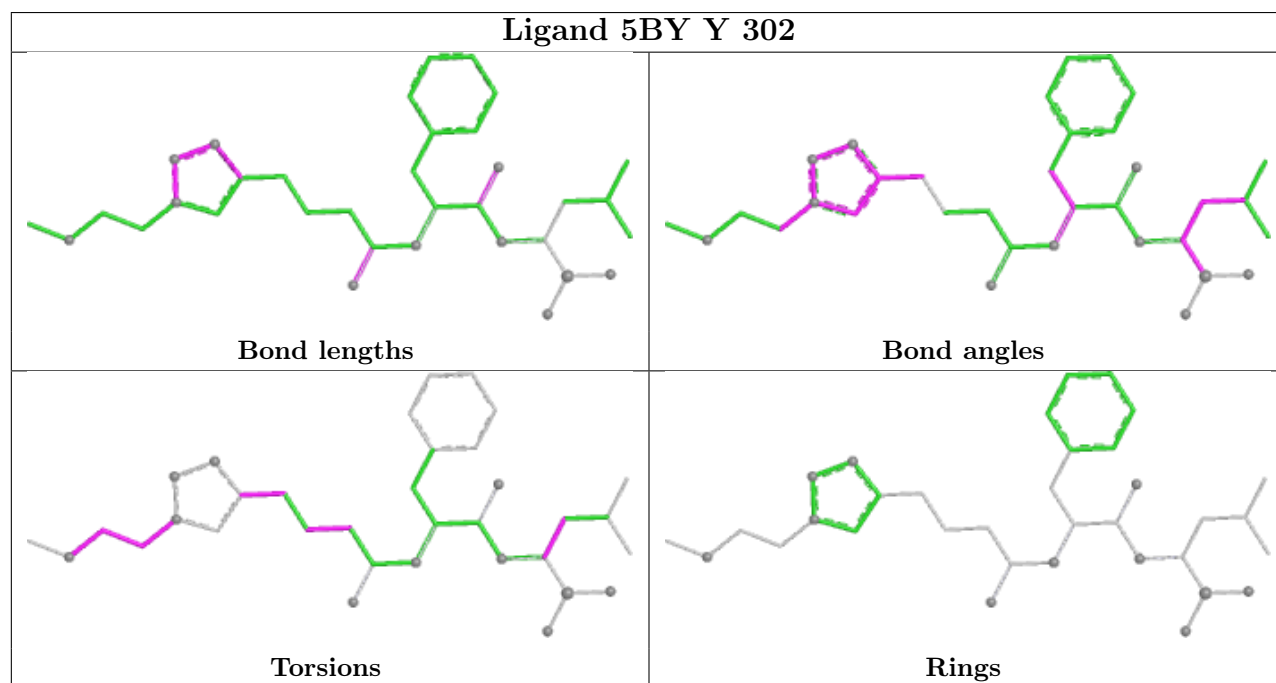
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	V	302	5BY	1	0
17	H	301	5BY	1	0

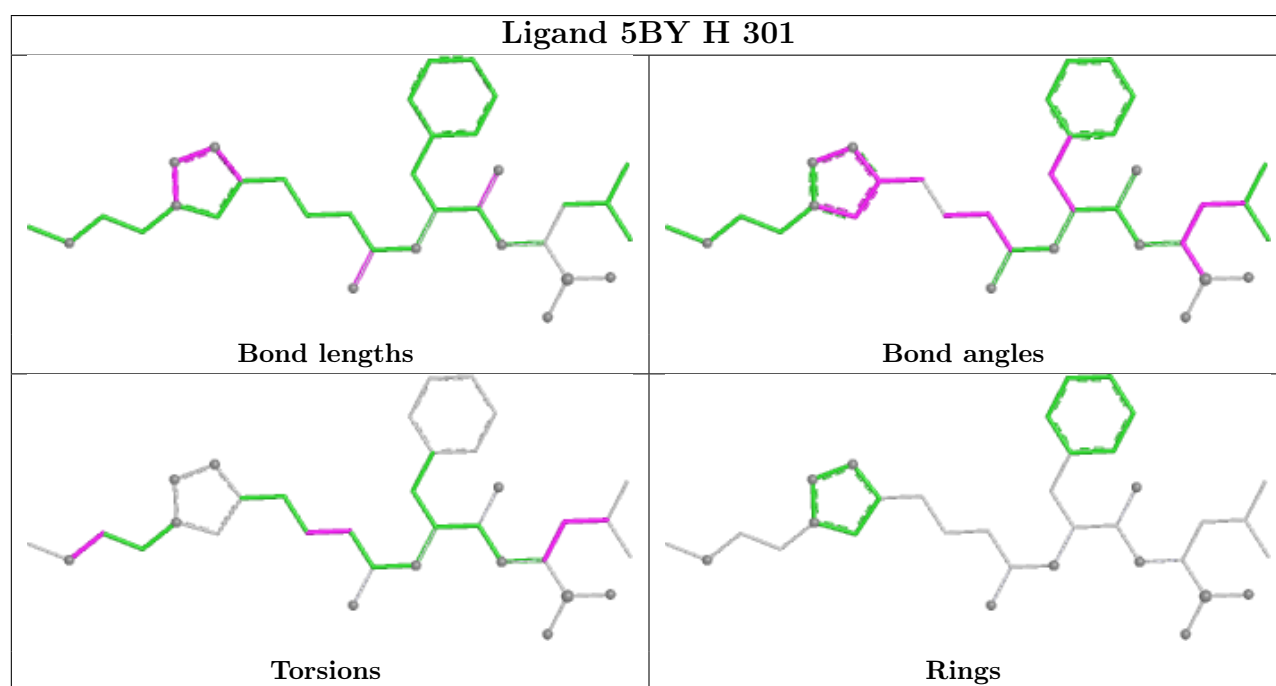
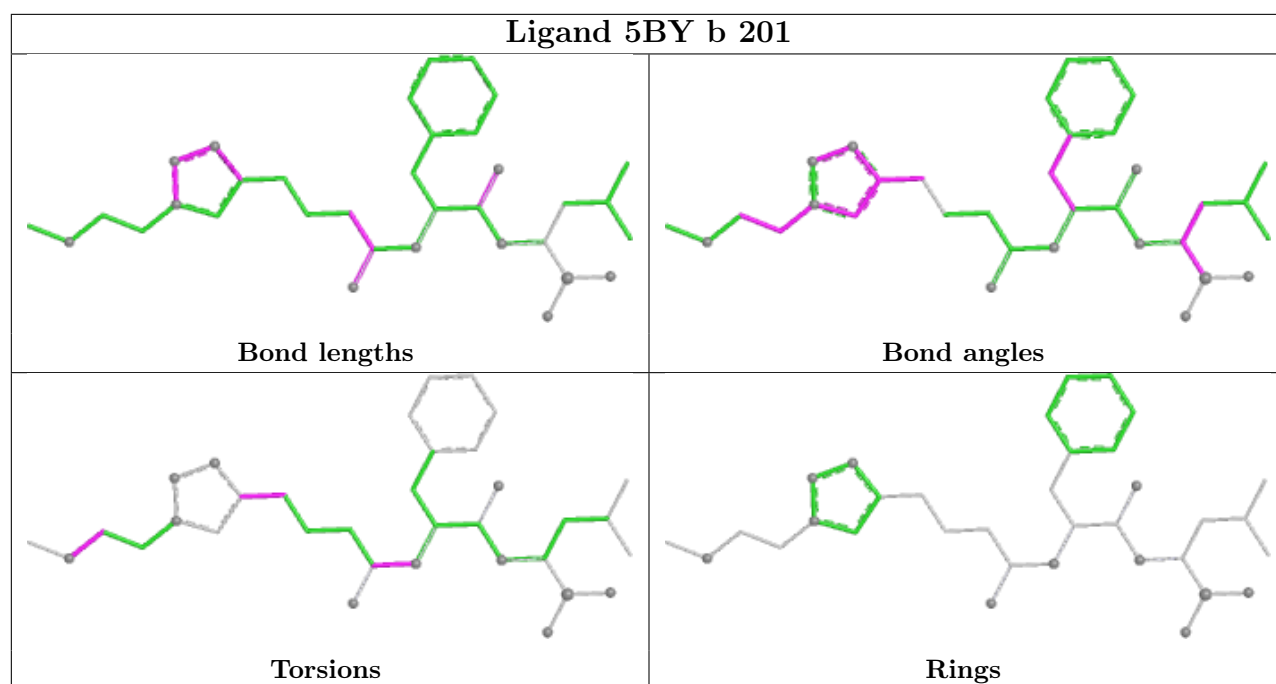
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

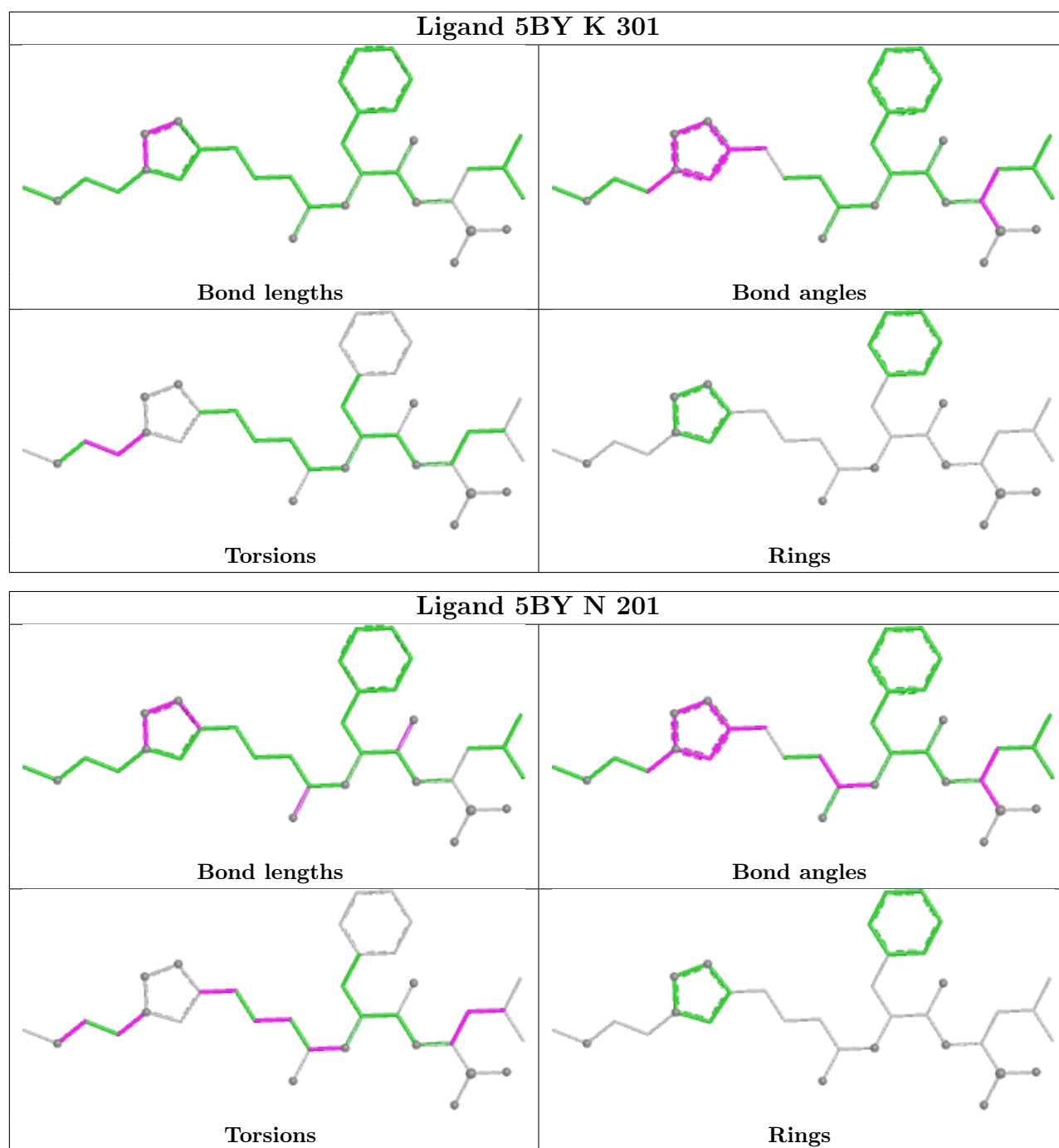
Ligand 5BY V 302



Ligand 5BY Y 302







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 ⓘ

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, 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%)	-0.38	0 100 100	36, 54, 93, 132	0
1	O	250/250 (100%)	-0.34	2 (0%) 82 75	42, 63, 109, 142	0
2	B	244/258 (94%)	-0.18	2 (0%) 82 75	41, 62, 107, 162	0
2	P	244/258 (94%)	-0.17	5 (2%) 65 56	45, 66, 109, 160	0
3	C	240/254 (94%)	-0.21	3 (1%) 75 66	40, 65, 130, 162	0
3	Q	240/254 (94%)	0.04	8 (3%) 49 39	48, 78, 162, 184	0
4	D	235/260 (90%)	-0.23	3 (1%) 75 66	46, 68, 103, 149	0
4	R	235/260 (90%)	-0.07	2 (0%) 81 74	55, 74, 115, 142	0
5	E	231/234 (98%)	-0.17	0 100 100	48, 69, 106, 146	0
5	S	231/234 (98%)	-0.06	2 (0%) 81 74	51, 72, 113, 149	0
6	F	243/288 (84%)	-0.28	2 (0%) 82 75	42, 63, 108, 138	0
6	T	243/288 (84%)	-0.15	6 (2%) 58 48	41, 68, 125, 157	0
7	G	241/252 (95%)	-0.33	0 100 100	40, 59, 98, 156	0
7	U	241/252 (95%)	-0.31	0 100 100	42, 58, 94, 136	0
8	H	226/232 (97%)	-0.32	1 (0%) 88 84	40, 54, 95, 166	0
8	V	226/232 (97%)	-0.39	1 (0%) 88 84	43, 56, 99, 182	0
9	I	204/205 (99%)	-0.47	0 100 100	36, 52, 83, 111	0
9	W	204/205 (99%)	-0.54	0 100 100	37, 55, 82, 112	0
10	J	195/198 (98%)	-0.29	3 (1%) 72 63	39, 56, 86, 124	0
10	X	195/198 (98%)	-0.32	3 (1%) 72 63	40, 58, 86, 133	0
11	K	212/212 (100%)	-0.14	7 (3%) 49 39	40, 57, 92, 110	0
11	Y	212/212 (100%)	-0.06	6 (2%) 55 45	41, 57, 97, 115	0
12	L	222/222 (100%)	-0.10	13 (5%) 28 21	39, 59, 111, 149	0
12	Z	222/222 (100%)	-0.15	13 (5%) 28 21	36, 56, 107, 141	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.44	2 (0%) 81 74	37, 56, 83, 104	0
13	a	233/246 (94%)	-0.51	1 (0%) 88 84	37, 54, 77, 95	0
14	N	196/196 (100%)	-0.49	0 100 100	37, 51, 82, 106	0
14	b	196/196 (100%)	-0.52	0 100 100	37, 52, 83, 112	0
All	All	6344/6614 (95%)	-0.27	85 (1%) 75 66	36, 61, 107, 184	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	L	174	TYR	6.8
10	X	1	MET	6.1
10	J	1	MET	6.1
12	Z	174	TYR	6.0
3	Q	50	LEU	5.7
12	L	165	ASN	5.7
11	Y	208	ASN	4.3
8	H	223	ILE	4.2
11	Y	211	ILE	4.2
12	Z	168	VAL	4.1
12	Z	169	LYS	4.0
12	Z	165	ASN	4.0
2	B	218	GLY	3.7
6	T	243	ILE	3.6
11	Y	148	LEU	3.5
12	L	172	LEU	3.5
12	L	170	LYS	3.5
13	a	1	THR	3.5
11	Y	209	ASN	3.5
12	Z	172	LEU	3.3
11	K	208	ASN	3.3
12	L	168	VAL	3.3
6	F	202	ASP	3.2
11	K	147	ASP	3.2
12	Z	173	LYS	3.2
11	K	211	ILE	3.2
3	Q	205	ALA	3.1
12	Z	166	GLY	3.1
12	Z	163	GLY	3.0
8	V	223	ILE	3.0
12	L	136	CYS	3.0
4	D	241	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
11	K	209	ASN	2.9
13	M	1	THR	2.9
2	P	222	GLY	2.8
6	T	215	CYS	2.8
11	K	146	TRP	2.8
2	P	52	THR	2.7
11	K	148	LEU	2.7
12	Z	162	PRO	2.7
12	L	167	LYS	2.7
12	Z	170	LYS	2.7
6	F	215	CYS	2.7
12	L	164	THR	2.7
6	T	204	LYS	2.6
2	P	218	GLY	2.6
12	L	169	LYS	2.6
12	L	166	GLY	2.6
11	Y	147	ASP	2.6
4	R	239	GLU	2.5
12	Z	136	CYS	2.5
12	L	162	PRO	2.5
6	T	205	GLU	2.5
1	O	1	MET	2.4
5	S	207	VAL	2.4
13	M	233	ILE	2.4
3	C	51	LYS	2.4
3	Q	240	GLU	2.4
2	P	1	GLY	2.4
3	Q	206	LYS	2.4
11	K	212	GLY	2.4
5	S	122	TYR	2.4
6	T	14	ASP	2.3
3	C	50	LEU	2.3
3	Q	203	THR	2.3
2	P	219	ALA	2.3
10	X	142	SER	2.3
2	B	52	THR	2.3
11	Y	150	VAL	2.3
1	O	53	SER	2.3
3	Q	51	LYS	2.2
3	Q	204	GLY	2.2
4	D	117	GLU	2.2
4	R	125	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
12	L	173	LYS	2.2
3	C	205	ALA	2.2
10	J	174	MET	2.1
12	L	171	PRO	2.1
4	D	240	ALA	2.1
10	J	142	SER	2.1
3	Q	234	ILE	2.1
6	T	244	ASN	2.1
12	Z	171	PRO	2.0
12	Z	135	GLN	2.0
10	X	143	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.

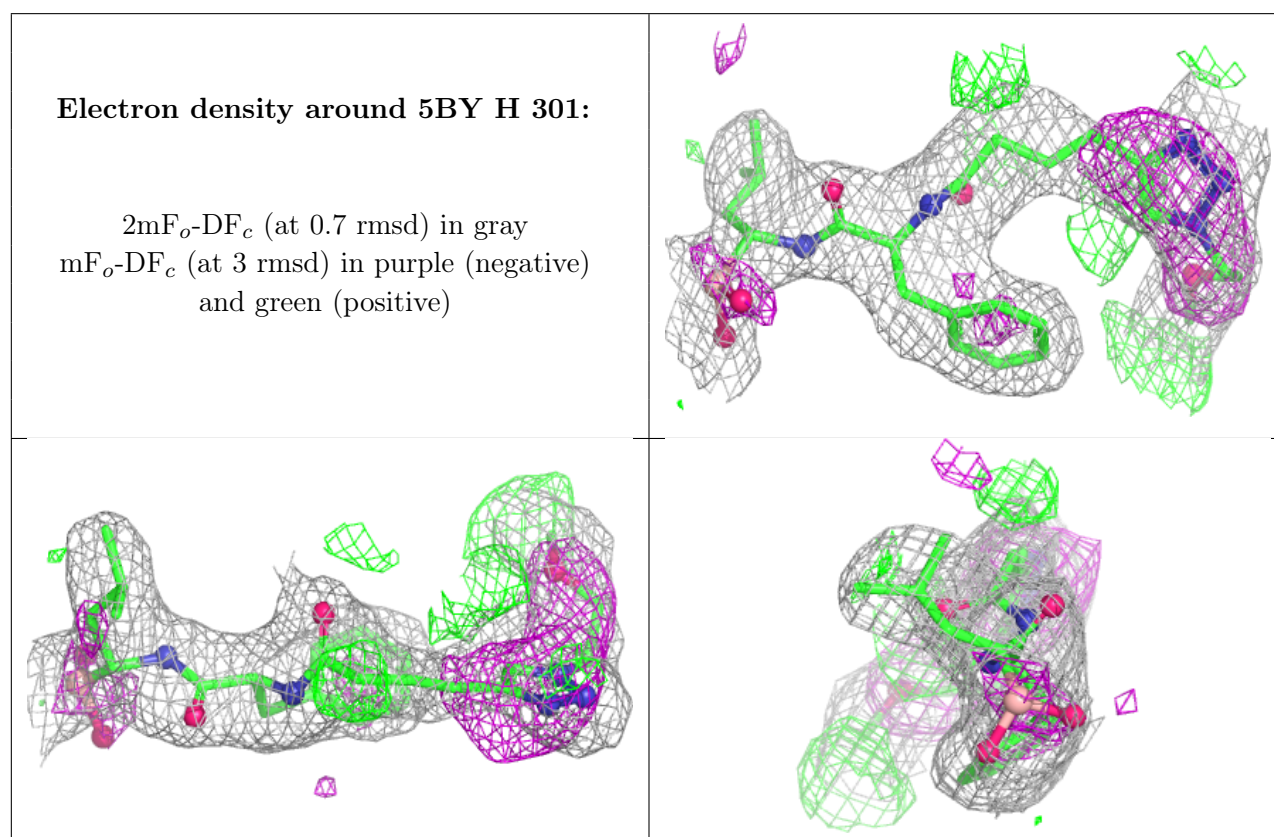
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
17	5BY	H	301	34/43	0.80	0.14	44,50,59,68	0
17	5BY	b	201	34/43	0.80	0.14	30,52,56,58	0
17	5BY	V	302	34/43	0.82	0.14	42,52,60,66	0
17	5BY	Y	302	34/43	0.84	0.13	41,50,59,66	0
17	5BY	N	201	34/43	0.85	0.13	40,50,56,59	0
17	5BY	K	301	34/43	0.85	0.12	41,51,60,63	0
15	MG	Z	301	1/1	0.91	0.09	67,67,67,67	0
15	MG	I	301	1/1	0.94	0.10	65,65,65,65	0
15	MG	K	302	1/1	0.98	0.07	60,60,60,60	0
16	CL	N	203	1/1	0.98	0.04	53,53,53,53	0
16	CL	U	301	1/1	0.98	0.07	47,47,47,47	0
16	CL	b	202	1/1	0.98	0.13	65,65,65,65	0

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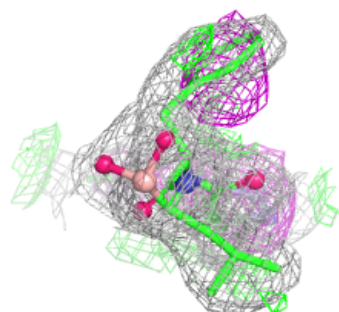
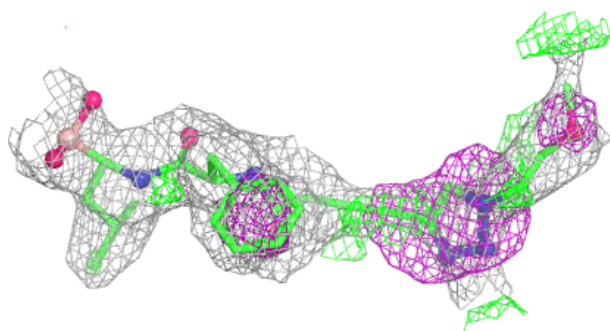
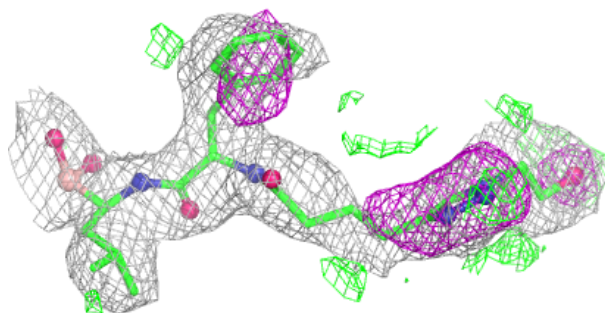
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	MG	V	301	1/1	0.98	0.07	67,67,67,67	0
16	CL	G	302	1/1	0.99	0.10	45,45,45,45	0
15	MG	N	202	1/1	0.99	0.04	52,52,52,52	0
15	MG	J	201	1/1	0.99	0.16	49,49,49,49	0
15	MG	Y	301	1/1	0.99	0.06	55,55,55,55	0
15	MG	G	301	1/1	0.99	0.06	53,53,53,53	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.

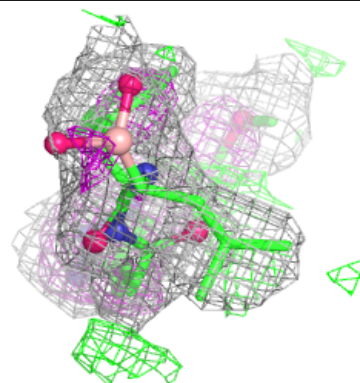
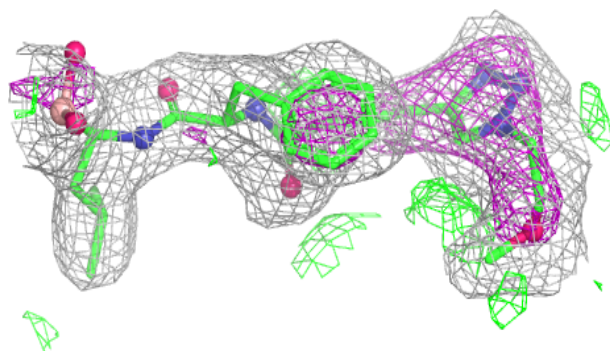
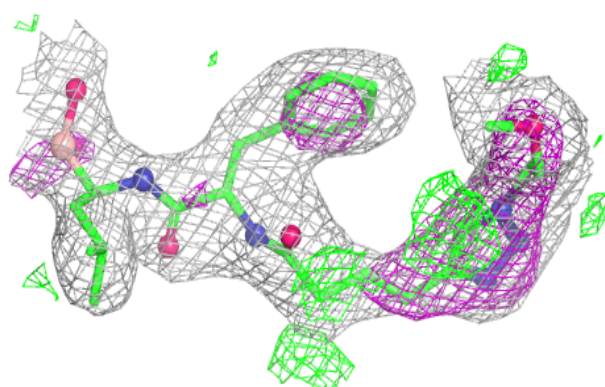


Electron density around 5BY b 201:

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

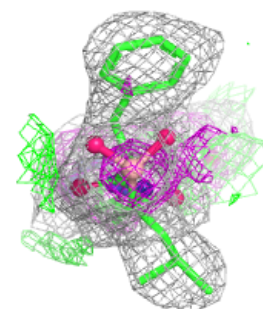
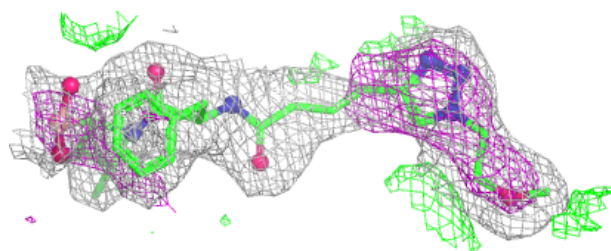
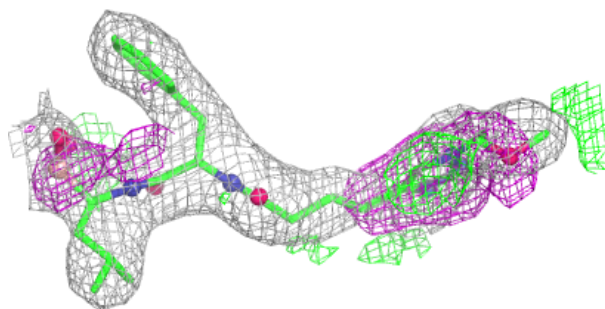
**Electron density around 5BY V 302:**

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

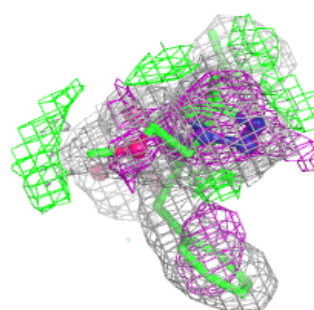
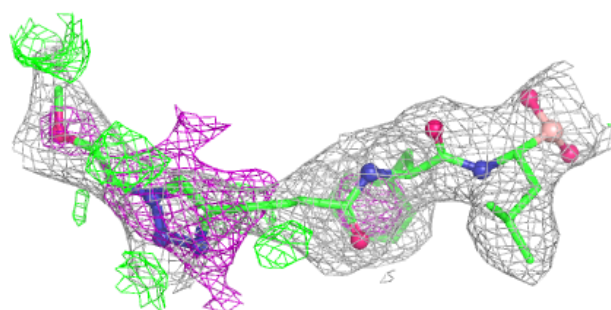
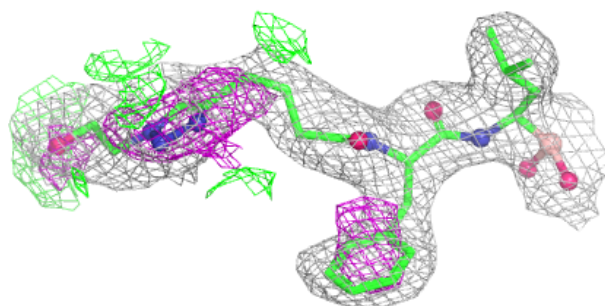


Electron density around 5BY Y 302:

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

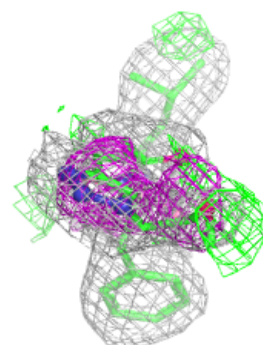
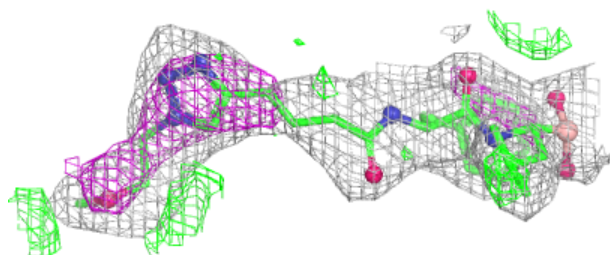
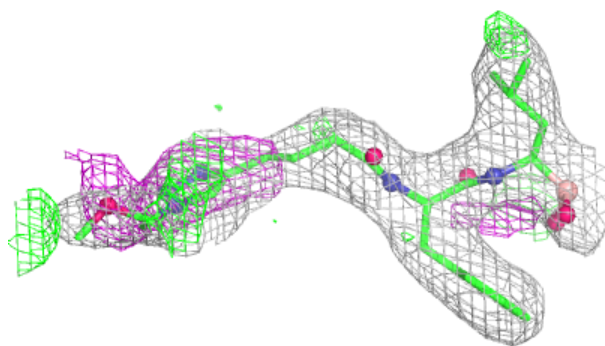
**Electron density around 5BY N 201:**

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



Electron density around 5BY K 301:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.