



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:26 PM UTC

PDB ID : 9FT0 / pdb_00009ft0
Title : Yeast 20S proteasome in complex with epoxyketone inhibitor 16
Authors : Maurits, E.; Huber, E.M.; Dekker, P.M.; Wang, X.; Heinemeyer, W.; Florea, B.I.; Groll, M.; Overkleeft, H.S.
Deposited on : 2024-06-23
Resolution : 2.75 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:

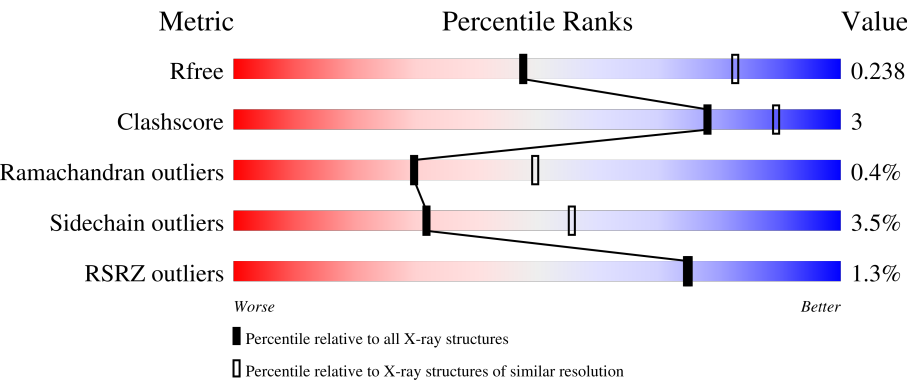
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

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

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	94%6%•
1	O	250	% 92%7%•
2	B	258	2% 85%9%5%
2	P	258	3% 86%9%5%
3	C	254	3% 86%8%•5%

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Mol	Chain	Length	Quality of chain
3	Q	254	
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	231	
8	V	231	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	211	
11	Y	211	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	196	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	SO4	V	302	-	-	X	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 49929 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	241	Total	C	N	O	S	0	0	0
			1890	1181	331	374	4			
3	Q	241	Total	C	N	O	S	0	0	0
			1890	1181	331	374	4			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	221	Total	C	N	O	S	0	0	0
			1677	1057	292	321	7			
8	V	221	Total	C	N	O	S	0	0	0
			1677	1057	292	321	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	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	211	Total	C	N	O	S	0	0	0
			1637	1041	279	310	7			
11	Y	211	Total	C	N	O	S	0	0	0
			1637	1041	279	310	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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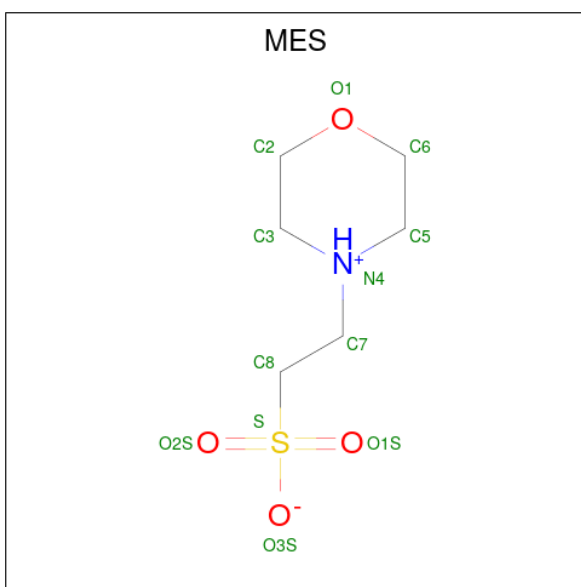
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	K	1	Total 1	Mg 1	0	0
15	N	1	Total 1	Mg 1	0	0
15	V	1	Total 1	Mg 1	0	0
15	W	1	Total 1	Mg 1	0	0
15	X	1	Total 1	Mg 1	0	0
15	Y	1	Total 1	Mg 1	0	0
15	Z	1	Total 1	Mg 1	0	0

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

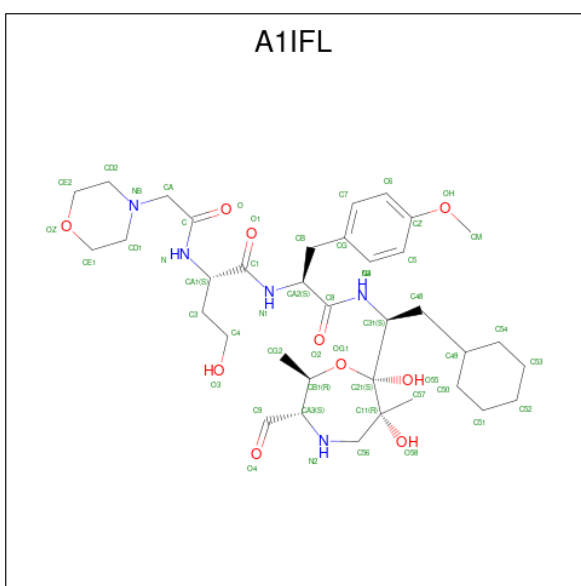
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	G	1	Total 1	Cl 1	0	0
16	N	2	Total 2	Cl 2	0	0
16	U	1	Total 1	Cl 1	0	0
16	b	1	Total 1	Cl 1	0	0

- Molecule 17 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



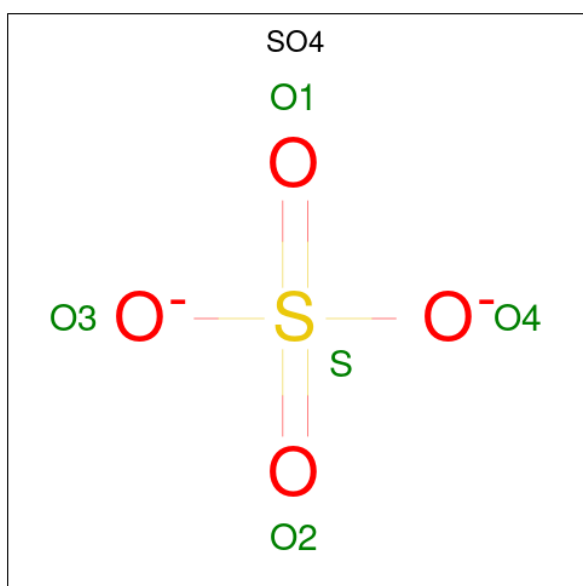
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
17	K	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
17	X	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 18 is (2S)-N-[(2S)-1-[(1S)-2-cyclohexyl-1-[(2R,3S,6R,7S)-3-methanoyl-2,6-dimethyl-6,7-bis(oxidanyl)-1,4-oxazepan-7-yl]ethyl]amino]-3-(4-methoxyphenyl)-1-oxidanylidene-propan-2-yl]-2-(2-morpholin-4-ylethanoylamino)-4-oxidanyl-butanamide (CCD ID: A1IFL) (formula: C₃₆H₅₇N₅O₁₀) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	H	1	Total	C	N	O	0	0
			51	36	5	10		
18	K	1	Total	C	N	O	0	0
			51	36	5	10		
18	V	1	Total	C	N	O	0	0
			51	36	5	10		
18	Y	1	Total	C	N	O	0	0
			51	36	5	10		

- Molecule 19 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	K	1	Total	O	S	0	0
			5	4	1		
19	V	1	Total	O	S	0	0
			5	4	1		
19	Y	1	Total	O	S	0	0
			5	4	1		

- Molecule 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	2	Total	O	0	0
			2	2		
20	B	6	Total	O	0	0
			6	6		
20	C	3	Total	O	0	0
			3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	D	2	Total O 2 2	0	0
20	E	4	Total O 4 4	0	0
20	F	5	Total O 5 5	0	0
20	G	4	Total O 4 4	0	0
20	H	4	Total O 4 4	0	0
20	I	3	Total O 3 3	0	0
20	J	7	Total O 7 7	0	0
20	K	6	Total O 6 6	0	0
20	L	5	Total O 5 5	0	0
20	M	5	Total O 5 5	0	0
20	N	8	Total O 8 8	0	0
20	O	2	Total O 2 2	0	0
20	P	6	Total O 6 6	0	0
20	Q	3	Total O 3 3	0	0
20	R	2	Total O 2 2	0	0
20	S	4	Total O 4 4	0	0
20	T	7	Total O 7 7	0	0
20	U	8	Total O 8 8	0	0
20	V	4	Total O 4 4	0	0
20	W	5	Total O 5 5	0	0
20	X	11	Total O 11 11	0	0

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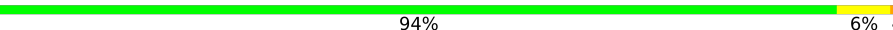
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	Y	7	Total 7	O 7	0	0
20	Z	10	Total 10	O 10	0	0
20	a	10	Total 10	O 10	0	0
20	b	7	Total 7	O 7	0	0

3 Residue-property plots [i](#)

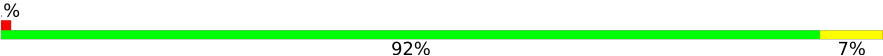
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

Chain A:  94% 6%



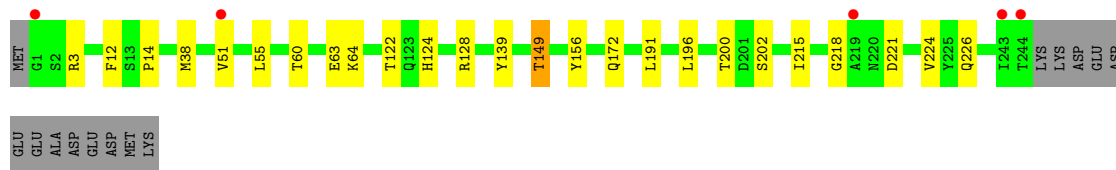
- Molecule 1: Proteasome subunit alpha type-2

Chain O:  92% 7%



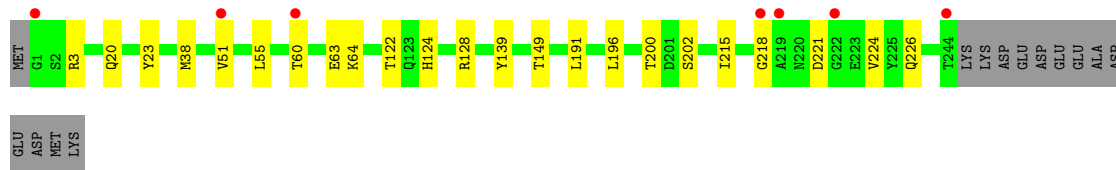
- Molecule 2: Proteasome subunit alpha type-3

Chain B:  85% 9% 5%



- Molecule 2: Proteasome subunit alpha type-3

Chain P:  86% 9% 5% 3%

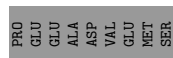
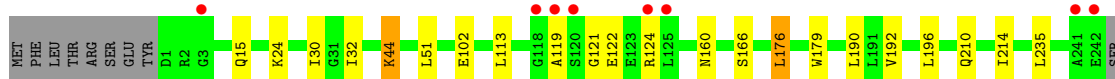


- Molecule 3: Proteasome subunit alpha type-4

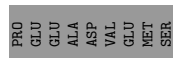
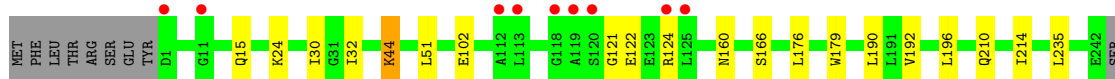
Chain C:  86% 8% 5% 3%



- Molecule 4: Proteasome subunit alpha type-5



- Molecule 4: Proteasome subunit alpha type-5



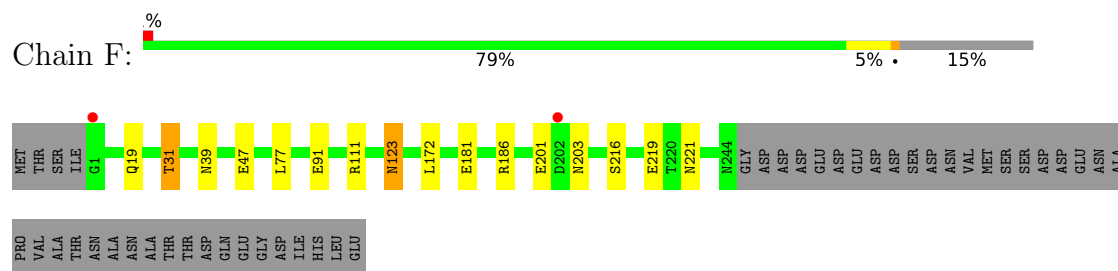
- Molecule 5: Proteasome subunit alpha type-6



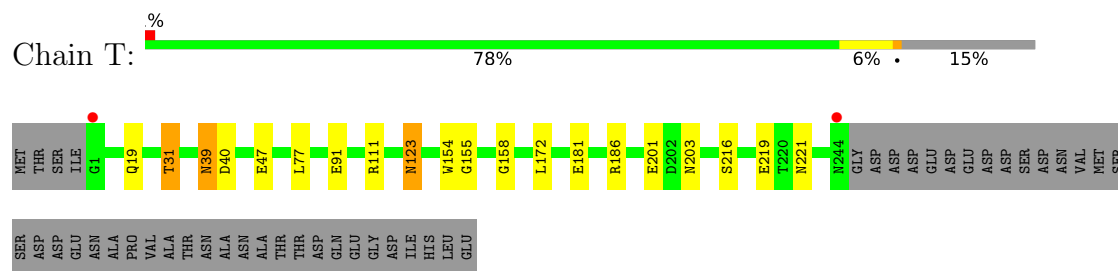
- Molecule 5: Proteasome subunit alpha type-6



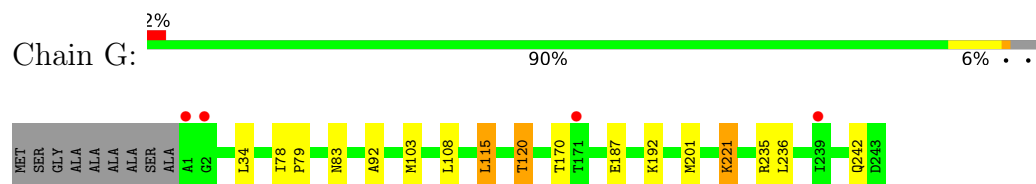
- Molecule 6: Probable proteasome subunit alpha type-7



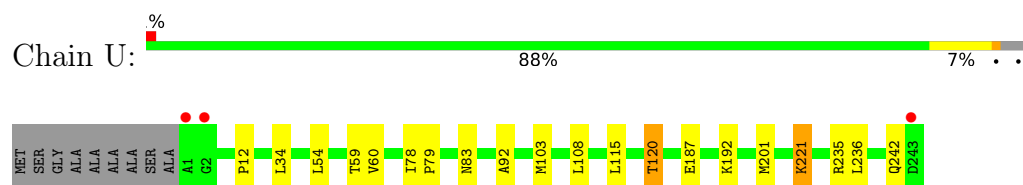
- Molecule 6: Probable proteasome subunit alpha type-7



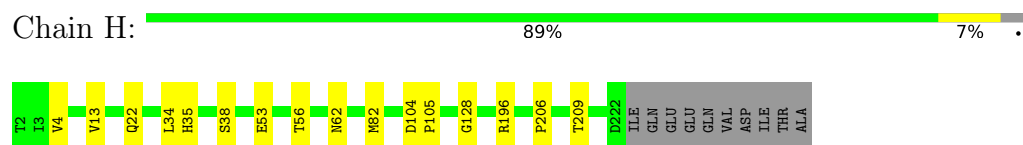
- Molecule 7: Proteasome subunit alpha type-1



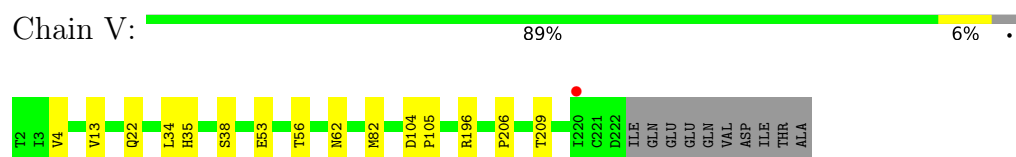
- Molecule 7: Proteasome subunit alpha type-1



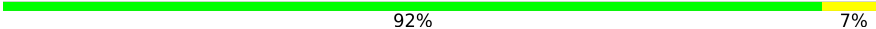
- Molecule 8: Proteasome subunit beta type-2

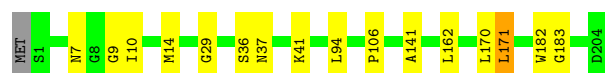


- Molecule 8: Proteasome subunit beta type-2



- Molecule 9: Proteasome subunit beta type-3

Chain I:  92% 7%



- Molecule 9: Proteasome subunit beta type-3

Chain W:  91% 8%

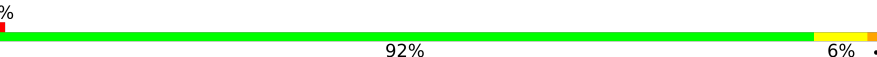


- Molecule 10: Proteasome subunit beta type-4

Chain J:  2% 89% 9% ..



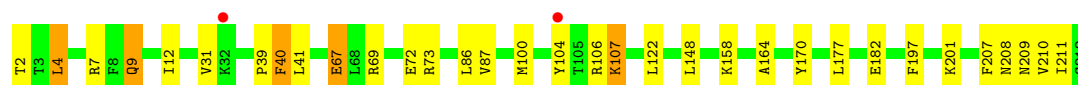
- Molecule 10: Proteasome subunit beta type-4

Chain X:  2% 92% 6% .



- Molecule 11: Proteasome subunit beta type-5

Chain K:  2% 84% 13% .



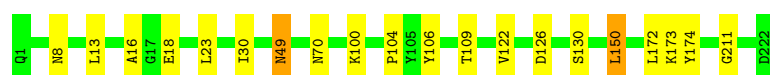
- Molecule 11: Proteasome subunit beta type-5

Chain Y:  2% 85% 12% .



- Molecule 12: Proteasome subunit beta type-6

Chain L:  91% 8% .



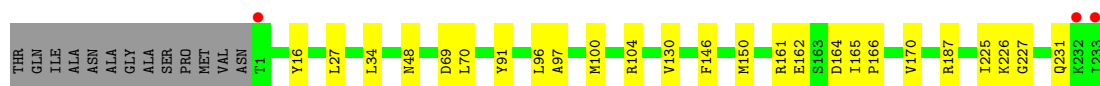
- Molecule 12: Proteasome subunit beta type-6

Chain Z:  91% 8% .



- Molecule 13: Proteasome subunit beta type-7

Chain M:  85% 10% 5%



- Molecule 13: Proteasome subunit beta type-7

Chain a:  83% 11% 5%

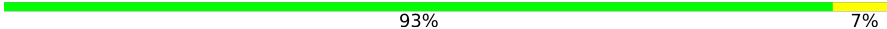


- Molecule 14: Proteasome subunit beta type-1

Chain N:  90% 10%



- Molecule 14: Proteasome subunit beta type-1

Chain b:  93% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.52Å 299.48Å 145.00Å 90.00° 112.90° 90.00°	Depositor
Resolution (Å)	30.00 – 2.75 30.00 – 2.75	Depositor EDS
% Data completeness (in resolution range)	96.3 (30.00-2.75) 96.3 (30.00-2.75)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.76Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.190 , 0.232 (Not available) , 0.238	Depositor DCC
R_{free} test set	13235 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	56.2	Xtriage
Anisotropy	0.750	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	49929	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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: CL, SO4, A1IFL, MES, MG

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	1.03	0/1952	1.43	0/2642
1	O	1.03	0/1952	1.42	0/2642
2	B	1.03	0/1934	1.47	0/2618
2	P	1.03	0/1934	1.47	0/2618
3	C	1.04	0/1919	1.49	0/2598
3	Q	1.04	0/1919	1.49	0/2598
4	D	1.04	0/1886	1.48	0/2541
4	R	1.04	0/1886	1.49	0/2541
5	E	1.03	0/1823	1.45	0/2463
5	S	1.03	0/1823	1.45	2/2463 (0.1%)
6	F	1.02	0/1936	1.48	2/2614 (0.1%)
6	T	1.03	0/1936	1.49	2/2614 (0.1%)
7	G	1.01	0/1959	1.43	0/2652
7	U	1.01	0/1959	1.43	0/2652
8	H	1.04	0/1708	1.43	2/2316 (0.1%)
8	V	1.04	0/1708	1.45	2/2316 (0.1%)
9	I	1.02	0/1611	1.43	1/2174 (0.0%)
9	W	1.02	0/1611	1.43	1/2174 (0.0%)
10	J	1.03	1/1613 (0.1%)	1.45	2/2173 (0.1%)
10	X	1.03	1/1613 (0.1%)	1.43	1/2173 (0.0%)
11	K	1.00	0/1674	1.47	1/2264 (0.0%)
11	Y	1.01	0/1674	1.49	5/2264 (0.2%)
12	L	1.02	0/1795	1.41	0/2420
12	Z	1.02	0/1795	1.41	0/2420
13	M	1.03	0/1855	1.39	2/2514 (0.1%)
13	a	1.03	0/1855	1.39	0/2514
14	N	1.02	0/1541	1.45	0/2087
14	b	1.03	0/1541	1.45	0/2087
All	All	1.03	2/50412 (0.0%)	1.45	23/68152 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	X	133	HIS	CE1-NE2	-8.07	1.24	1.32
10	J	133	HIS	CE1-NE2	-7.46	1.25	1.32

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	T	77	LEU	CA-C-N	7.34	124.87	120.24
6	T	77	LEU	C-N-CA	7.34	124.87	120.24
10	J	145	ASP	CA-CB-CG	6.77	119.37	112.60
11	Y	211	ILE	N-CA-CB	-6.42	103.69	111.21
11	K	107	LYS	CB-CA-C	-5.67	102.23	110.96
9	I	183	GLY	CA-C-O	-5.59	118.37	122.23
11	Y	210	VAL	CA-C-N	5.55	130.01	122.90
11	Y	210	VAL	C-N-CA	5.55	130.01	122.90
10	X	133	HIS	CB-CG-ND1	5.54	131.01	122.70
6	F	77	LEU	CA-C-N	5.53	124.75	120.33
6	F	77	LEU	C-N-CA	5.53	124.75	120.33
11	Y	107	LYS	CB-CA-C	-5.51	102.48	110.96
11	Y	211	ILE	CA-CB-CG1	5.48	119.72	110.40
9	W	183	GLY	CA-C-O	-5.44	118.48	122.23
13	M	164	ASP	CA-C-N	5.31	124.58	120.33
13	M	164	ASP	C-N-CA	5.31	124.58	120.33
8	V	4	VAL	CA-C-N	5.21	125.20	121.65
8	V	4	VAL	C-N-CA	5.21	125.20	121.65
10	J	133	HIS	CB-CG-ND1	5.15	130.43	122.70
8	H	4	VAL	CA-C-N	5.10	125.12	121.65
8	H	4	VAL	C-N-CA	5.10	125.12	121.65
5	S	35	VAL	CA-C-N	5.08	125.10	121.65
5	S	35	VAL	C-N-CA	5.08	125.10	121.65

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	1915	0	1929	11	0
2	B	1904	0	1904	12	0
2	P	1904	0	1904	10	0
3	C	1890	0	1903	11	0
3	Q	1890	0	1903	8	0
4	D	1861	0	1839	11	0
4	R	1861	0	1839	8	0
5	E	1795	0	1800	19	0
5	S	1795	0	1800	15	0
6	F	1896	0	1889	5	0
6	T	1896	0	1889	9	0
7	G	1921	0	1913	11	0
7	U	1921	0	1913	12	0
8	H	1677	0	1678	6	0
8	V	1677	0	1678	4	0
9	I	1581	0	1574	8	0
9	W	1581	0	1574	10	0
10	J	1585	0	1590	15	0
10	X	1585	0	1590	14	0
11	K	1637	0	1585	20	0
11	Y	1637	0	1585	23	0
12	L	1757	0	1711	11	0
12	Z	1757	0	1711	14	0
13	M	1824	0	1832	8	0
13	a	1824	0	1832	11	0
14	N	1512	0	1481	13	0
14	b	1512	0	1481	8	0
15	G	1	0	0	0	0
15	I	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	W	1	0	0	0	0
15	X	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	2	0	0	1	0
16	U	1	0	0	0	0
16	b	1	0	0	0	0
17	H	12	0	13	2	0
17	K	12	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	X	12	0	13	0	0
18	H	51	0	0	1	0
18	K	51	0	0	2	0
18	V	51	0	0	4	0
18	Y	51	0	0	4	0
19	K	5	0	0	0	0
19	V	5	0	0	2	0
19	Y	5	0	0	0	0
20	A	2	0	0	0	0
20	B	6	0	0	0	0
20	C	3	0	0	0	0
20	D	2	0	0	0	0
20	E	4	0	0	0	0
20	F	5	0	0	0	0
20	G	4	0	0	0	0
20	H	4	0	0	0	0
20	I	3	0	0	0	0
20	J	7	0	0	1	0
20	K	6	0	0	0	0
20	L	5	0	0	0	0
20	M	5	0	0	0	0
20	N	8	0	0	0	0
20	O	2	0	0	0	0
20	P	6	0	0	0	0
20	Q	3	0	0	0	0
20	R	2	0	0	0	0
20	S	4	0	0	0	0
20	T	7	0	0	0	0
20	U	8	0	0	0	0
20	V	4	0	0	0	0
20	W	5	0	0	0	0
20	X	11	0	0	0	0
20	Y	7	0	0	0	0
20	Z	10	0	0	0	0
20	a	10	0	0	0	0
20	b	7	0	0	0	0
All	All	49929	0	49295	273	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 3.

All (273) 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:Y:104:TYR:CZ	11:Y:182:GLU:HG3	2.07	0.90
11:K:104:TYR:CZ	11:K:182:GLU:HG3	2.08	0.88
19:V:302:SO4:O3	18:V:303:A1IFL:O58	1.92	0.87
6:T:91:GLU:HG2	6:T:111:ARG:HB3	1.67	0.76
6:F:91:GLU:HG2	6:F:111:ARG:HB3	1.68	0.75
7:G:92:ALA:HA	7:G:103:MET:HE2	1.68	0.75
7:U:92:ALA:HA	7:U:103:MET:HE2	1.66	0.74
11:K:104:TYR:CE1	11:K:182:GLU:HG3	2.22	0.74
11:K:208:ASN:ND2	10:X:148:TYR:O	2.21	0.73
8:H:128:GLY:H	17:H:301:MES:H31	1.52	0.73
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.54	0.72
11:Y:104:TYR:CE1	11:Y:182:GLU:HG3	2.24	0.71
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.54	0.71
10:J:174:MET:HA	10:X:174:MET:HA	1.73	0.71
12:L:18:GLU:HA	12:L:174:TYR:CE2	2.28	0.69
11:K:209:ASN:O	9:W:37:ASN:ND2	2.27	0.68
12:Z:18:GLU:HA	12:Z:174:TYR:CE2	2.28	0.68
6:T:31:THR:HG21	6:T:47:GLU:O	1.96	0.66
6:F:31:THR:HG21	6:F:47:GLU:O	1.96	0.64
1:O:128:ARG:HH21	7:U:120:THR:HG22	1.63	0.63
1:A:128:ARG:HH21	7:G:120:THR:HG22	1.64	0.62
10:X:174:MET:SD	10:X:174:MET:N	2.73	0.62
5:S:92:ASN:HD21	12:Z:70:ASN:HD21	1.48	0.61
10:X:25:ILE:HG13	10:X:25:ILE:O	2.01	0.60
5:S:12:PHE:H	6:T:19:GLN:HE22	1.49	0.60
7:G:78:ILE:N	7:G:79:PRO:HD2	2.16	0.60
7:U:78:ILE:N	7:U:79:PRO:HD2	2.16	0.59
11:K:4:LEU:HD22	11:K:4:LEU:C	2.28	0.59
10:J:174:MET:SD	10:J:174:MET:N	2.73	0.59
11:Y:4:LEU:C	11:Y:4:LEU:HD22	2.28	0.59
11:Y:167:ARG:HH21	11:Y:209:ASN:ND2	2.02	0.58
11:K:211:ILE:HD11	9:W:38:LYS:HG2	1.86	0.58
10:X:1:MET:N	10:X:1:MET:HE2	2.21	0.56
5:E:92:ASN:HD21	12:L:70:ASN:HD21	1.51	0.56
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.36	0.56
5:E:87:LEU:HD11	5:E:107:ALA:HB1	1.88	0.56
10:X:7:ILE:HD11	10:X:144:LEU:HD22	1.87	0.56
11:K:67:GLU:HA	11:K:72:GLU:O	2.07	0.55
8:H:206:PRO:O	8:H:209:THR:OG1	2.22	0.55
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.36	0.55
5:S:87:LEU:HD11	5:S:107:ALA:HB1	1.88	0.55
3:C:157:TRP:CE2	4:D:51:LEU:HD23	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:V:303:A1IFL:C8	18:V:303:A1IFL:C57	2.86	0.53
18:Y:303:A1IFL:C8	18:Y:303:A1IFL:C57	2.85	0.53
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.90	0.53
3:C:35:LYS:HG2	3:C:158:SER:O	2.09	0.53
18:V:303:A1IFL:C57	18:V:303:A1IFL:N4	2.72	0.53
10:J:101:ASN:HB3	10:J:133:HIS:ND1	2.24	0.52
11:K:2:THR:HG21	11:K:164:ALA:CB	2.39	0.52
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.74	0.52
10:X:1:MET:HE2	10:X:1:MET:CA	2.39	0.52
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.91	0.51
2:B:12:PHE:H	3:C:17:GLN:HE22	1.59	0.51
11:K:170:TYR:O	18:K:304:A1IFL:C56	2.59	0.51
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.10	0.51
6:T:155:GLY:HA3	7:U:59:THR:HG21	1.92	0.51
3:Q:157:TRP:CE2	4:R:51:LEU:HD23	2.46	0.51
5:E:12:PHE:H	6:F:19:GLN:HE22	1.58	0.50
11:Y:40:PHE:HE1	11:Y:182:GLU:O	1.95	0.50
1:O:30:GLN:HA	1:O:30:GLN:HE21	1.76	0.50
5:S:92:ASN:ND2	12:Z:70:ASN:HD21	2.09	0.50
5:S:127:TYR:O	5:S:148:PRO:HB3	2.10	0.50
13:M:97:ALA:HA	13:M:130:VAL:HG21	1.94	0.50
1:A:30:GLN:HE21	1:A:30:GLN:HA	1.76	0.50
14:N:132:THR:O	14:b:133:PHE:HA	2.11	0.50
2:B:3:ARG:HB2	5:E:122:TYR:OH	2.11	0.49
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.94	0.49
13:M:27:LEU:HD21	13:M:34:LEU:HD22	1.94	0.49
5:E:127:TYR:O	5:E:148:PRO:HB3	2.12	0.49
12:L:49:ASN:HD21	12:L:211:GLY:HA2	1.77	0.49
11:Y:2:THR:HG21	11:Y:164:ALA:CB	2.42	0.49
7:U:103:MET:HE3	7:U:108:LEU:HD13	1.95	0.49
3:C:9:PHE:H	4:D:15:GLN:HE22	1.61	0.49
13:a:27:LEU:HD21	13:a:34:LEU:HD22	1.94	0.49
12:Z:49:ASN:HD21	12:Z:211:GLY:HA2	1.78	0.48
13:a:97:ALA:HA	13:a:130:VAL:HG21	1.94	0.48
1:O:12:PHE:H	2:P:20:GLN:HE22	1.61	0.48
3:C:161:THR:HG21	3:C:169:VAL:HG13	1.95	0.48
2:P:196:LEU:O	2:P:200:THR:OG1	2.31	0.48
12:L:8:ASN:HA	12:L:30:ILE:O	2.13	0.48
3:Q:161:THR:HG21	3:Q:169:VAL:HG13	1.94	0.48
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.94	0.48
4:D:119:ALA:HA	5:E:124:GLY:HA2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:200:LEU:HD11	5:E:205:LEU:HD22	1.96	0.48
10:J:39:SER:HB2	10:J:40:PRO:HD2	1.95	0.48
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.49	0.48
8:V:206:PRO:O	8:V:209:THR:OG1	2.22	0.48
10:X:172:MET:HE2	10:X:174:MET:HE1	1.95	0.48
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.14	0.48
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.96	0.48
11:K:201:LYS:HG3	11:K:207:PHE:HB2	1.96	0.48
7:G:103:MET:HE3	7:G:108:LEU:HD13	1.95	0.48
5:S:200:LEU:HD11	5:S:205:LEU:HD22	1.96	0.48
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.96	0.48
11:Y:201:LYS:HG3	11:Y:207:PHE:HB2	1.96	0.48
2:B:196:LEU:O	2:B:200:THR:OG1	2.31	0.47
11:K:197:PHE:HZ	11:K:210:VAL:HG21	1.78	0.47
6:T:158:GLY:O	7:U:54:LEU:HB3	2.14	0.47
10:X:39:SER:HB2	10:X:40:PRO:HD2	1.94	0.47
2:P:200:THR:HG22	2:P:202:SER:H	1.79	0.47
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.49	0.47
5:S:92:ASN:HD21	12:Z:70:ASN:ND2	2.12	0.47
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.50	0.47
14:b:175:MET:HB2	14:b:186:LEU:HB2	1.96	0.47
14:N:175:MET:HB2	14:N:186:LEU:HB2	1.96	0.47
12:Z:126:ASP:C	12:Z:126:ASP:OD2	2.57	0.47
11:K:40:PHE:HE1	11:K:182:GLU:O	1.98	0.47
11:Y:167:ARG:NH2	11:Y:209:ASN:ND2	2.63	0.47
2:B:172:GLN:HG2	3:C:50:LEU:HD12	1.95	0.47
2:B:200:THR:HG22	2:B:202:SER:H	1.80	0.46
5:S:9:THR:HG21	5:S:119:THR:HA	1.97	0.46
13:a:16:TYR:CE2	13:a:170:VAL:HG22	2.51	0.46
5:E:9:THR:HG21	5:E:119:THR:HA	1.97	0.46
5:E:205:LEU:H	5:E:205:LEU:HD23	1.80	0.46
4:D:44:LYS:HE3	4:D:210:GLN:HB2	1.97	0.46
10:J:21:VAL:HG11	11:K:122:LEU:HD11	1.98	0.46
13:M:16:TYR:CE2	13:M:170:VAL:HG22	2.50	0.46
5:E:226:GLY:O	5:E:229:VAL:HG22	2.16	0.46
5:S:205:LEU:HD23	5:S:205:LEU:H	1.80	0.46
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.41	0.46
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.80	0.45
11:K:86:LEU:C	11:K:86:LEU:HD13	2.41	0.45
4:R:44:LYS:HE3	4:R:210:GLN:HB2	1.97	0.45
18:H:302:A1IFL:C57	18:H:302:A1IFL:N4	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:2:THR:HG21	11:Y:164:ALA:HB3	1.98	0.45
9:W:36:SER:HB2	10:X:126:VAL:HG21	1.98	0.45
12:Z:18:GLU:HB2	12:Z:174:TYR:CD2	2.51	0.45
5:S:226:GLY:O	5:S:229:VAL:HG22	2.17	0.45
10:J:150:PRO:HD3	11:Y:208:ASN:HD22	1.81	0.45
2:P:63:GLU:HG3	2:P:64:LYS:HG3	1.99	0.45
11:Y:7:ARG:HG3	11:Y:12:ILE:HG12	1.98	0.45
12:Z:16:ALA:HB2	12:Z:122:VAL:HG23	1.98	0.45
18:K:304:A1IFL:N4	18:K:304:A1IFL:C57	2.80	0.45
10:X:172:MET:HE2	10:X:174:MET:CE	2.46	0.45
12:L:16:ALA:HB2	12:L:122:VAL:HG23	1.99	0.45
2:P:139:TYR:CD1	2:P:224:VAL:HG21	2.52	0.45
11:Y:170:TYR:O	18:Y:303:A1IFL:C56	2.65	0.45
11:K:7:ARG:HG3	11:K:12:ILE:HG12	1.98	0.44
11:K:9:GLN:NE2	11:K:148:LEU:O	2.50	0.44
11:K:4:LEU:HD22	11:K:4:LEU:O	2.18	0.44
2:B:139:TYR:CD1	2:B:224:VAL:HG21	2.52	0.44
4:D:113:LEU:HD12	5:E:78:PRO:HB2	1.99	0.44
14:N:7:THR:OG1	14:N:123:PRO:O	2.32	0.44
2:B:63:GLU:HG3	2:B:64:LYS:HG3	1.99	0.44
5:E:98:PHE:O	13:M:91:TYR:HA	2.18	0.44
12:L:18:GLU:HB2	12:L:174:TYR:CD2	2.52	0.44
6:T:123:ASN:C	6:T:123:ASN:HD22	2.26	0.44
11:Y:9:GLN:NE2	11:Y:148:LEU:O	2.51	0.44
5:E:92:ASN:ND2	12:L:70:ASN:HD21	2.15	0.44
5:E:197:SER:HA	5:E:200:LEU:HG	2.00	0.44
12:L:13:LEU:HD11	12:L:150:LEU:HD21	2.00	0.44
5:E:80:ALA:HB2	5:E:129:VAL:HG21	2.00	0.43
13:M:165:ILE:N	13:M:166:PRO:HD2	2.33	0.43
3:C:108:THR:HG21	3:C:146:TYR:HB3	2.00	0.43
10:J:145:ASP:OD1	11:Y:209:ASN:ND2	2.51	0.43
11:K:4:LEU:C	11:K:4:LEU:CD2	2.91	0.43
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.53	0.43
5:S:77:ALA:N	5:S:78:PRO:CD	2.81	0.43
1:A:55:LEU:HD12	7:G:170:THR:HG23	2.01	0.43
1:O:119:GLN:O	1:O:122:THR:HB	2.18	0.43
19:V:302:SO4:S	18:V:303:A1IFL:O58	2.74	0.43
10:X:149:ARG:HB2	10:X:152:MET:HG3	2.00	0.43
4:D:30:ILE:HD12	4:D:196:LEU:HG	2.00	0.43
8:H:35:HIS:HB2	8:H:56:THR:HG21	2.00	0.43
1:O:14:PRO:HA	2:P:23:TYR:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:4:LEU:C	11:Y:4:LEU:CD2	2.91	0.43
14:N:45:ARG:NH2	16:N:203:CL:CL	2.82	0.43
5:S:197:SER:HA	5:S:200:LEU:HG	1.99	0.43
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.67	0.43
12:Z:100:LYS:O	12:Z:104:PRO:HA	2.18	0.43
6:F:123:ASN:C	6:F:123:ASN:HD22	2.26	0.43
10:J:48:GLY:HA2	20:J:207:HOH:O	2.19	0.43
9:W:10:ILE:HD12	9:W:170:LEU:HD12	2.01	0.43
14:N:26:ILE:HB	13:a:187:ARG:HA	2.01	0.43
14:N:136:GLY:HA2	14:b:161:GLN:HE21	1.84	0.43
13:a:165:ILE:N	13:a:166:PRO:HD2	2.33	0.43
5:E:77:ALA:N	5:E:78:PRO:CD	2.82	0.43
11:Y:197:PHE:HZ	11:Y:210:VAL:HG21	1.83	0.43
9:I:10:ILE:HD12	9:I:170:LEU:HD12	2.01	0.43
1:A:149:GLN:O	1:A:156:TYR:HA	2.19	0.42
4:D:176:LEU:HD22	5:E:55:LEU:HD13	2.01	0.42
9:I:94:LEU:HD11	9:I:106:PRO:HG2	2.01	0.42
1:O:149:GLN:O	1:O:156:TYR:HA	2.19	0.42
11:Y:104:TYR:CD1	11:Y:104:TYR:C	2.98	0.42
3:C:204:GLY:HA3	3:C:207:ASN:HB2	2.01	0.42
7:G:34:LEU:C	7:G:34:LEU:HD12	2.43	0.42
2:P:3:ARG:HB2	5:S:122:TYR:OH	2.19	0.42
3:Q:108:THR:HG21	3:Q:146:TYR:HB3	2.00	0.42
6:T:216:SER:HB3	6:T:219:GLU:HB2	2.01	0.42
8:V:35:HIS:HB2	8:V:56:THR:HG21	2.00	0.42
9:W:36:SER:CB	10:X:126:VAL:HG21	2.49	0.42
13:a:96:LEU:O	13:a:100:MET:HG2	2.18	0.42
6:F:216:SER:HB3	6:F:219:GLU:HB2	2.02	0.42
9:I:36:SER:HB2	10:J:126:VAL:HG21	2.01	0.42
10:J:1:MET:HB2	10:J:1:MET:HE3	1.25	0.42
4:R:24:LYS:O	4:R:166:SER:HA	2.19	0.42
7:G:78:ILE:N	7:G:79:PRO:CD	2.81	0.42
14:b:176:VAL:HG12	14:b:178:LEU:HD13	2.01	0.42
4:D:24:LYS:O	4:D:166:SER:HA	2.20	0.42
10:J:172:MET:HE2	10:J:174:MET:CE	2.49	0.42
14:N:176:VAL:HG12	14:N:178:LEU:HD13	2.01	0.42
11:Y:211:ILE:HD13	11:Y:211:ILE:HG21	1.63	0.42
13:a:227:GLY:HA3	13:a:231:GLN:HB3	2.02	0.42
4:R:160:ASN:HB3	4:R:179:TRP:CZ2	2.55	0.42
2:B:124:HIS:HB3	3:C:124:VAL:HG12	2.02	0.42
9:W:14:MET:HB3	9:W:162:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:4:LEU:HD22	11:Y:4:LEU:O	2.19	0.42
13:M:150:MET:HE1	13:M:187:ARG:HG3	2.02	0.42
4:R:32:ILE:HD12	4:R:192:VAL:HG23	2.02	0.42
14:N:161:GLN:HE21	14:b:136:GLY:HA2	1.84	0.41
4:R:30:ILE:HD12	4:R:196:LEU:HG	2.01	0.41
12:Z:18:GLU:HA	12:Z:174:TYR:HE2	1.83	0.41
9:I:14:MET:HB3	9:I:162:LEU:HD11	2.02	0.41
10:J:149:ARG:HB2	10:J:152:MET:HG3	2.01	0.41
14:N:146:MET:HE1	14:N:154:PHE:HB2	2.02	0.41
14:N:171:GLY:HA2	13:a:219:TRP:CH2	2.55	0.41
3:Q:204:GLY:HA3	3:Q:207:ASN:HB2	2.01	0.41
12:Z:13:LEU:HD11	12:Z:150:LEU:HD21	2.01	0.41
14:b:146:MET:HE1	14:b:154:PHE:HB2	2.02	0.41
1:A:110:LEU:O	1:A:114:VAL:HG23	2.20	0.41
4:D:32:ILE:HD12	4:D:192:VAL:HG23	2.03	0.41
4:D:160:ASN:HB3	4:D:179:TRP:CZ2	2.55	0.41
7:U:78:ILE:N	7:U:79:PRO:CD	2.81	0.41
11:Y:41:LEU:HD23	11:Y:41:LEU:HA	1.88	0.41
12:Z:18:GLU:CB	12:Z:174:TYR:CD2	3.03	0.41
1:A:75:TYR:HB3	1:A:82:TYR:CD1	2.55	0.41
12:L:18:GLU:CB	12:L:174:TYR:CD2	3.03	0.41
9:W:7:ASN:HA	9:W:29:GLY:O	2.20	0.41
11:Y:45:MET:HE2	18:Y:303:A1IFL:C51	2.49	0.41
2:B:215:ILE:HG12	2:B:226:GLN:HG2	2.02	0.41
14:N:133:PHE:HA	14:b:132:THR:O	2.20	0.41
2:P:215:ILE:HG12	2:P:226:GLN:HG2	2.03	0.41
9:I:7:ASN:HA	9:I:29:GLY:O	2.20	0.41
9:I:171:LEU:HD12	9:I:171:LEU:HA	1.92	0.41
7:U:221:LYS:HA	7:U:221:LYS:HE3	2.02	0.41
9:W:94:LEU:HD11	9:W:106:PRO:HG2	2.01	0.41
1:A:68:THR:HB	1:A:69:PRO:HD2	2.03	0.41
7:G:103:MET:HE3	7:G:108:LEU:HB2	2.03	0.41
8:H:128:GLY:N	17:H:301:MES:H31	2.28	0.41
13:M:96:LEU:O	13:M:100:MET:HG2	2.21	0.41
13:M:227:GLY:HA3	13:M:231:GLN:HB3	2.02	0.41
1:O:110:LEU:O	1:O:114:VAL:HG23	2.20	0.41
5:E:70:GLY:HA3	5:E:221:PHE:CE2	2.56	0.41
7:G:221:LYS:HE3	7:G:221:LYS:HA	2.02	0.41
1:O:68:THR:HB	1:O:69:PRO:HD2	2.03	0.41
5:S:80:ALA:HB2	5:S:129:VAL:HG21	2.01	0.41
8:V:62:ASN:HB3	8:V:82:MET:HE1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:26:ASN:HA	13:a:39:VAL:O	2.21	0.41
13:a:150:MET:HE1	13:a:187:ARG:HG3	2.03	0.41
1:O:75:TYR:HB3	1:O:82:TYR:CD1	2.55	0.41
6:T:154:TRP:CZ3	7:U:60:VAL:HA	2.57	0.41
13:a:15:LYS:HB3	13:a:20:VAL:HG12	2.03	0.40
14:b:163:ILE:HG23	14:b:170:GLY:HA2	2.03	0.40
10:J:101:ASN:HB3	10:J:133:HIS:CE1	2.56	0.40
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	2.03	0.40
6:T:39:ASN:HD22	6:T:40:ASP:N	2.19	0.40
7:U:34:LEU:C	7:U:34:LEU:HD12	2.45	0.40
8:H:62:ASN:HB3	8:H:82:MET:HE1	2.03	0.40
10:J:169:GLU:O	10:X:177:LYS:NZ	2.54	0.40
12:L:100:LYS:O	12:L:104:PRO:HA	2.21	0.40
14:N:45:ARG:NH1	14:N:52:THR:OG1	2.55	0.40
7:U:187:GLU:HG2	7:U:192:LYS:HB2	2.03	0.40
18:Y:303:A1IFL:C57	18:Y:303:A1IFL:N4	2.82	0.40
2:B:14:PRO:HA	3:C:20:TYR:CD1	2.57	0.40
5:E:28:ILE:HD11	5:E:148:PRO:CD	2.51	0.40
7:G:115:LEU:HD12	7:G:115:LEU:HA	1.88	0.40
10:J:53:THR:HG23	10:J:54:VAL:HG23	2.04	0.40
11:K:39:PRO:HB2	11:K:40:PHE:CD2	2.56	0.40
11:K:158:LYS:HB2	11:K:177:LEU:HD11	2.04	0.40
2:B:149:THR:O	2:B:156:TYR:HA	2.22	0.40
7:G:187:GLU:HG2	7:G:192:LYS:HB2	2.04	0.40
5:S:70:GLY:HA3	5:S:221:PHE:CE2	2.56	0.40
11:Y:211:ILE:O	11:Y:211:ILE:CG2	2.69	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%)	240 (97%)	6 (2%)	2 (1%)	16	30
1	O	248/250 (99%)	241 (97%)	5 (2%)	2 (1%)	16	30
2	B	242/258 (94%)	232 (96%)	7 (3%)	3 (1%)	10	20
2	P	242/258 (94%)	232 (96%)	7 (3%)	3 (1%)	10	20
3	C	239/254 (94%)	227 (95%)	9 (4%)	3 (1%)	9	18
3	Q	239/254 (94%)	228 (95%)	8 (3%)	3 (1%)	9	18
4	D	240/260 (92%)	230 (96%)	8 (3%)	2 (1%)	16	30
4	R	240/260 (92%)	230 (96%)	8 (3%)	2 (1%)	16	30
5	E	231/234 (99%)	218 (94%)	11 (5%)	2 (1%)	14	28
5	S	231/234 (99%)	218 (94%)	11 (5%)	2 (1%)	14	28
6	F	242/288 (84%)	234 (97%)	8 (3%)	0	100	100
6	T	242/288 (84%)	234 (97%)	8 (3%)	0	100	100
7	G	241/252 (96%)	234 (97%)	6 (2%)	1 (0%)	30	50
7	U	241/252 (96%)	234 (97%)	6 (2%)	1 (0%)	30	50
8	H	219/231 (95%)	214 (98%)	5 (2%)	0	100	100
8	V	219/231 (95%)	214 (98%)	5 (2%)	0	100	100
9	I	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
9	W	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
10	J	196/198 (99%)	191 (97%)	5 (3%)	0	100	100
10	X	196/198 (99%)	191 (97%)	5 (3%)	0	100	100
11	K	209/211 (99%)	204 (98%)	5 (2%)	0	100	100
11	Y	209/211 (99%)	205 (98%)	4 (2%)	0	100	100
12	L	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
12	Z	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
13	M	231/246 (94%)	220 (95%)	11 (5%)	0	100	100
13	a	231/246 (94%)	221 (96%)	10 (4%)	0	100	100
14	N	194/196 (99%)	186 (96%)	8 (4%)	0	100	100
14	b	194/196 (99%)	185 (95%)	9 (5%)	0	100	100
All	All	6308/6610 (95%)	6081 (96%)	201 (3%)	26 (0%)	30	50

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	LYS
3	C	203	THR
5	E	201	ARG
1	O	166	LYS
3	Q	203	THR
5	S	201	ARG
2	B	51	VAL
2	B	221	ASP
4	D	121	GLY
5	E	227	GLU
2	P	51	VAL
2	P	221	ASP
4	R	121	GLY
5	S	227	GLU
3	C	52	LEU
4	D	122	GLU
3	Q	52	LEU
4	R	122	GLU
1	A	2	THR
3	C	183	PRO
7	G	242	GLN
1	O	2	THR
3	Q	183	PRO
7	U	242	GLN
2	B	218	GLY
2	P	218	GLY

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	70
1	O	209/209 (100%)	205 (98%)	4 (2%)	50	70
2	B	203/216 (94%)	197 (97%)	6 (3%)	36	60
2	P	203/216 (94%)	197 (97%)	6 (3%)	36	60
3	C	213/226 (94%)	206 (97%)	7 (3%)	33	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Q	213/226 (94%)	206 (97%)	7 (3%)	33	57
4	D	198/215 (92%)	191 (96%)	7 (4%)	32	56
4	R	198/215 (92%)	191 (96%)	7 (4%)	32	56
5	E	192/193 (100%)	186 (97%)	6 (3%)	35	59
5	S	192/193 (100%)	186 (97%)	6 (3%)	35	59
6	F	201/239 (84%)	192 (96%)	9 (4%)	24	46
6	T	201/239 (84%)	192 (96%)	9 (4%)	24	46
7	G	207/210 (99%)	200 (97%)	7 (3%)	32	57
7	U	207/210 (99%)	200 (97%)	7 (3%)	32	57
8	H	180/189 (95%)	174 (97%)	6 (3%)	33	57
8	V	180/189 (95%)	174 (97%)	6 (3%)	33	57
9	I	172/173 (99%)	169 (98%)	3 (2%)	53	71
9	W	172/173 (99%)	169 (98%)	3 (2%)	53	71
10	J	175/175 (100%)	166 (95%)	9 (5%)	21	40
10	X	175/175 (100%)	169 (97%)	6 (3%)	32	57
11	K	168/168 (100%)	156 (93%)	12 (7%)	13	25
11	Y	168/168 (100%)	156 (93%)	12 (7%)	13	25
12	L	185/185 (100%)	176 (95%)	9 (5%)	22	43
12	Z	185/185 (100%)	176 (95%)	9 (5%)	22	43
13	M	199/208 (96%)	190 (96%)	9 (4%)	24	46
13	a	199/208 (96%)	190 (96%)	9 (4%)	24	46
14	N	162/162 (100%)	160 (99%)	2 (1%)	63	78
14	b	162/162 (100%)	160 (99%)	2 (1%)	63	78
All	All	5328/5536 (96%)	5139 (96%)	189 (4%)	32	56

All (189) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	61	LEU
1	A	122	THR
1	A	157	PHE
2	B	38	MET
2	B	55	LEU

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Mol	Chain	Res	Type
2	B	60	THR
2	B	122	THR
2	B	149	THR
2	B	191	LEU
3	C	4	ARG
3	C	19	GLU
3	C	51	LYS
3	C	61	LYS
3	C	160	GLN
3	C	169	VAL
3	C	171	GLU
4	D	44	LYS
4	D	102	GLU
4	D	124	ARG
4	D	176	LEU
4	D	190	LEU
4	D	214	ILE
4	D	235	LEU
5	E	9	THR
5	E	29	LYS
5	E	188	LEU
5	E	198	GLN
5	E	227	GLU
5	E	231	LYS
6	F	31	THR
6	F	39	ASN
6	F	123	ASN
6	F	172	LEU
6	F	181	GLU
6	F	186	ARG
6	F	201	GLU
6	F	203	ASN
6	F	221	ASN
7	G	83	ASN
7	G	115	LEU
7	G	120	THR
7	G	201	MET
7	G	221	LYS
7	G	235	ARG
7	G	236	LEU
8	H	13	VAL
8	H	22	GLN

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Mol	Chain	Res	Type
8	H	34	LEU
8	H	38	SER
8	H	53	GLU
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
9	I	182	TRP
10	J	1	MET
10	J	7	ILE
10	J	25	ILE
10	J	26	SER
10	J	110	LYS
10	J	127	GLU
10	J	145	ASP
10	J	172	MET
10	J	174	MET
11	K	4	LEU
11	K	9	GLN
11	K	31	VAL
11	K	40	PHE
11	K	41	LEU
11	K	67	GLU
11	K	69	ARG
11	K	73	ARG
11	K	87	VAL
11	K	100	MET
11	K	106	ARG
11	K	107	LYS
12	L	23	LEU
12	L	49	ASN
12	L	106	TYR
12	L	109	THR
12	L	126	ASP
12	L	130	SER
12	L	150	LEU
12	L	172	LEU
12	L	173	LYS
13	M	48	ASN
13	M	69	ASP
13	M	70	LEU
13	M	104	ARG
13	M	146	PHE

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Mol	Chain	Res	Type
13	M	161	ARG
13	M	162	GLU
13	M	225	ILE
13	M	226	LYS
14	N	46	SER
14	N	119	VAL
1	O	30	GLN
1	O	61	LEU
1	O	122	THR
1	O	157	PHE
2	P	38	MET
2	P	55	LEU
2	P	60	THR
2	P	122	THR
2	P	149	THR
2	P	191	LEU
3	Q	4	ARG
3	Q	19	GLU
3	Q	51	LYS
3	Q	61	LYS
3	Q	160	GLN
3	Q	169	VAL
3	Q	171	GLU
4	R	44	LYS
4	R	102	GLU
4	R	124	ARG
4	R	176	LEU
4	R	190	LEU
4	R	214	ILE
4	R	235	LEU
5	S	9	THR
5	S	29	LYS
5	S	188	LEU
5	S	198	GLN
5	S	227	GLU
5	S	231	LYS
6	T	31	THR
6	T	39	ASN
6	T	123	ASN
6	T	172	LEU
6	T	181	GLU
6	T	186	ARG

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Mol	Chain	Res	Type
6	T	201	GLU
6	T	203	ASN
6	T	221	ASN
7	U	83	ASN
7	U	115	LEU
7	U	120	THR
7	U	201	MET
7	U	221	LYS
7	U	235	ARG
7	U	236	LEU
8	V	13	VAL
8	V	22	GLN
8	V	34	LEU
8	V	38	SER
8	V	53	GLU
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
9	W	182	TRP
10	X	1	MET
10	X	7	ILE
10	X	110	LYS
10	X	127	GLU
10	X	172	MET
10	X	174	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	31	VAL
11	Y	41	LEU
11	Y	67	GLU
11	Y	69	ARG
11	Y	71	LYS
11	Y	73	ARG
11	Y	87	VAL
11	Y	100	MET
11	Y	106	ARG
11	Y	107	LYS
12	Z	23	LEU
12	Z	49	ASN
12	Z	106	TYR
12	Z	109	THR
12	Z	126	ASP

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Mol	Chain	Res	Type
12	Z	130	SER
12	Z	150	LEU
12	Z	172	LEU
12	Z	173	LYS
13	a	48	ASN
13	a	69	ASP
13	a	70	LEU
13	a	104	ARG
13	a	146	PHE
13	a	161	ARG
13	a	162	GLU
13	a	225	ILE
13	a	226	LYS
14	b	46	SER
14	b	119	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (154) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	149	GLN
2	B	20	GLN
2	B	69	ASN
2	B	88	ASN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
3	C	17	GLN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
3	C	241	GLN
4	D	15	GLN
4	D	91	HIS
4	D	100	ASN
4	D	106	GLN
4	D	146	GLN
4	D	160	ASN
4	D	225	ASN

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Mol	Chain	Res	Type
5	E	59	GLN
5	E	68	HIS
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	147	GLN
5	E	151	ASN
5	E	184	ASN
5	E	198	GLN
6	F	19	GLN
6	F	39	ASN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
7	G	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	167	GLN
7	G	175	ASN
7	G	184	HIS
7	G	186	ASN
8	H	66	HIS
8	H	144	GLN
8	H	172	ASN
9	I	88	GLN
10	J	37	GLN
10	J	55	GLN
10	J	63	ASN
10	J	166	GLN
11	K	9	GLN
11	K	85	ASN
11	K	133	GLN
11	K	143	ASN
11	K	176	ASN
11	K	209	ASN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	80	ASN

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Mol	Chain	Res	Type
12	L	158	ASN
12	L	165	ASN
12	L	197	GLN
13	M	2	GLN
13	M	18	ASN
13	M	26	ASN
13	M	48	ASN
13	M	102	GLN
13	M	108	ASN
13	M	213	GLN
14	N	161	GLN
1	O	30	GLN
1	O	149	GLN
2	P	20	GLN
2	P	69	ASN
2	P	88	ASN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	155	ASN
2	P	176	GLN
2	P	220	ASN
3	Q	17	GLN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
3	Q	241	GLN
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
4	R	106	GLN
4	R	146	GLN
4	R	160	ASN
4	R	225	ASN
5	S	68	HIS
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	147	GLN
5	S	151	ASN

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Mol	Chain	Res	Type
5	S	184	ASN
5	S	198	GLN
6	T	19	GLN
6	T	39	ASN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	167	GLN
7	U	186	ASN
7	U	231	ASN
8	V	144	GLN
8	V	165	ASN
8	V	172	ASN
9	W	37	ASN
9	W	44	HIS
9	W	88	GLN
10	X	37	GLN
10	X	55	GLN
10	X	63	ASN
10	X	86	GLN
10	X	147	HIS
11	Y	9	GLN
11	Y	85	ASN
11	Y	143	ASN
11	Y	166	HIS
11	Y	176	ASN
11	Y	209	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	79	HIS
12	Z	80	ASN
12	Z	158	ASN
12	Z	165	ASN
12	Z	197	GLN
13	a	18	ASN
13	a	48	ASN

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Mol	Chain	Res	Type
13	a	102	GLN
13	a	108	ASN
13	a	213	GLN
14	b	69	GLN
14	b	161	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 14 are monoatomic - leaving 10 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	A1IFL	Y	303	11	49,54,54	1.63	7 (14%)	58,75,75	1.10	3 (5%)
19	SO4	K	303	-	4,4,4	0.58	0	6,6,6	0.09	0
19	SO4	Y	302	-	4,4,4	0.33	0	6,6,6	0.08	0
17	MES	X	202	-	12,12,12	0.75	0	15,16,16	0.33	0
19	SO4	V	302	-	4,4,4	0.49	0	6,6,6	0.12	0
18	A1IFL	V	303	8	49,54,54	1.18	3 (6%)	58,75,75	1.14	5 (8%)
18	A1IFL	H	302	8	49,54,54	1.15	2 (4%)	58,75,75	1.25	7 (12%)
17	MES	H	301	-	12,12,12	0.70	0	15,16,16	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	MES	K	302	-	12,12,12	0.73	0	15,16,16	0.45	0
18	A1IFL	K	304	11	49,54,54	1.86	9 (18%)	58,75,75	1.17	6 (10%)

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	A1IFL	Y	303	11	-	9/37/85/85	0/3/4/4
17	MES	X	202	-	-	2/6/14/14	0/1/1/1
18	A1IFL	V	303	8	-	6/37/85/85	0/3/4/4
18	A1IFL	H	302	8	-	13/37/85/85	0/3/4/4
17	MES	H	301	-	-	2/6/14/14	0/1/1/1
17	MES	K	302	-	-	4/6/14/14	0/1/1/1
18	A1IFL	K	304	11	-	12/37/85/85	0/3/4/4

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	K	304	A1IFL	CB-CG	-6.89	1.35	1.51
18	H	302	A1IFL	CB-CG	-6.21	1.36	1.51
18	Y	303	A1IFL	CB-CG	-6.14	1.36	1.51
18	V	303	A1IFL	CB-CG	-5.45	1.38	1.51
18	K	304	A1IFL	O58-C11	-5.12	1.37	1.44
18	Y	303	A1IFL	O58-C11	-4.63	1.38	1.44
18	V	303	A1IFL	OG1-CB1	-4.23	1.38	1.43
18	K	304	A1IFL	OG1-CB1	-3.62	1.39	1.43
18	Y	303	A1IFL	OG1-CB1	-3.47	1.39	1.43
18	K	304	A1IFL	OG1-C21	-3.41	1.37	1.43
18	H	302	A1IFL	OG1-CB1	-2.70	1.40	1.43
18	K	304	A1IFL	C54-C49	-2.66	1.44	1.52
18	Y	303	A1IFL	C48-C31	-2.56	1.50	1.52
18	Y	303	A1IFL	OG1-C21	-2.49	1.38	1.43
18	Y	303	A1IFL	C57-C11	-2.43	1.49	1.52
18	K	304	A1IFL	C53-C54	-2.39	1.47	1.53
18	K	304	A1IFL	C48-C31	-2.39	1.50	1.52
18	V	303	A1IFL	OG1-C21	-2.33	1.38	1.43
18	K	304	A1IFL	C21-C31	-2.16	1.50	1.54
18	Y	303	A1IFL	C54-C49	-2.16	1.46	1.52
18	K	304	A1IFL	CB-CA2	-2.11	1.49	1.54

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	H	302	A1IFL	CM-OH-CZ	-3.86	109.22	117.50
18	V	303	A1IFL	CB1-CA3-N2	-3.05	104.88	111.75
18	V	303	A1IFL	CE2-CD2-NB	3.04	114.74	110.12
18	H	302	A1IFL	CA-NB-CD2	-2.82	106.75	111.14
18	H	302	A1IFL	C3-CA1-N	-2.73	105.51	110.91
18	K	304	A1IFL	O55-C21-C11	2.72	112.63	106.08
18	K	304	A1IFL	CB1-CA3-N2	-2.60	105.91	111.75
18	K	304	A1IFL	C4-C3-CA1	-2.55	109.69	113.53
18	K	304	A1IFL	C53-C54-C49	-2.45	106.93	112.08
18	Y	303	A1IFL	CB1-CA3-N2	-2.43	106.28	111.75
18	K	304	A1IFL	CM-OH-CZ	-2.36	112.44	117.50
18	H	302	A1IFL	O55-C21-C11	2.32	111.66	106.08
18	Y	303	A1IFL	CM-OH-CZ	-2.24	112.70	117.50
18	V	303	A1IFL	CM-OH-CZ	-2.22	112.73	117.50
18	V	303	A1IFL	CA-NB-CD2	-2.22	107.69	111.14
18	V	303	A1IFL	C3-CA1-N	-2.19	106.58	110.91
18	Y	303	A1IFL	C7-C6-CZ	2.11	122.14	119.73
18	H	302	A1IFL	C53-C54-C49	-2.03	107.82	112.08
18	H	302	A1IFL	CD2-NB-CD1	-2.02	104.49	108.84
18	K	304	A1IFL	C3-CA1-N	-2.01	106.93	110.91
18	H	302	A1IFL	CG-CB-CA2	-2.00	108.03	113.36

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	K	302	MES	C7-C8-S-O1S
17	X	202	MES	C8-C7-N4-C3
18	H	302	A1IFL	CA1-C3-C4-O3
18	H	302	A1IFL	C21-C31-C48-C49
18	H	302	A1IFL	C31-C48-C49-C54
18	K	304	A1IFL	C21-C31-C48-C49
18	V	303	A1IFL	CA1-C3-C4-O3
18	V	303	A1IFL	C21-C31-C48-C49
18	V	303	A1IFL	C31-C48-C49-C54
18	Y	303	A1IFL	CA1-C3-C4-O3
18	Y	303	A1IFL	C21-C31-C48-C49
18	H	302	A1IFL	C6-CZ-OH-CM
18	H	302	A1IFL	N4-C31-C48-C49
18	Y	303	A1IFL	N4-C31-C48-C49
18	H	302	A1IFL	C5-CZ-OH-CM

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Mol	Chain	Res	Type	Atoms
18	K	304	A1IFL	N4-C31-C48-C49
18	V	303	A1IFL	N4-C31-C48-C49
17	K	302	MES	C7-C8-S-O3S
18	K	304	A1IFL	N1-CA2-CB-CG
18	Y	303	A1IFL	N1-CA2-CB-CG
18	K	304	A1IFL	C4-C3-CA1-N
18	H	302	A1IFL	N-C-CA-NB
18	H	302	A1IFL	C4-C3-CA1-C1
17	K	302	MES	C8-C7-N4-C3
18	H	302	A1IFL	C31-C48-C49-C50
18	V	303	A1IFL	C31-C48-C49-C50
18	Y	303	A1IFL	C31-C48-C49-C54
18	H	302	A1IFL	O-C-CA-NB
18	K	304	A1IFL	O2-C8-CA2-N1
17	K	302	MES	C7-C8-S-O2S
18	K	304	A1IFL	C4-C3-CA1-C1
18	K	304	A1IFL	N4-C8-CA2-N1
18	H	302	A1IFL	C4-C3-CA1-N
17	H	301	MES	C8-C7-N4-C5
18	K	304	A1IFL	C31-C48-C49-C54
18	Y	303	A1IFL	O1-C1-CA1-N
18	Y	303	A1IFL	N1-C1-CA1-N
18	K	304	A1IFL	C8-CA2-CB-CG
18	H	302	A1IFL	O2-C8-CA2-N1
17	X	202	MES	C7-C8-S-O1S
18	K	304	A1IFL	N-C-CA-NB
17	H	301	MES	C8-C7-N4-C3
18	H	302	A1IFL	N4-C8-CA2-N1
18	K	304	A1IFL	C31-C48-C49-C50
18	Y	303	A1IFL	C31-C48-C49-C50
18	K	304	A1IFL	C6-CZ-OH-CM
18	V	303	A1IFL	O1-C1-CA1-N
18	Y	303	A1IFL	C8-CA2-CB-CG

There are no ring outliers.

6 monomers are involved in 13 short contacts:

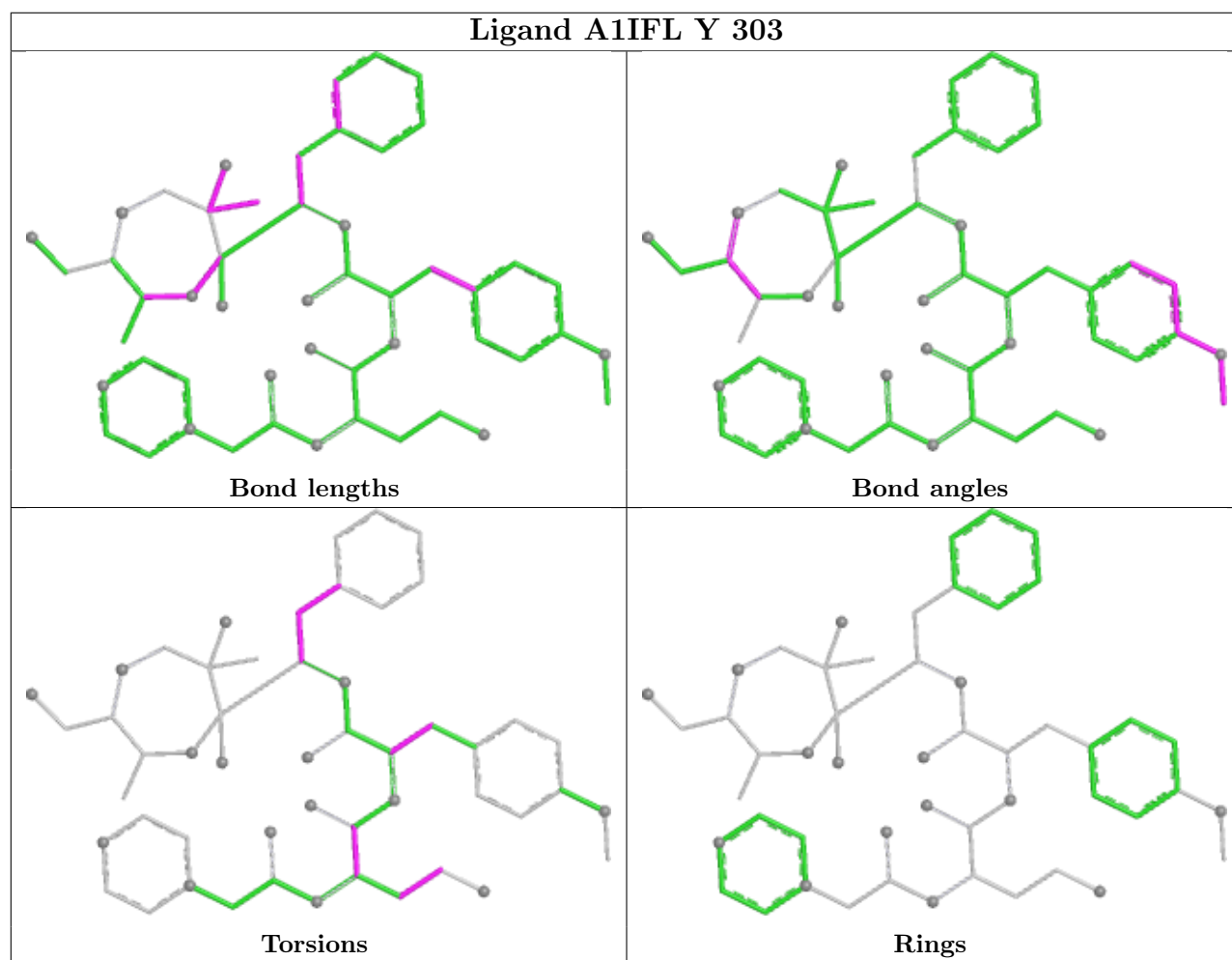
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	Y	303	A1IFL	4	0
19	V	302	SO4	2	0
18	V	303	A1IFL	4	0
18	H	302	A1IFL	1	0

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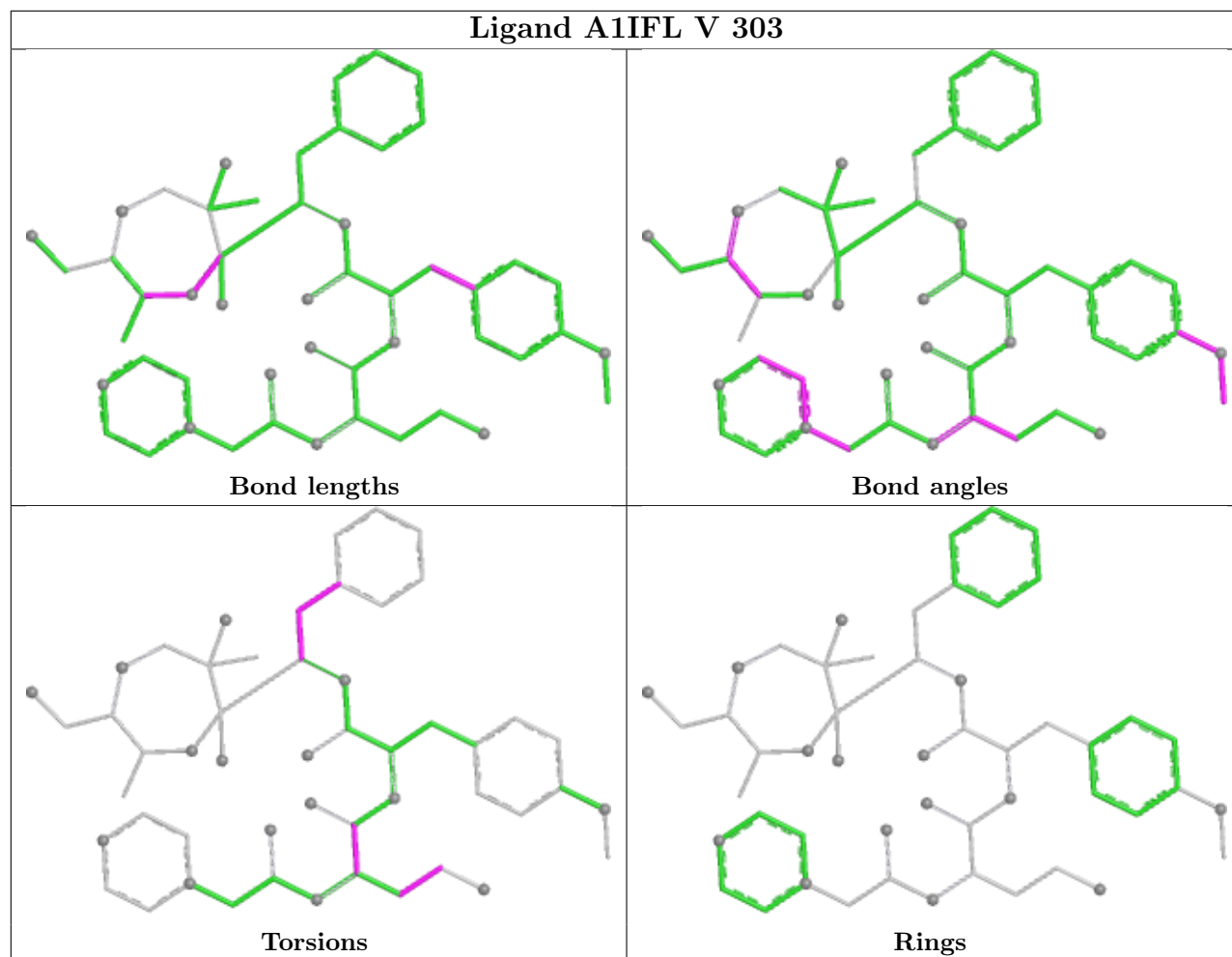
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	H	301	MES	2	0
18	K	304	A1IFL	2	0

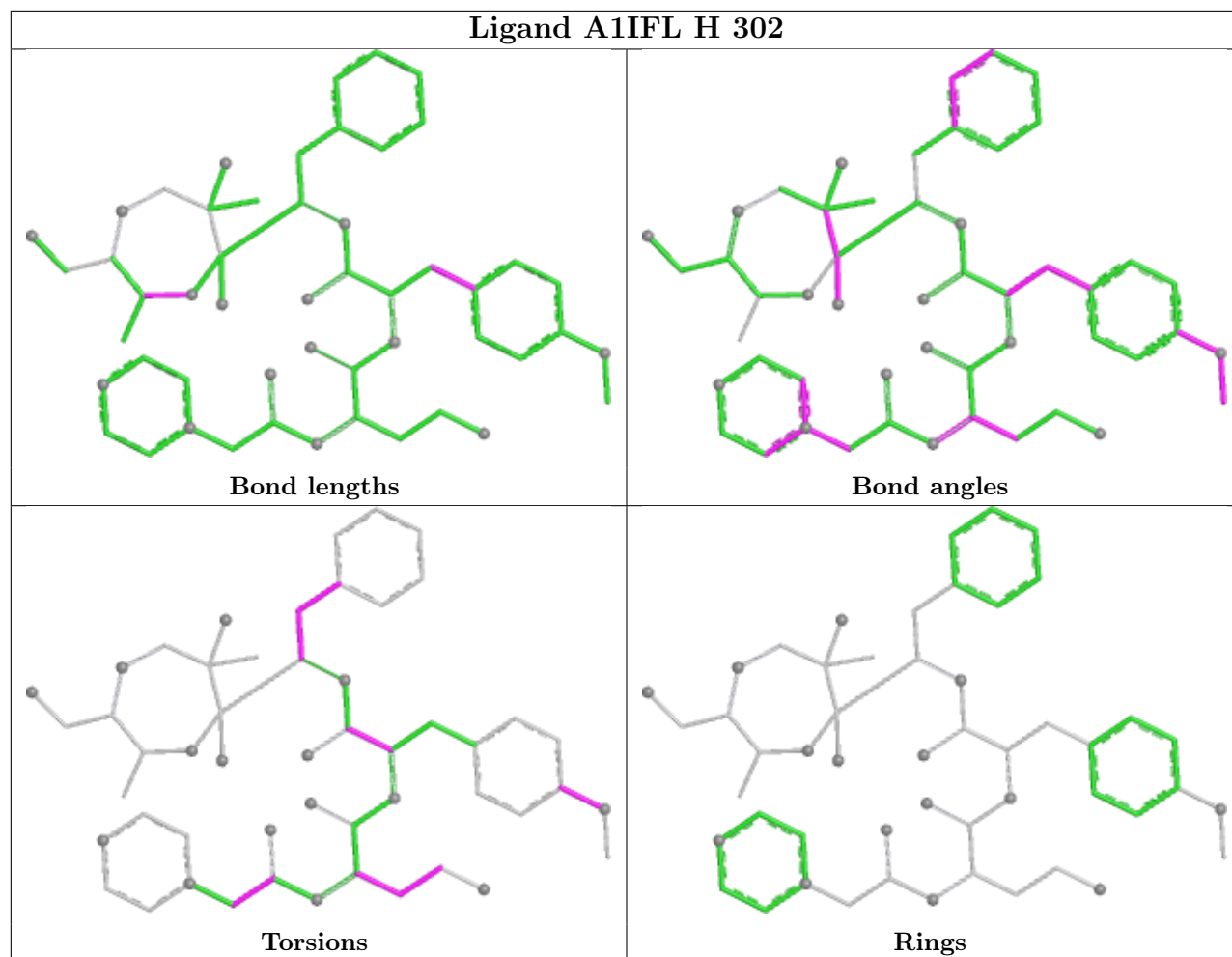
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

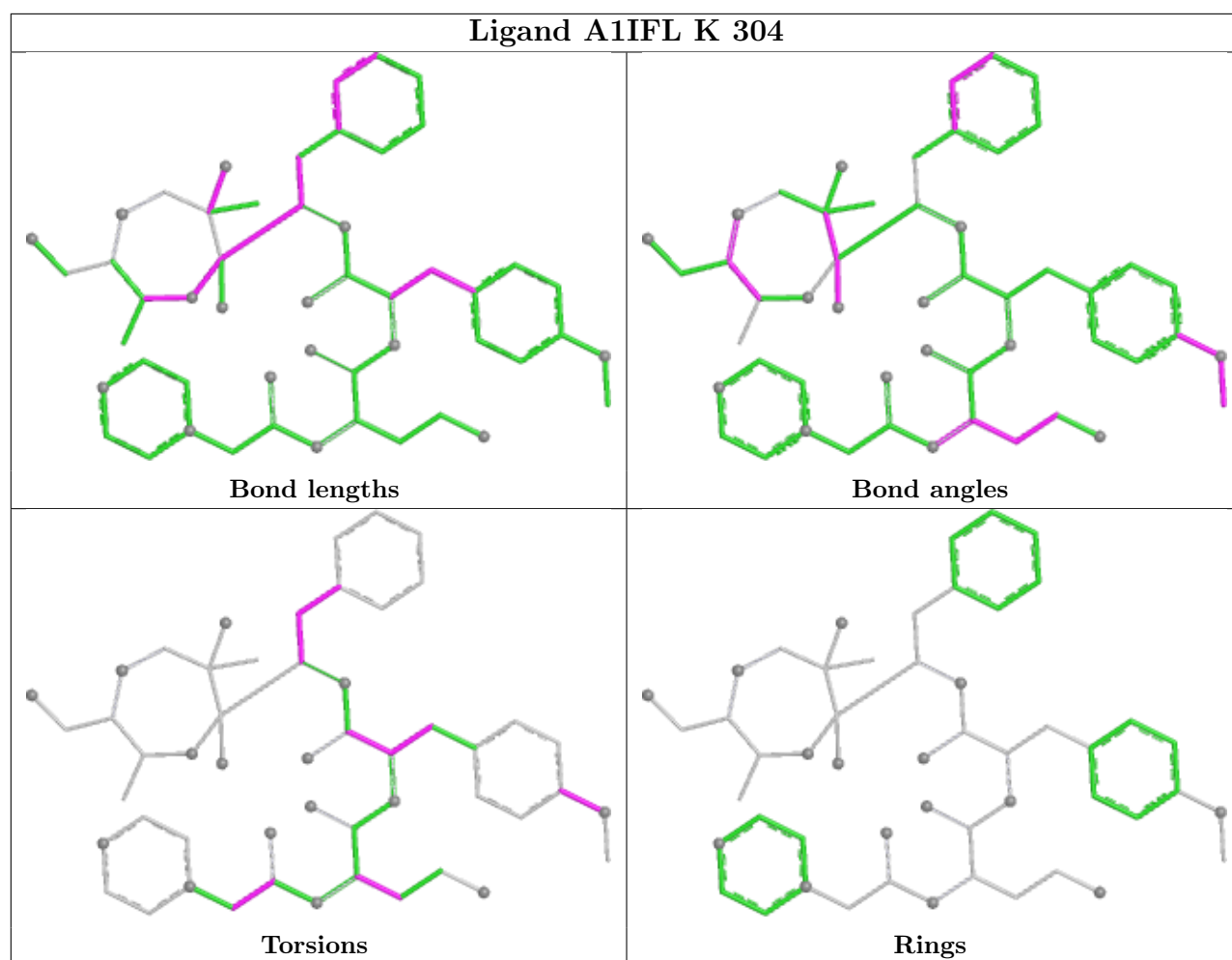


Ligand A1IFL V 303



Ligand A1IFL H 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%)	-0.21	1 (0%) 88 89	49, 65, 94, 137	0
1	O	250/250 (100%)	-0.13	3 (1%) 76 76	56, 73, 106, 145	0
2	B	244/258 (94%)	0.12	5 (2%) 65 63	53, 72, 114, 147	0
2	P	244/258 (94%)	0.03	7 (2%) 53 52	56, 73, 120, 153	0
3	C	241/254 (94%)	0.03	8 (3%) 49 47	53, 75, 131, 143	0
3	Q	241/254 (94%)	0.12	6 (2%) 58 56	57, 84, 146, 165	0
4	D	242/260 (93%)	0.07	8 (3%) 49 47	55, 76, 114, 153	0
4	R	242/260 (93%)	0.10	9 (3%) 45 42	58, 81, 121, 162	0
5	E	233/234 (99%)	0.09	3 (1%) 75 75	57, 77, 112, 140	0
5	S	233/234 (99%)	0.16	5 (2%) 63 61	57, 80, 114, 160	0
6	F	244/288 (84%)	-0.04	2 (0%) 82 82	52, 70, 106, 138	0
6	T	244/288 (84%)	-0.02	2 (0%) 82 82	55, 73, 112, 138	0
7	G	243/252 (96%)	-0.12	4 (1%) 70 69	50, 65, 96, 148	0
7	U	243/252 (96%)	-0.19	3 (1%) 76 76	53, 66, 93, 148	0
8	H	221/231 (95%)	-0.13	0 100 100	51, 62, 86, 141	0
8	V	221/231 (95%)	-0.12	1 (0%) 87 87	53, 66, 92, 136	0
9	I	204/205 (99%)	-0.26	0 100 100	48, 61, 84, 112	0
9	W	204/205 (99%)	-0.32	1 (0%) 87 87	46, 64, 85, 102	0
10	J	198/198 (100%)	-0.15	4 (2%) 65 63	48, 64, 90, 148	0
10	X	198/198 (100%)	-0.20	2 (1%) 79 79	51, 66, 90, 149	0
11	K	211/211 (100%)	-0.14	2 (0%) 81 81	48, 63, 90, 111	0
11	Y	211/211 (100%)	-0.12	3 (1%) 73 73	52, 63, 91, 109	0
12	L	222/222 (100%)	-0.21	0 100 100	48, 65, 88, 103	0
12	Z	222/222 (100%)	-0.18	0 100 100	50, 65, 92, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.23	3 (1%) 75 75	48, 63, 84, 110	0
13	a	233/246 (94%)	-0.23	2 (0%) 81 81	46, 62, 82, 111	0
14	N	196/196 (100%)	-0.26	0 100 100	47, 59, 88, 113	0
14	b	196/196 (100%)	-0.29	0 100 100	46, 59, 86, 108	0
All	All	6364/6610 (96%)	-0.09	84 (1%) 75 75	46, 68, 108, 165	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	50	LEU	5.9
4	D	119	ALA	5.8
4	R	125	LEU	5.0
3	C	50	LEU	4.6
3	Q	49	THR	4.5
10	J	1	MET	4.4
5	E	1	PHE	4.2
5	S	1	PHE	4.2
4	R	118	GLY	4.2
4	R	120	SER	4.1
3	C	49	THR	4.0
4	D	125	LEU	3.9
7	G	1	ALA	3.9
4	R	113	LEU	3.7
10	X	1	MET	3.7
2	B	244	THR	3.6
4	D	118	GLY	3.6
4	R	124	ARG	3.6
7	U	1	ALA	3.5
4	R	119	ALA	3.4
10	J	197	ALA	3.3
13	M	1	THR	3.3
4	D	124	ARG	3.1
4	D	120	SER	3.1
11	K	104	TYR	3.0
7	U	243	ASP	3.0
2	P	1	GLY	3.0
7	G	239	ILE	2.9
5	S	207	VAL	2.9
1	A	1	MET	2.8
7	G	2	GLY	2.8
2	B	51	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
2	P	51	VAL	2.8
3	C	51	LYS	2.8
2	P	60	THR	2.8
13	M	233	ILE	2.7
2	B	243	ILE	2.7
11	K	32	LYS	2.7
6	T	244	ASN	2.6
2	B	219	ALA	2.6
11	Y	104	TYR	2.6
3	Q	51	LYS	2.6
6	F	1	GLY	2.6
3	C	205	ALA	2.6
1	O	4	ARG	2.5
3	C	52	LEU	2.4
4	R	11	GLY	2.4
13	M	232	LYS	2.4
7	U	2	GLY	2.4
1	O	249	ALA	2.4
4	D	242	GLU	2.3
5	S	204	SER	2.3
6	T	1	GLY	2.3
2	P	222	GLY	2.3
3	Q	205	ALA	2.3
8	V	220	ILE	2.3
3	C	206	LYS	2.3
4	R	1	ASP	2.3
1	O	1	MET	2.2
7	G	171	THR	2.2
3	C	48	SER	2.2
13	a	1	THR	2.2
2	P	218	GLY	2.2
2	P	219	ALA	2.2
6	F	202	ASP	2.2
10	J	198	GLN	2.1
5	E	202	ASP	2.1
4	R	112	ALA	2.1
11	Y	211	ILE	2.1
9	W	1	SER	2.1
2	B	1	GLY	2.1
4	D	3	GLY	2.1
5	E	16	GLY	2.1
3	Q	203	THR	2.1

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Mol	Chain	Res	Type	RSRZ
13	a	38	GLY	2.1
5	S	202	ASP	2.0
10	J	145	ASP	2.0
4	D	241	ALA	2.0
3	Q	61	LYS	2.0
2	P	244	THR	2.0
5	S	196	ILE	2.0
11	Y	182	GLU	2.0
3	C	238	LYS	2.0
10	X	197	ALA	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
15	MG	Z	301	1/1	0.61	0.26	98,98,98,98	0
17	MES	H	301	12/12	0.88	0.24	60,64,68,68	12
18	A1IFL	H	302	51/51	0.90	0.15	50,65,74,76	51
18	A1IFL	V	303	51/51	0.90	0.15	55,66,83,84	51
15	MG	G	301	1/1	0.91	0.08	75,75,75,75	0
15	MG	K	301	1/1	0.92	0.13	89,89,89,89	0
16	CL	N	203	1/1	0.93	0.12	95,95,95,95	0
18	A1IFL	Y	303	51/51	0.93	0.10	46,56,72,72	0
18	A1IFL	K	304	51/51	0.94	0.09	48,52,76,76	0
15	MG	V	301	1/1	0.94	0.13	112,112,112,112	0
15	MG	W	301	1/1	0.94	0.12	78,78,78,78	0
19	SO4	V	302	5/5	0.94	0.12	78,83,88,88	5
19	SO4	K	303	5/5	0.95	0.16	100,107,110,110	0

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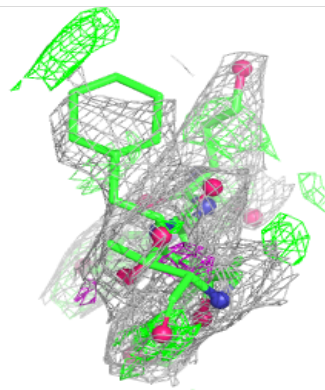
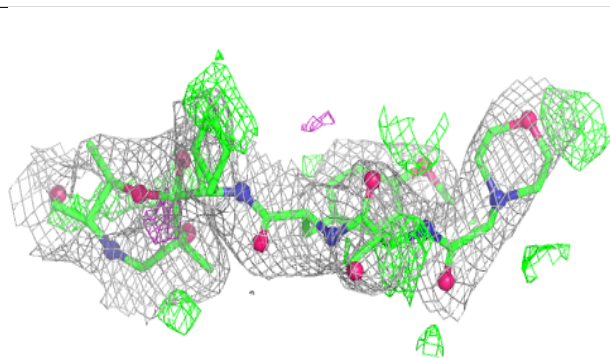
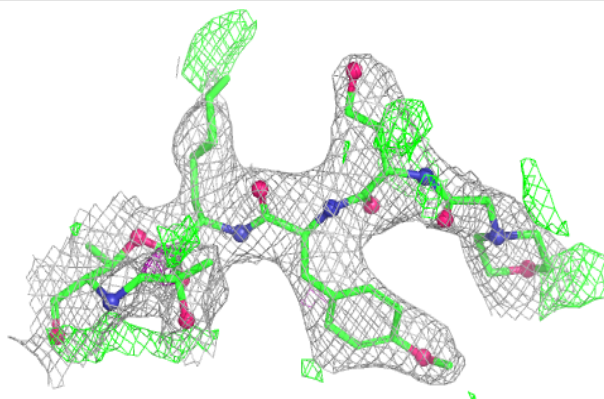
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
17	MES	K	302	12/12	0.95	0.11	75,82,86,88	0
15	MG	N	201	1/1	0.96	0.09	74,74,74,74	0
15	MG	Y	301	1/1	0.96	0.06	84,84,84,84	0
17	MES	X	202	12/12	0.96	0.11	69,78,84,86	0
15	MG	I	301	1/1	0.97	0.06	75,75,75,75	0
16	CL	G	302	1/1	0.98	0.03	59,59,59,59	0
16	CL	U	301	1/1	0.98	0.05	66,66,66,66	0
16	CL	b	201	1/1	0.98	0.05	70,70,70,70	0
19	SO4	Y	302	5/5	0.98	0.10	70,72,73,76	5
16	CL	N	202	1/1	0.99	0.06	70,70,70,70	0
15	MG	X	201	1/1	0.99	0.14	52,52,52,52	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.

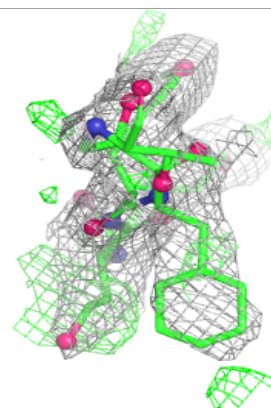
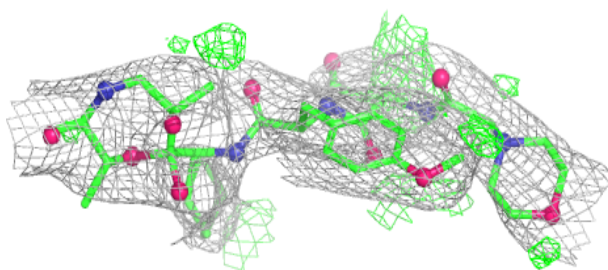
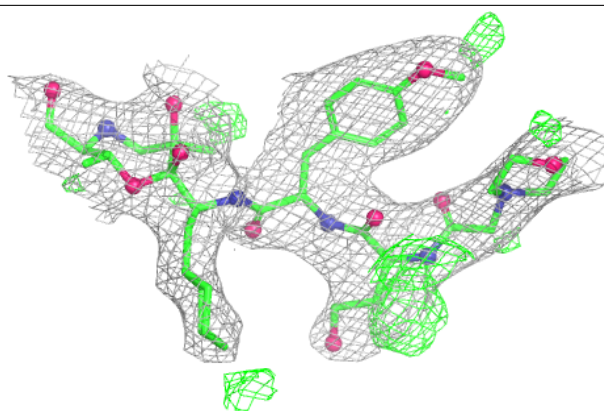
Electron density around A1IFL H 302:

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

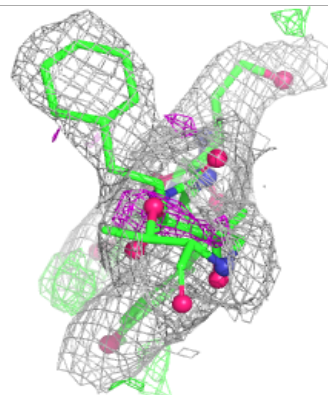
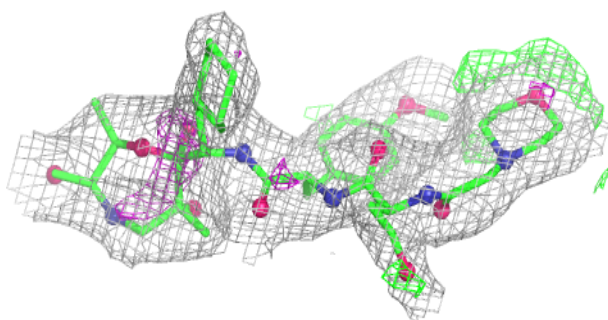
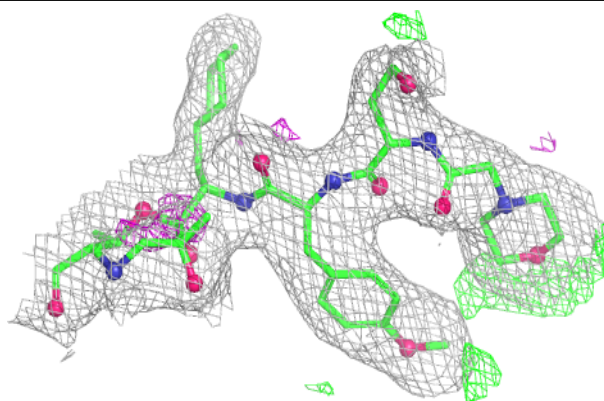


Electron density around A1IFL V 303:

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

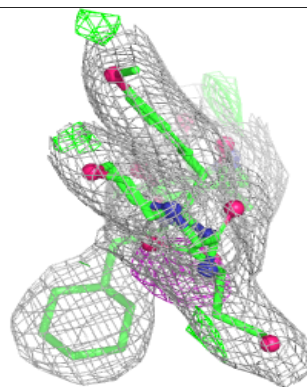
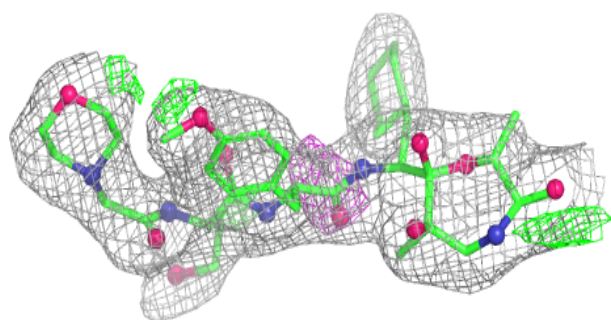
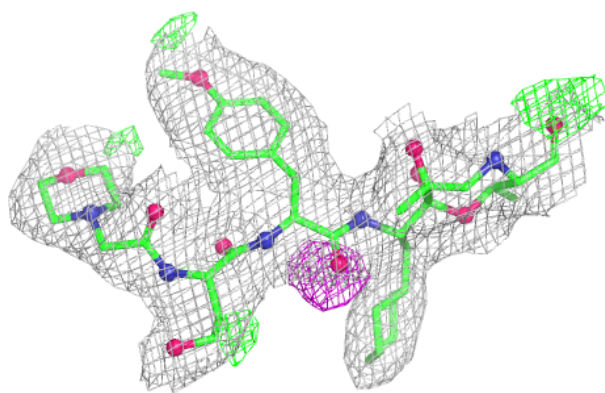
**Electron density around A1IFL Y 303:**

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



Electron density around A1IFL K 304:

$2mF_o - DF_c$ (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.