Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 06:17 pm BST

PDB ID	:	6OCZ
Title	:	Crystal Structure of Mycobacterium tuberculosis Proteasome in Complex with Phenylimidazole-based Inhibitor A86
Authors	:	Hsu, H.C.; Li, H.
Deposited on	:	2019-03-25
Resolution	:	2.65 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 following versions of software and data (see references ⓘ) were used in the production of this report:

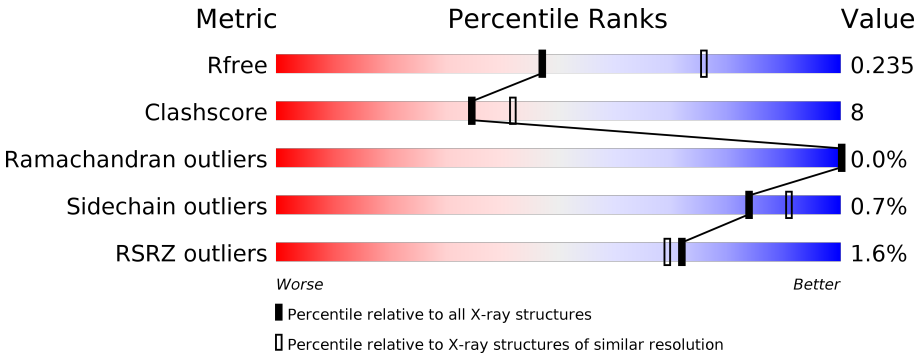
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.65 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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

Mol	Chain	Length	Quality of chain
1	A	240	% 68% 23% 9%
1	B	240	5% 68% 21% 10%
1	C	240	5% 65% 25% 10%
1	D	240	3% 69% 20% 10%
1	E	240	3% 66% 24% 10%
1	F	240	4% 69% 21% 10%

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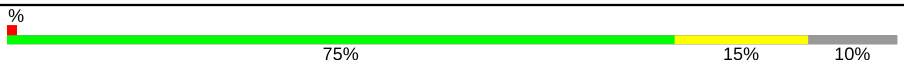
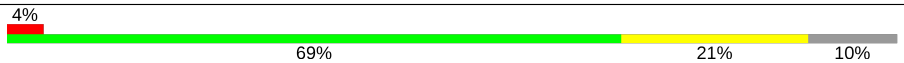
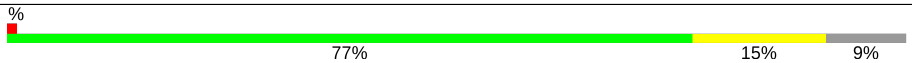
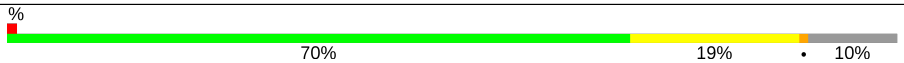
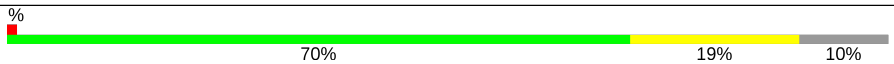
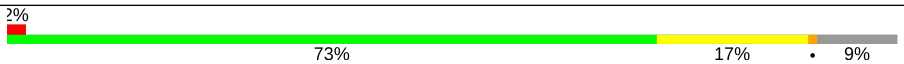
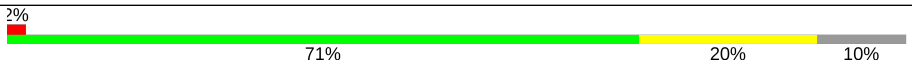
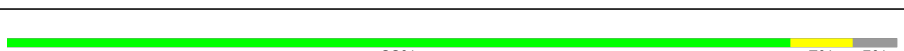
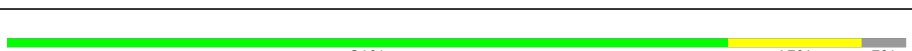
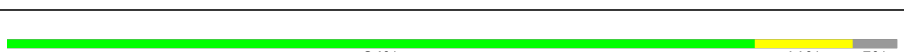
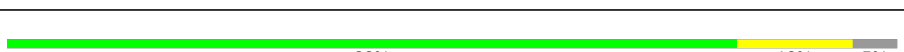
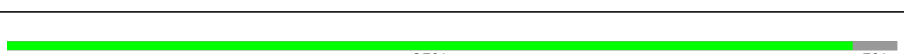
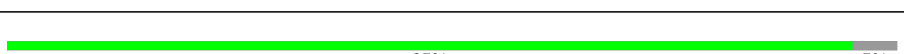
Mol	Chain	Length	Quality of chain
1	G	240	
1	O	240	
1	P	240	
1	Q	240	
1	R	240	
1	S	240	
1	T	240	
1	U	240	
2	H	234	
2	I	234	
2	J	234	
2	K	234	
2	L	234	
2	M	234	
2	N	234	
2	V	234	
2	W	234	
2	X	234	
2	Y	234	
2	Z	234	
2	a	234	
2	b	234	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 48235 atoms, of which 210 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1677	1050	306	317	4			
1	B	215	Total	C	N	O	S	0	0	0
			1660	1041	303	312	4			
1	C	217	Total	C	N	O	S	0	0	0
			1672	1047	305	316	4			
1	D	215	Total	C	N	O	S	0	0	0
			1655	1035	303	313	4			
1	E	217	Total	C	N	O	S	0	0	0
			1670	1046	305	315	4			
1	F	216	Total	C	N	O	S	0	0	0
			1663	1041	304	314	4			
1	G	216	Total	C	N	O	S	0	0	0
			1661	1039	304	314	4			
1	O	217	Total	C	N	O	S	0	0	0
			1670	1045	305	316	4			
1	P	219	Total	C	N	O	S	0	0	0
			1685	1054	307	320	4			
1	Q	216	Total	C	N	O	S	0	0	0
			1668	1045	304	315	4			
1	R	215	Total	C	N	O	S	0	0	0
			1657	1038	303	312	4			
1	S	218	Total	C	N	O	S	0	0	0
			1678	1050	306	318	4			
1	T	217	Total	C	N	O	S	0	0	0
			1671	1047	305	315	4			
1	U	216	Total	C	N	O	S	0	0	0
			1664	1043	304	313	4			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	MET	-	initiating methionine	UNP P9WHU1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	9	MET	-	initiating methionine	UNP P9WHU1
C	9	MET	-	initiating methionine	UNP P9WHU1
D	9	MET	-	initiating methionine	UNP P9WHU1
E	9	MET	-	initiating methionine	UNP P9WHU1
F	9	MET	-	initiating methionine	UNP P9WHU1
G	9	MET	-	initiating methionine	UNP P9WHU1
O	9	MET	-	initiating methionine	UNP P9WHU1
P	9	MET	-	initiating methionine	UNP P9WHU1
Q	9	MET	-	initiating methionine	UNP P9WHU1
R	9	MET	-	initiating methionine	UNP P9WHU1
S	9	MET	-	initiating methionine	UNP P9WHU1
T	9	MET	-	initiating methionine	UNP P9WHU1
U	9	MET	-	initiating methionine	UNP P9WHU1

- Molecule 2 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	I	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	J	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	K	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			
2	L	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			
2	M	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	N	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			
2	V	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			
2	W	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			
2	X	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	Y	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			
2	Z	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	a	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			

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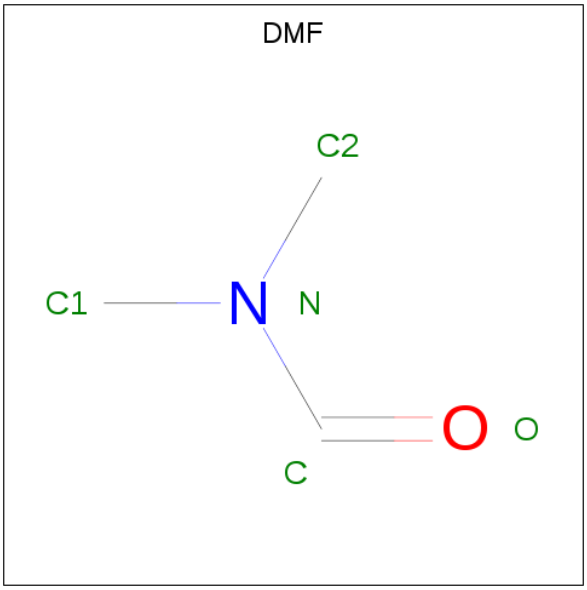
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	b	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			

- Molecule 3 is DIMETHYLFORMAMIDE (three-letter code: DMF) (formula: C_3H_7NO).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			12	3	7	1	1		
3	B	1	Total	C	H	N	O	0	0
			12	3	7	1	1		
3	C	1	Total	C	H	N	O	0	0
			12	3	7	1	1		
3	E	1	Total	C	H	N	O	0	0
			12	3	7	1	1		
3	F	1	Total	C	H	N	O	0	0
			12	3	7	1	1		
3	F	1	Total	C	H	N	O	0	0
			12	3	7	1	1		
3	G	1	Total	C	H	N	O	0	0
			12	3	7	1	1		
3	G	1	Total	C	H	N	O	0	0
			12	3	7	1	1		
3	I	1	Total	C	H	N	O	0	0
			12	3	7	1	1		
3	J	1	Total	C	H	N	O	0	0
			12	3	7	1	1		

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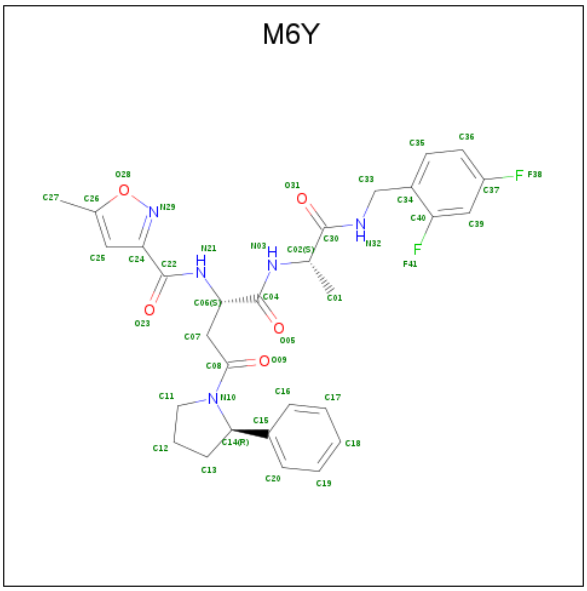
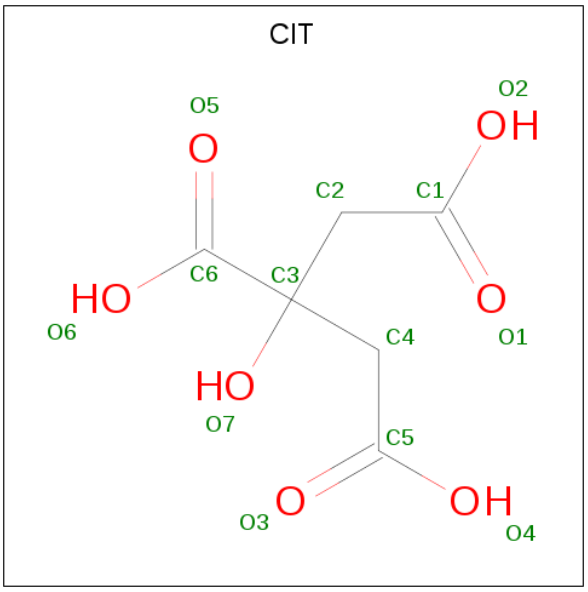
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	J	1	Total	C	H	N	O	0	0
			12	3	7	1	1		
3	O	1	Total	C	H	N	O	0	0
			12	3	7	1	1		
3	P	1	Total	C	H	N	O	0	0
			12	3	7	1	1		
3	Q	1	Total	C	H	N	O	0	0
			12	3	7	1	1		
3	R	1	Total	C	H	N	O	0	0
			12	3	7	1	1		
3	R	1	Total	C	H	N	O	0	0
			12	3	7	1	1		
3	S	1	Total	C	H	N	O	0	0
			12	3	7	1	1		
3	S	1	Total	C	H	N	O	0	0
			12	3	7	1	1		
3	T	1	Total	C	H	N	O	0	0
			12	3	7	1	1		
3	U	1	Total	C	H	N	O	0	0
			12	3	7	1	1		

- Molecule 4 is N-{(2S)-1-({(2S)-1-[(2,4-difluorobenzyl)amino]-1-oxopropan-2-yl}amino)-1,4-dioxo-4-[(2R)-2-phenylpyrrolidin-1-yl]butan-2-yl}-5-methyl-1,2-oxazole-3-carboxamide (non-preferred name) (three-letter code: M6Y) (formula: $C_{29}H_{31}F_2N_5O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	H	1	Total	C	F	N	O	0	0
			41	29	2	5	5		
4	I	1	Total	C	F	N	O	0	0
			41	29	2	5	5		
4	J	1	Total	C	F	N	O	0	0
			41	29	2	5	5		
4	K	1	Total	C	F	N	O	0	0
			41	29	2	5	5		
4	L	1	Total	C	F	N	O	0	0
			41	29	2	5	5		
4	M	1	Total	C	F	N	O	0	0
			41	29	2	5	5		
4	N	1	Total	C	F	N	O	0	0
			41	29	2	5	5		
4	V	1	Total	C	F	N	O	0	0
			41	29	2	5	5		
4	W	1	Total	C	F	N	O	0	0
			41	29	2	5	5		
4	X	1	Total	C	F	N	O	0	0
			41	29	2	5	5		
4	Y	1	Total	C	F	N	O	0	0
			41	29	2	5	5		
4	Z	1	Total	C	F	N	O	0	0
			41	29	2	5	5		
4	a	1	Total	C	F	N	O	0	0
			41	29	2	5	5		
4	b	1	Total	C	F	N	O	0	0
			41	29	2	5	5		

- Molecule 5 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	1	Total C H O 18 6 5 7	0	0
5	I	1	Total C H O 18 6 5 7	0	0
5	J	1	Total C H O 18 6 5 7	0	0
5	K	1	Total C H O 18 6 5 7	0	0
5	L	1	Total C H O 18 6 5 7	0	0
5	M	1	Total C H O 18 6 5 7	0	0
5	N	1	Total C H O 18 6 5 7	0	0
5	V	1	Total C H O 18 6 5 7	0	0
5	W	1	Total C H O 18 6 5 7	0	0
5	X	1	Total C H O 18 6 5 7	0	0
5	Y	1	Total C H O 18 6 5 7	0	0
5	Z	1	Total C H O 18 6 5 7	0	0
5	a	1	Total C H O 18 6 5 7	0	0
5	b	1	Total C H O 18 6 5 7	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	27	Total O 27 27	0	0
6	B	20	Total O 20 20	0	0
6	C	29	Total O 29 29	0	0
6	D	20	Total O 20 20	0	0
6	E	24	Total O 24 24	0	0
6	F	16	Total O 16 16	0	0
6	G	21	Total O 21 21	0	0
6	H	36	Total O 36 36	0	0
6	I	49	Total O 49 49	0	0
6	J	36	Total O 36 36	0	0
6	K	41	Total O 41 41	0	0
6	L	42	Total O 42 42	0	0
6	M	35	Total O 35 35	0	0
6	N	34	Total O 34 34	0	0
6	O	17	Total O 17 17	0	0
6	P	26	Total O 26 26	0	0
6	Q	31	Total O 31 31	0	0
6	R	28	Total O 28 28	0	0
6	S	28	Total O 28 28	0	0
6	T	13	Total O 13 13	0	0
6	U	27	Total O 27 27	0	0

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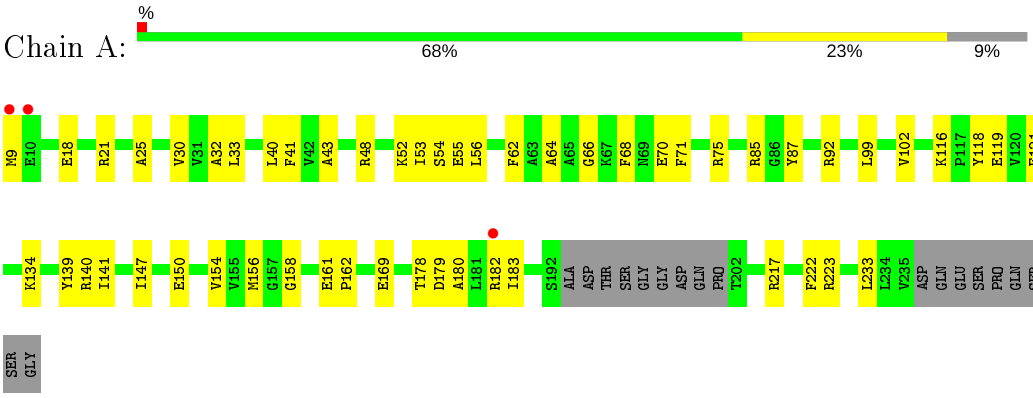
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	V	42	Total O 42 42	0	0
6	W	39	Total O 39 39	0	0
6	X	35	Total O 35 35	0	0
6	Y	40	Total O 40 40	0	0
6	Z	37	Total O 37 37	0	0
6	a	29	Total O 29 29	0	0
6	b	32	Total O 32 32	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

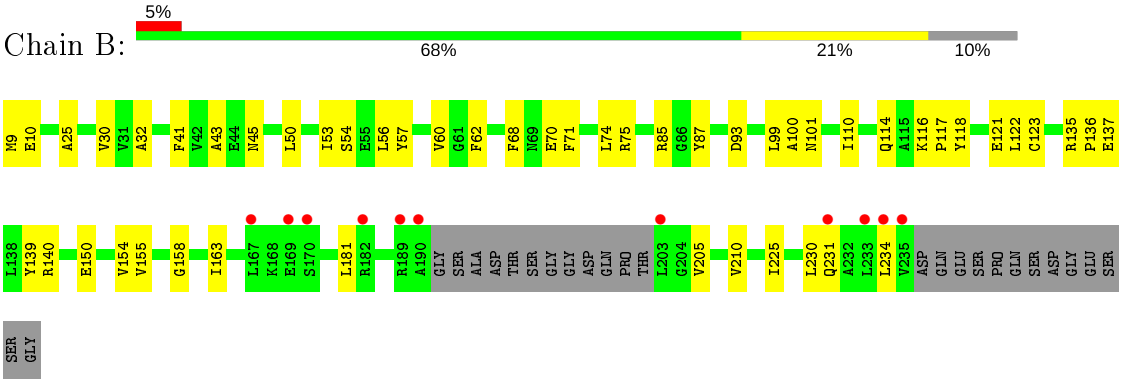
- Molecule 1: Proteasome subunit alpha

Chain A:



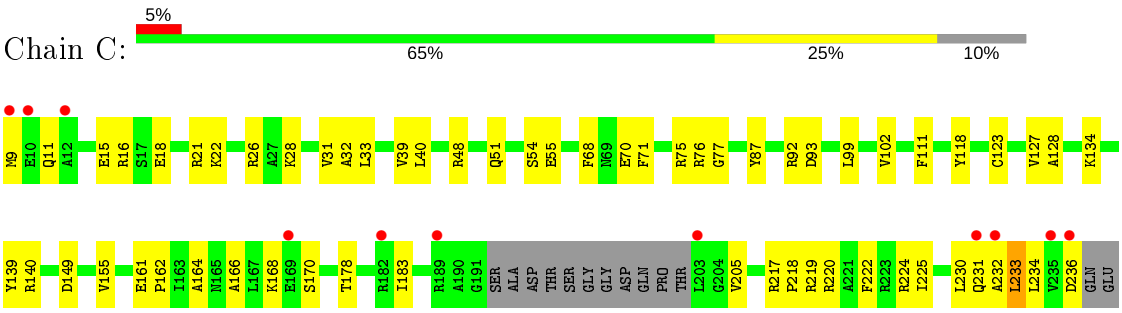
- Molecule 1: Proteasome subunit alpha

Chain B:



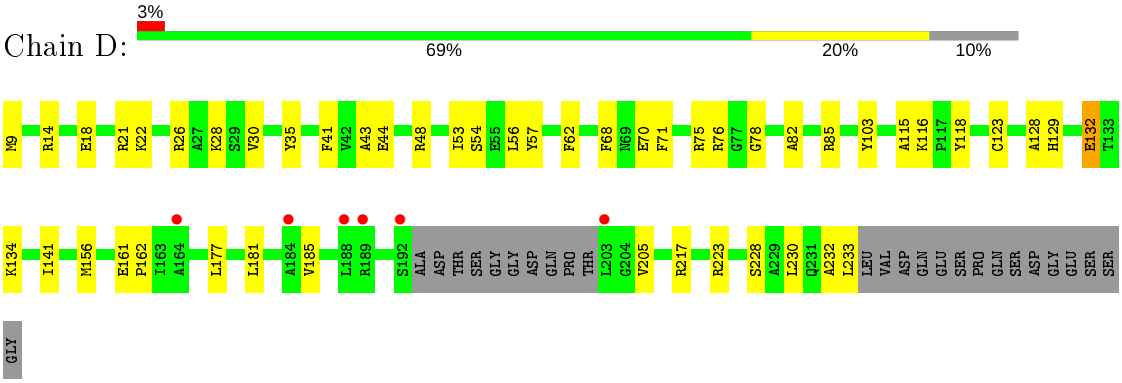
- Molecule 1: Proteasome subunit alpha

Chain C:



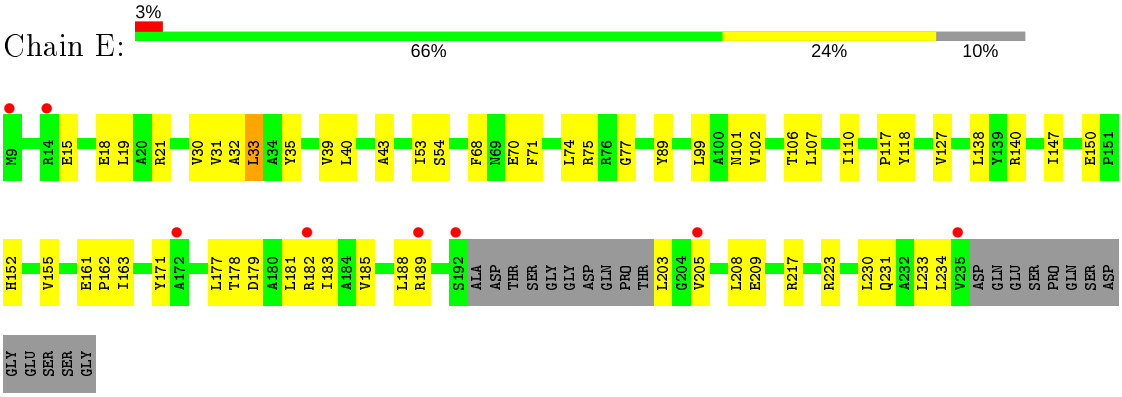
- Molecule 1: Proteasome subunit alpha

Chain D:



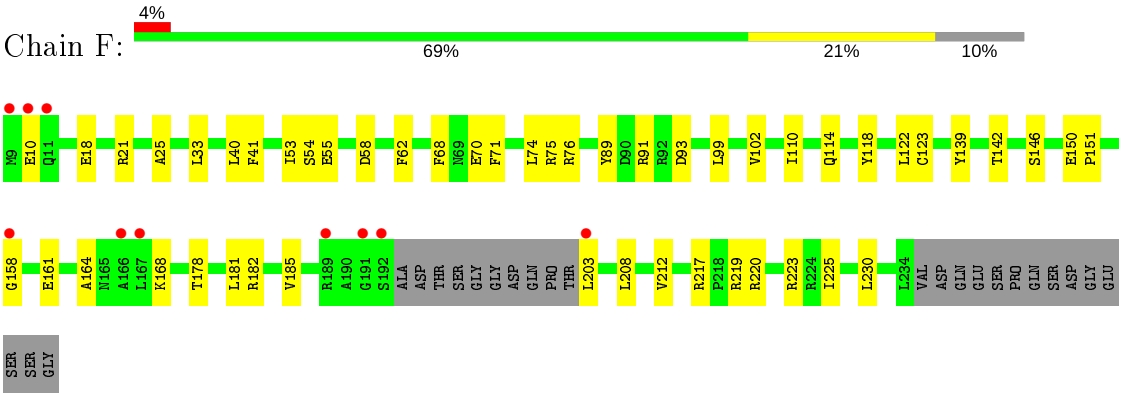
- Molecule 1: Proteasome subunit alpha

Chain E:



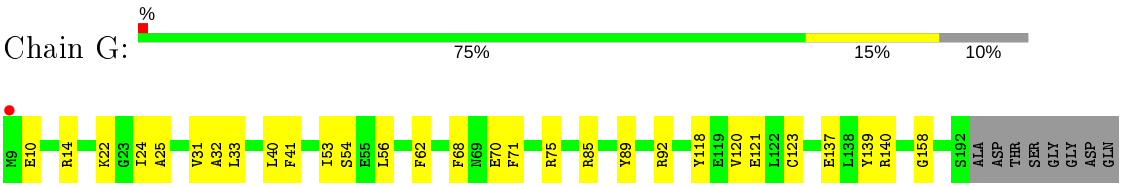
- Molecule 1: Proteasome subunit alpha

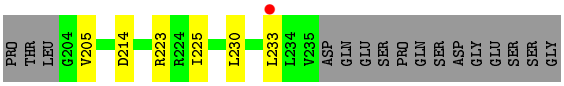
Chain F:



- Molecule 1: Proteasome subunit alpha

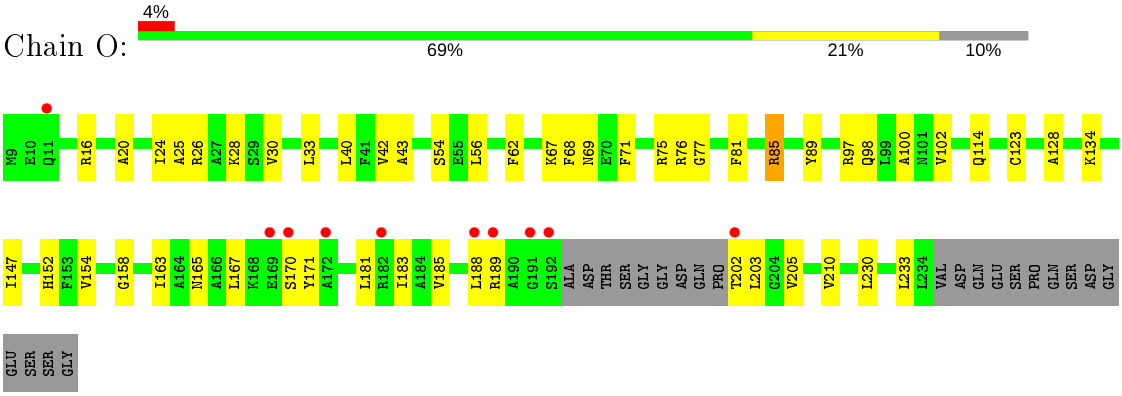
Chain G:





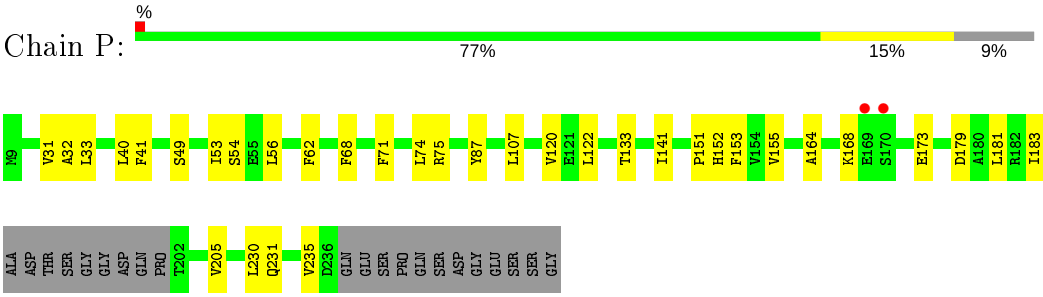
- Molecule 1: Proteasome subunit alpha

Chain O:



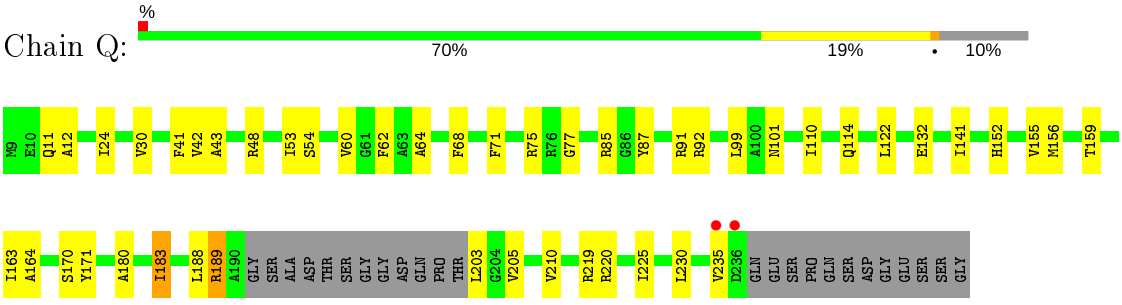
- Molecule 1: Proteasome subunit alpha

Chain P:



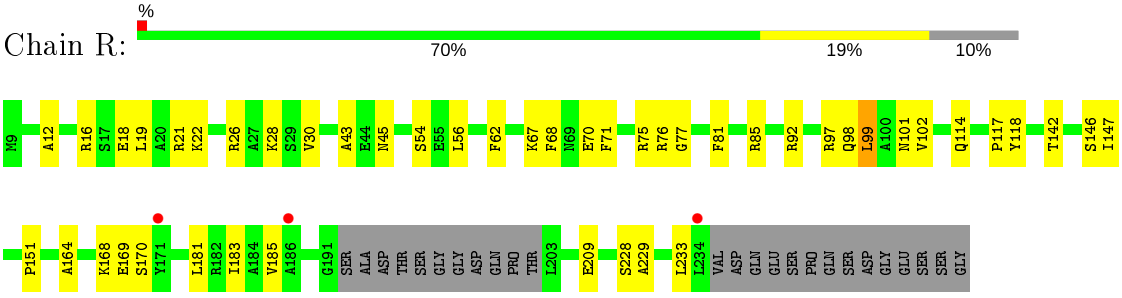
- Molecule 1: Proteasome subunit alpha

Chain Q:



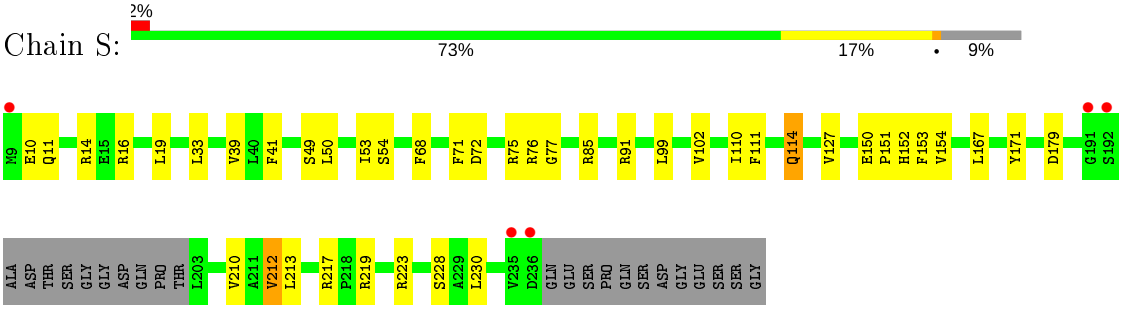
- Molecule 1: Proteasome subunit alpha

Chain R:



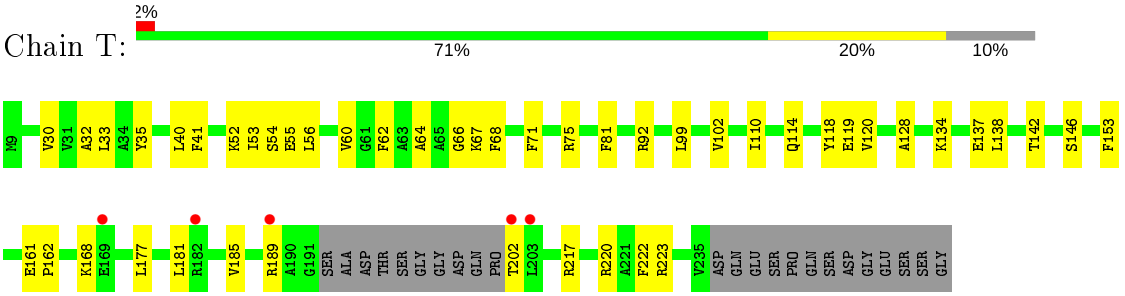
- Molecule 1: Proteasome subunit alpha

Chain S:



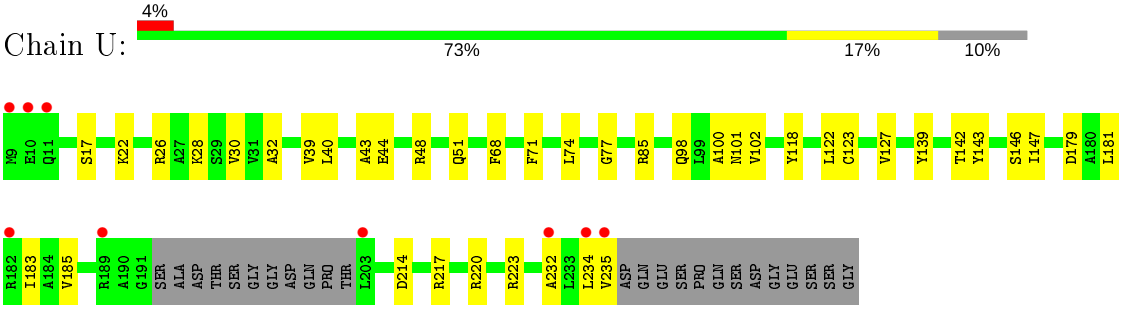
• Molecule 1: Proteasome subunit alpha

Chain T:



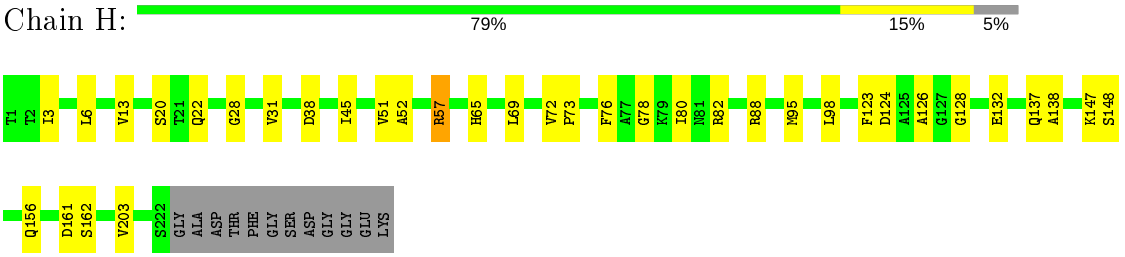
• Molecule 1: Proteasome subunit alpha

Chain U:



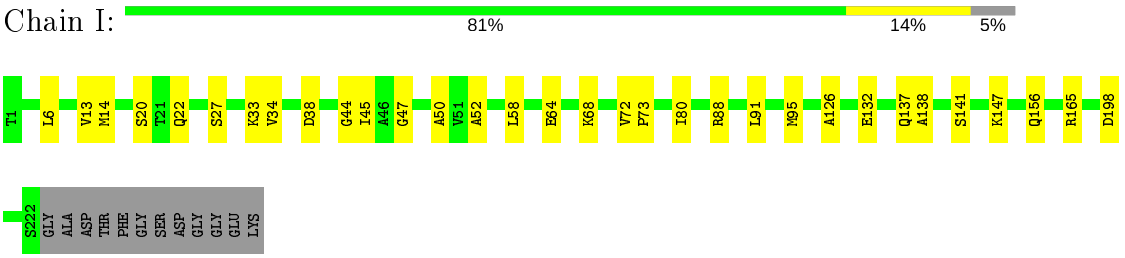
• Molecule 2: Proteasome subunit beta

Chain H:



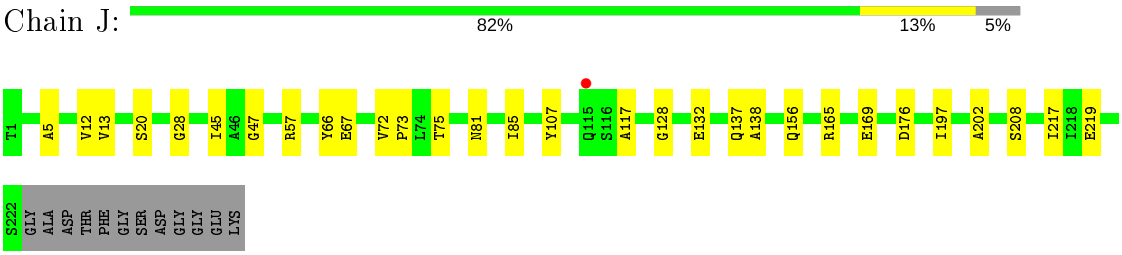
• Molecule 2: Proteasome subunit beta

Chain I:



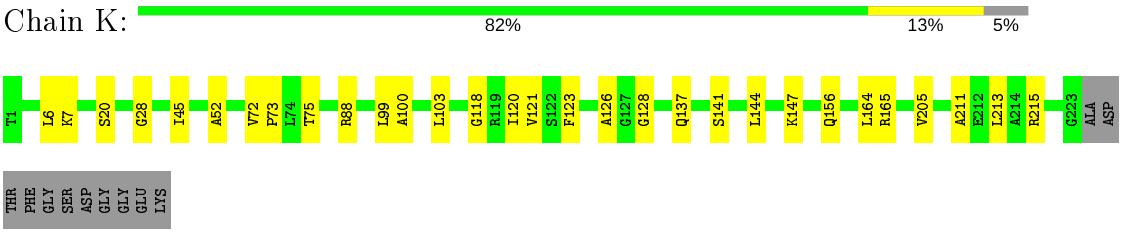
- Molecule 2: Proteasome subunit beta

Chain J:



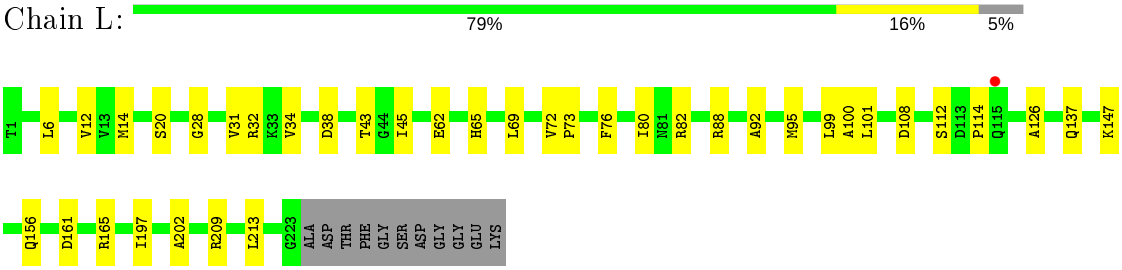
- Molecule 2: Proteasome subunit beta

Chain K:



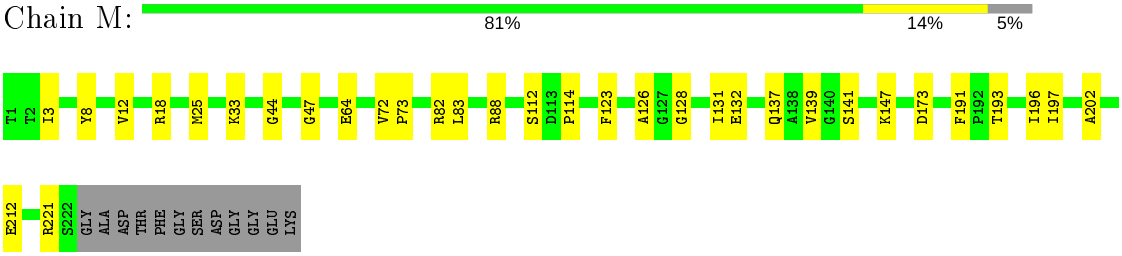
- Molecule 2: Proteasome subunit beta

Chain L:



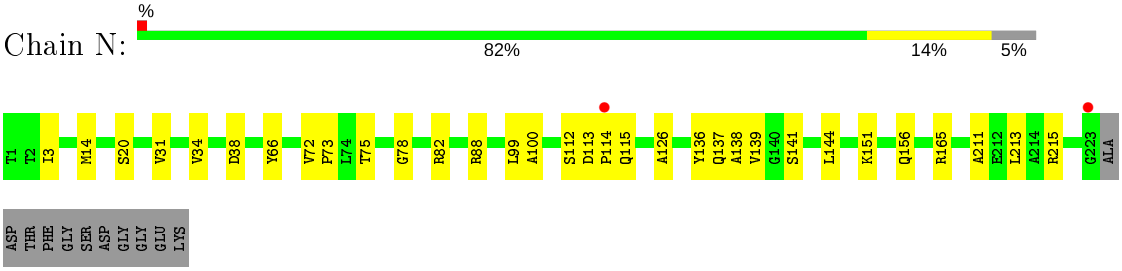
- Molecule 2: Proteasome subunit beta

Chain M:



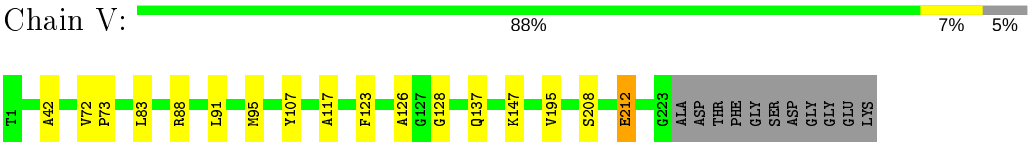
- Molecule 2: Proteasome subunit beta

Chain N:



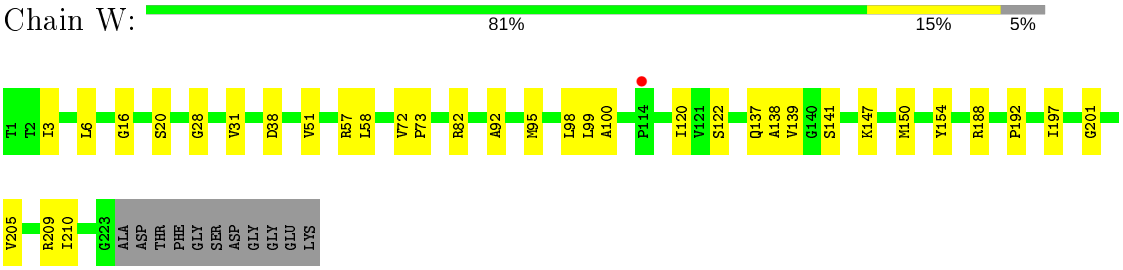
- Molecule 2: Proteasome subunit beta

Chain V:



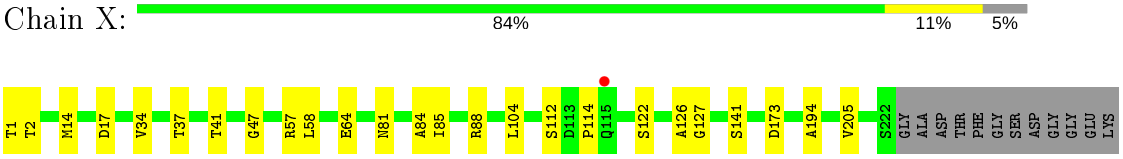
• Molecule 2: Proteasome subunit beta

Chain W:



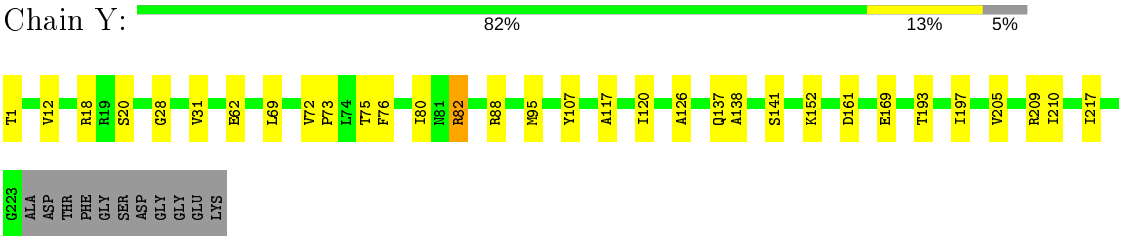
• Molecule 2: Proteasome subunit beta

Chain X:



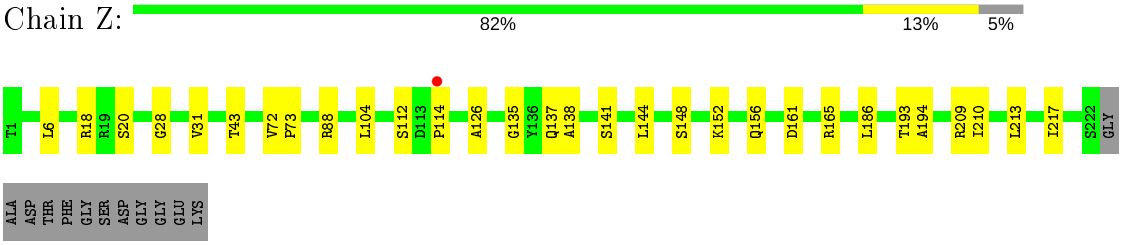
• Molecule 2: Proteasome subunit beta

Chain Y:



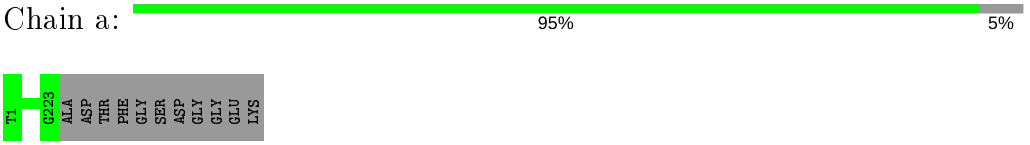
• Molecule 2: Proteasome subunit beta

Chain Z:



• Molecule 2: Proteasome subunit beta

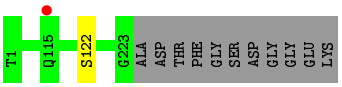
Chain a:



• Molecule 2: Proteasome subunit beta

Chain b:


95%
5%


T1
Q115
S122
G223
ALA
ASP
THR
PHE
GLY
SER
ASP
GLY
GLY
GLU
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	120.77Å 198.06Å 167.92Å 90.00° 103.72° 90.00°	Depositor
Resolution (Å)	42.92 – 2.65 42.92 – 2.65	Depositor EDS
% Data completeness (in resolution range)	93.5 (42.92-2.65) 93.5 (42.92-2.65)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 2.65Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.184 , 0.235 0.184 , 0.235	Depositor DCC
R_{free} test set	10226 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	35.4	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	48235	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: M6Y, DMF, CIT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.27	0/1701	0.47	0/2297
1	B	0.26	0/1684	0.44	0/2274
1	C	0.26	0/1696	0.45	0/2290
1	D	0.27	0/1679	0.46	0/2266
1	E	0.26	0/1694	0.45	0/2287
1	F	0.33	0/1687	0.47	0/2277
1	G	0.27	0/1684	0.46	0/2272
1	O	0.33	0/1694	0.50	2/2287 (0.1%)
1	P	0.26	0/1709	0.45	0/2308
1	Q	0.27	0/1692	0.46	0/2285
1	R	0.27	0/1681	0.46	0/2269
1	S	0.27	0/1702	0.46	0/2298
1	T	0.26	0/1695	0.45	0/2289
1	U	0.31	0/1688	0.48	0/2279
2	H	0.27	0/1662	0.48	0/2254
2	I	0.27	0/1662	0.47	0/2254
2	J	0.27	0/1662	0.48	0/2254
2	K	0.28	0/1666	0.49	0/2259
2	L	0.27	0/1666	0.48	0/2259
2	M	0.26	0/1662	0.47	0/2254
2	N	0.27	0/1666	0.48	0/2259
2	V	0.31	0/1666	0.48	0/2259
2	W	0.27	0/1666	0.48	0/2259
2	X	0.27	0/1662	0.47	0/2254
2	Y	0.34	0/1666	0.50	0/2259
2	Z	0.27	0/1662	0.48	0/2254
2	a	0.29	0/1666	0.46	0/2259
2	b	0.27	0/1666	0.47	0/2259
All	All	0.28	0/46986	0.47	2/63574 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	85	ARG	CG-CD-NE	-5.90	99.41	111.80
1	O	85	ARG	NE-CZ-NH2	-5.78	117.41	120.30

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	1677	0	1680	42	0
1	B	1660	0	1665	43	0
1	C	1672	0	1672	47	0
1	D	1655	0	1653	38	0
1	E	1670	0	1673	45	0
1	F	1663	0	1664	36	0
1	G	1661	0	1659	25	0
1	O	1670	0	1671	44	0
1	P	1685	0	1684	27	0
1	Q	1668	0	1669	40	0
1	R	1657	0	1659	39	0
1	S	1678	0	1677	36	0
1	T	1671	0	1675	34	0
1	U	1664	0	1668	29	0
2	H	1638	0	1633	26	0
2	I	1638	0	1633	22	0
2	J	1638	0	1633	23	0
2	K	1642	0	1636	21	0
2	L	1642	0	1636	28	0
2	M	1638	0	1633	27	0
2	N	1642	0	1636	23	0
2	V	1642	0	1636	10	0
2	W	1642	0	1636	25	0
2	X	1638	0	1633	18	0
2	Y	1642	0	1636	21	0
2	Z	1638	0	1633	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	a	1642	0	1636	0	0
2	b	1642	0	1636	0	0
3	A	5	7	7	0	0
3	B	5	7	7	0	0
3	C	5	7	7	1	0
3	E	5	7	7	2	0
3	F	10	14	14	1	0
3	G	10	14	14	0	0
3	I	5	7	7	1	0
3	J	10	14	14	2	0
3	O	5	7	7	1	0
3	P	5	7	7	0	0
3	Q	5	7	7	1	0
3	R	10	14	14	2	0
3	S	10	14	14	2	0
3	T	5	7	7	0	0
3	U	5	7	7	1	0
4	H	41	0	0	1	0
4	I	41	0	0	1	0
4	J	41	0	0	0	0
4	K	41	0	0	0	0
4	L	41	0	0	0	0
4	M	41	0	0	0	0
4	N	41	0	0	0	0
4	V	41	0	0	0	0
4	W	41	0	0	0	0
4	X	41	0	0	0	0
4	Y	41	0	0	0	0
4	Z	41	0	0	0	0
4	a	41	0	0	0	0
4	b	41	0	0	0	0
5	H	13	5	5	0	0
5	I	13	5	5	2	0
5	J	13	5	5	1	0
5	K	13	5	5	2	0
5	L	13	5	5	0	0
5	M	13	5	5	2	0
5	N	13	5	5	1	0
5	V	13	5	5	0	0
5	W	13	5	5	1	0
5	X	13	5	5	2	0
5	Y	13	5	5	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	Z	13	5	5	1	0
5	a	13	5	5	0	0
5	b	13	5	5	0	0
6	A	27	0	0	4	0
6	B	20	0	0	2	0
6	C	29	0	0	2	0
6	D	20	0	0	3	0
6	E	24	0	0	1	0
6	F	16	0	0	0	0
6	G	21	0	0	1	0
6	H	36	0	0	0	0
6	I	49	0	0	2	0
6	J	36	0	0	0	0
6	K	41	0	0	0	0
6	L	42	0	0	1	0
6	M	35	0	0	3	0
6	N	34	0	0	0	0
6	O	17	0	0	3	0
6	P	26	0	0	2	0
6	Q	31	0	0	4	0
6	R	28	0	0	2	0
6	S	28	0	0	3	0
6	T	13	0	0	0	0
6	U	27	0	0	3	0
6	V	42	0	0	0	0
6	W	39	0	0	0	0
6	X	35	0	0	1	0
6	Y	40	0	0	1	0
6	Z	37	0	0	1	0
6	a	29	0	0	0	0
6	b	32	0	0	0	0
All	All	48025	210	46465	727	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 8.

All (727) 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)
1:U:217:ARG:HD2	1:U:223:ARG:HH21	0.99	1.08
1:Q:30:VAL:HG13	1:Q:43:ALA:HB2	1.42	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:217:ARG:HD2	1:U:223:ARG:NH2	1.78	0.97
1:E:177:LEU:HD12	1:E:233:LEU:HD22	1.59	0.85
1:U:217:ARG:CD	1:U:223:ARG:HH21	1.86	0.85
2:M:8:TYR:HE2	2:M:196:ILE:HD11	1.43	0.83
1:T:33:LEU:HD23	1:T:153:PHE:HB3	1.58	0.83
2:L:88:ARG:HD3	2:L:126:ALA:O	1.79	0.82
1:F:217:ARG:NH1	1:F:223:ARG:HB3	1.95	0.81
2:X:14:MET:CE	2:X:34:VAL:HG13	2.10	0.80
1:E:30:VAL:HG13	1:E:43:ALA:HB2	1.63	0.80
2:M:8:TYR:CE2	2:M:196:ILE:HD11	2.17	0.79
1:B:205:VAL:HG21	1:B:231:GLN:HB3	1.66	0.78
1:A:87:TYR:O	2:H:57:ARG:NH1	2.17	0.77
1:G:41:PHE:HB3	1:G:53:ILE:HD13	1.66	0.77
1:E:205:VAL:HG21	1:E:231:GLN:HG2	1.66	0.77
1:C:87:TYR:O	2:J:57:ARG:NH2	2.19	0.76
1:C:77:GLY:HA3	3:C:301:DMF:H13	1.69	0.74
2:V:91:LEU:O	2:V:95:MET:HG2	1.88	0.74
1:D:9:MET:HE3	1:E:19:LEU:HD13	1.69	0.73
2:X:14:MET:HE3	2:X:34:VAL:HG13	1.69	0.73
2:Y:88:ARG:HD3	2:Y:126:ALA:O	1.86	0.72
1:R:170:SER:OG	1:R:183:ILE:HD11	1.90	0.72
1:A:178:THR:HG22	1:A:233:LEU:HD22	1.72	0.72
1:D:9:MET:CE	1:E:19:LEU:HD13	2.20	0.72
1:C:149:ASP:OD2	1:D:48:ARG:HG2	1.90	0.71
1:S:33:LEU:HD12	1:S:153:PHE:HB3	1.72	0.71
2:N:88:ARG:HD3	2:N:126:ALA:O	1.90	0.70
1:O:20:ALA:O	1:O:24:ILE:HD12	1.90	0.70
2:M:25:MET:HE1	2:N:144:LEU:HD21	1.75	0.69
2:Y:62:GLU:OE2	2:Y:82:ARG:HD2	1.93	0.69
1:Q:64:ALA:HA	1:Q:156:MET:HE1	1.75	0.69
1:A:9:MET:HE1	1:B:116:LYS:HA	1.75	0.69
1:F:217:ARG:HH11	1:F:223:ARG:HB3	1.56	0.69
1:Q:170:SER:OG	1:Q:183:ILE:HD11	1.93	0.69
1:B:32:ALA:HB3	1:B:154:VAL:HG22	1.75	0.69
1:Q:101:ASN:ND2	1:R:76:ARG:HH21	1.90	0.69
1:F:219:ARG:NH2	2:M:64:GLU:OE2	2.27	0.68
1:E:77:GLY:HA3	3:E:301:DMF:H22	1.74	0.68
2:M:88:ARG:HD3	2:M:126:ALA:O	1.93	0.68
1:T:110:ILE:HA	1:T:114:GLN:HG3	1.75	0.68
2:J:20:SER:HB3	2:J:28:GLY:HA3	1.75	0.68
1:T:68:PHE:HA	1:T:71:PHE:CZ	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:92:ARG:HB3	2:Y:75:THR:HG21	1.77	0.67
1:P:68:PHE:HA	1:P:71:PHE:CE2	2.28	0.67
1:D:128:ALA:HB2	1:D:134:LYS:HB3	1.77	0.67
1:D:14:ARG:NH2	6:D:301:HOH:O	2.28	0.67
1:B:110:ILE:HA	1:B:114:GLN:HG3	1.77	0.66
2:M:72:VAL:HG23	2:M:73:PRO:HD2	1.77	0.66
1:D:41:PHE:HB3	1:D:53:ILE:HD13	1.76	0.66
1:R:97:ARG:HH11	1:S:49:SER:HB2	1.60	0.66
1:C:164:ALA:O	1:C:168:LYS:HG3	1.95	0.66
2:M:3:ILE:HB	2:M:139:VAL:HG12	1.77	0.66
1:T:68:PHE:HA	1:T:71:PHE:CE2	2.31	0.66
1:A:48:ARG:NH2	1:G:137:GLU:HG2	2.11	0.66
1:R:85:ARG:HH21	1:R:98:GLN:HE21	1.44	0.66
1:D:9:MET:HB3	1:E:15:GLU:OE2	1.96	0.66
2:J:156:GLN:OE1	2:J:165:ARG:NH2	2.21	0.66
1:U:74:LEU:HD13	1:U:122:LEU:HD11	1.78	0.66
1:E:31:VAL:HG13	1:E:188:LEU:HD21	1.76	0.65
1:F:203:LEU:HD13	1:F:208:LEU:HD11	1.79	0.65
1:D:85:ARG:HD2	6:D:306:HOH:O	1.96	0.65
1:F:41:PHE:HB3	1:F:53:ILE:HD13	1.77	0.65
2:I:91:LEU:HG	2:I:95:MET:CE	2.26	0.65
1:R:68:PHE:HA	1:R:71:PHE:CE2	2.32	0.65
1:T:128:ALA:HB2	1:T:134:LYS:HB3	1.78	0.65
2:X:14:MET:HE2	2:X:34:VAL:HG13	1.78	0.65
1:A:68:PHE:HA	1:A:71:PHE:CE2	2.32	0.65
1:T:81:PHE:CE1	1:T:102:VAL:HG11	2.32	0.65
1:A:48:ARG:HH21	1:G:137:GLU:HG2	1.60	0.64
1:R:85:ARG:HH21	1:R:98:GLN:NE2	1.95	0.64
2:W:92:ALA:HA	2:W:95:MET:HE2	1.79	0.64
2:H:88:ARG:HD3	2:H:126:ALA:O	1.98	0.64
1:P:31:VAL:HG12	1:P:155:VAL:HG12	1.79	0.64
1:E:68:PHE:HA	1:E:71:PHE:CE2	2.33	0.64
1:C:170:SER:OG	1:C:183:ILE:HD11	1.97	0.64
2:M:212:GLU:HG3	6:M:420:HOH:O	1.96	0.64
1:P:33:LEU:HD13	1:P:153:PHE:HB3	1.80	0.64
1:R:101:ASN:ND2	1:S:76:ARG:HH21	1.96	0.64
1:C:92:ARG:HB2	2:K:75:THR:HG21	1.79	0.63
1:U:214:ASP:OD2	1:U:223:ARG:NH2	2.31	0.63
1:C:22:LYS:O	1:C:26:ARG:HG2	1.97	0.63
2:H:72:VAL:HG23	2:H:73:PRO:HD2	1.77	0.63
1:Q:30:VAL:HG13	1:Q:43:ALA:CB	2.25	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:88:ARG:HD3	2:V:126:ALA:O	1.98	0.63
1:S:85:ARG:HB3	6:S:425:HOH:O	1.98	0.63
1:E:74:LEU:HD11	1:E:107:LEU:HD21	1.80	0.63
1:Q:41:PHE:HB3	1:Q:53:ILE:HD13	1.81	0.63
1:R:92:ARG:HD2	6:R:425:HOH:O	1.97	0.63
1:P:56:LEU:HD11	1:P:62:PHE:HB2	1.81	0.63
1:G:214:ASP:OD2	1:G:223:ARG:NH2	2.32	0.62
1:Q:42:VAL:HG22	1:Q:210:VAL:CG2	2.29	0.62
1:F:18:GLU:OE2	1:F:21:ARG:NH1	2.33	0.62
2:N:20:SER:HB2	2:N:31:VAL:HG21	1.80	0.62
1:B:205:VAL:HG13	1:B:230:LEU:HD23	1.81	0.62
1:C:9:MET:CE	1:D:116:LYS:HG3	2.29	0.62
1:D:9:MET:HE1	1:E:117:PRO:HD2	1.81	0.62
1:U:85:ARG:NH1	1:U:98:GLN:OE1	2.33	0.62
1:R:30:VAL:HG13	1:R:43:ALA:HB2	1.82	0.62
1:S:77:GLY:HA3	3:S:301:DMF:H12	1.82	0.62
1:U:223:ARG:NH1	6:U:401:HOH:O	2.33	0.62
1:G:41:PHE:CB	1:G:53:ILE:HD13	2.29	0.62
2:M:132:GLU:HG2	6:M:414:HOH:O	1.99	0.62
1:G:85:ARG:HB3	6:G:401:HOH:O	1.98	0.62
1:A:147:ILE:HG23	1:B:50:LEU:HD21	1.82	0.61
1:P:181:LEU:O	1:P:185:VAL:HG23	2.00	0.61
1:Q:77:GLY:HA3	3:Q:301:DMF:C	2.30	0.61
2:N:156:GLN:OE1	2:N:165:ARG:NH1	2.30	0.61
2:Y:72:VAL:HG23	2:Y:73:PRO:HD2	1.82	0.61
1:O:210:VAL:HG21	1:O:230:LEU:HD13	1.83	0.61
1:U:100:ALA:HB1	1:U:147:ILE:HD11	1.81	0.61
2:Z:152:LYS:HD3	6:Z:429:HOH:O	2.01	0.61
2:J:72:VAL:HG23	2:J:73:PRO:HD2	1.83	0.61
1:C:31:VAL:HG22	1:C:155:VAL:HG12	1.83	0.60
1:Q:42:VAL:HG22	1:Q:210:VAL:HG22	1.82	0.60
2:K:99:LEU:HD12	2:K:100:ALA:N	2.15	0.60
2:M:137:GLN:OE1	2:M:147:LYS:HD3	2.00	0.60
2:Z:141:SER:HB3	5:Z:302:CIT:H41	1.84	0.60
1:A:70:GLU:HB3	1:A:118:TYR:CD2	2.37	0.60
1:Q:87:TYR:O	2:X:57:ARG:NH1	2.34	0.60
2:N:141:SER:HB3	5:N:302:CIT:H41	1.82	0.60
1:S:68:PHE:HA	1:S:71:PHE:CE2	2.37	0.60
1:E:18:GLU:OE1	1:E:21:ARG:NH1	2.35	0.60
1:A:150:GLU:HG3	6:A:417:HOH:O	2.02	0.59
2:V:137:GLN:OE1	2:V:147:LYS:HD3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:MET:HE2	1:D:116:LYS:HG3	1.84	0.59
1:A:64:ALA:HA	1:A:156:MET:HE1	1.84	0.59
2:I:132:GLU:HG2	6:I:403:HOH:O	2.02	0.59
2:J:197:ILE:HG12	2:J:202:ALA:CB	2.33	0.59
1:Q:87:TYR:CZ	2:X:58:LEU:HD13	2.37	0.59
1:C:178:THR:HG22	1:C:233:LEU:HD13	1.83	0.59
1:Q:85:ARG:HD2	6:Q:411:HOH:O	2.02	0.59
1:U:181:LEU:O	1:U:185:VAL:HG23	2.02	0.59
1:C:68:PHE:HA	1:C:71:PHE:CZ	2.37	0.59
1:D:129:HIS:HB2	1:D:132:GLU:HG3	1.84	0.59
1:D:30:VAL:HG13	1:D:43:ALA:HB2	1.85	0.59
2:I:47:GLY:HA2	5:I:302:CIT:H41	1.84	0.59
2:I:91:LEU:HG	2:I:95:MET:HE2	1.84	0.59
2:L:20:SER:HB2	2:L:31:VAL:HG21	1.83	0.59
3:F:301:DMF:H11	2:N:66:TYR:HA	1.85	0.59
1:C:68:PHE:HA	1:C:71:PHE:CE2	2.37	0.59
2:J:176:ASP:OD1	2:W:188:ARG:NH1	2.36	0.59
1:B:68:PHE:HA	1:B:71:PHE:CE2	2.38	0.58
1:Q:92:ARG:NH2	1:Q:132:GLU:OE1	2.37	0.58
2:H:20:SER:HB2	2:H:31:VAL:HG21	1.85	0.58
1:P:62:PHE:CE2	1:P:122:LEU:HD22	2.38	0.58
2:I:141:SER:HB3	5:I:302:CIT:H22	1.85	0.58
1:O:81:PHE:CE1	1:O:102:VAL:HG21	2.39	0.58
1:F:68:PHE:HA	1:F:71:PHE:CZ	2.39	0.58
1:F:99:LEU:O	1:F:102:VAL:HG12	2.03	0.58
2:L:108:ASP:HA	6:L:425:HOH:O	2.04	0.58
1:E:35:TYR:CZ	1:E:177:LEU:HD23	2.39	0.57
1:Q:91:ARG:HD2	6:Q:424:HOH:O	2.03	0.57
1:R:101:ASN:HD21	1:S:76:ARG:HH21	1.51	0.57
1:F:68:PHE:HA	1:F:71:PHE:CE2	2.39	0.57
1:B:41:PHE:HB3	1:B:53:ILE:HD13	1.85	0.57
2:V:83:LEU:HD23	2:V:123:PHE:CZ	2.39	0.57
2:N:3:ILE:HB	2:N:139:VAL:HG12	1.85	0.57
2:M:72:VAL:CG2	2:M:73:PRO:HD2	2.34	0.57
1:P:87:TYR:O	2:W:57:ARG:NH2	2.37	0.57
1:B:135:ARG:HD2	1:B:136:PRO:HD2	1.86	0.57
2:W:99:LEU:HD12	2:W:100:ALA:H	1.70	0.57
2:M:12:VAL:O	2:M:196:ILE:HD12	2.04	0.57
1:R:81:PHE:CZ	1:R:102:VAL:HG11	2.40	0.57
2:J:72:VAL:CG2	2:J:73:PRO:HD2	2.35	0.57
1:D:68:PHE:HA	1:D:71:PHE:CE2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:77:GLY:HA3	3:O:301:DMF:C	2.35	0.56
1:B:121:GLU:OE1	1:B:140:ARG:NH2	2.38	0.56
1:B:54:SER:CB	1:B:75:ARG:HD2	2.36	0.56
2:W:72:VAL:CG2	2:W:73:PRO:HD2	2.35	0.56
1:B:210:VAL:HG21	1:B:230:LEU:HD13	1.87	0.56
1:Q:180:ALA:O	1:Q:183:ILE:HG22	2.05	0.56
1:S:11:GLN:HG3	1:S:14:ARG:HH12	1.70	0.56
1:P:41:PHE:HB3	1:P:53:ILE:HD13	1.86	0.56
1:A:178:THR:HG22	1:A:233:LEU:CD2	2.35	0.56
2:K:137:GLN:OE1	2:K:147:LYS:HD3	2.05	0.56
1:R:12:ALA:O	1:R:16:ARG:HG3	2.04	0.56
1:R:28:LYS:HE3	6:R:421:HOH:O	2.04	0.56
1:S:39:VAL:HG23	1:S:127:VAL:HG12	1.88	0.56
1:F:110:ILE:HG23	1:F:114:GLN:HG3	1.86	0.56
2:K:72:VAL:HG23	2:K:73:PRO:HD2	1.88	0.56
2:W:20:SER:HB3	2:W:28:GLY:HA3	1.88	0.56
1:E:99:LEU:HA	1:E:102:VAL:HG12	1.89	0.55
1:U:179:ASP:O	1:U:183:ILE:HG23	2.05	0.55
1:E:152:HIS:HB3	1:E:171:TYR:CE2	2.42	0.55
2:Z:20:SER:HB3	2:Z:28:GLY:HA3	1.89	0.55
2:Z:43:THR:HG22	2:Z:104:LEU:HD12	1.88	0.55
1:S:41:PHE:HB3	1:S:53:ILE:HD13	1.87	0.55
1:C:232:ALA:O	1:C:236:ASP:HB2	2.07	0.55
1:E:217:ARG:NH2	1:E:223:ARG:HD3	2.21	0.55
1:F:161:GLU:OE1	1:F:161:GLU:N	2.26	0.55
1:F:164:ALA:O	1:F:168:LYS:HB2	2.06	0.55
1:B:70:GLU:HB3	1:B:118:TYR:CD2	2.42	0.55
2:M:197:ILE:HG12	2:M:202:ALA:CB	2.37	0.55
1:O:30:VAL:HG22	1:O:43:ALA:HB1	1.88	0.55
1:T:33:LEU:HD23	1:T:153:PHE:CB	2.31	0.55
1:F:74:LEU:HD13	1:F:122:LEU:HD11	1.89	0.55
1:S:91:ARG:HD3	1:S:219:ARG:NH2	2.21	0.55
1:T:30:VAL:CG2	1:T:52:LYS:HE2	2.37	0.55
1:U:142:THR:OG1	1:U:146:SER:HB2	2.07	0.55
1:O:81:PHE:CZ	1:O:102:VAL:HG21	2.42	0.55
1:B:30:VAL:HG22	1:B:43:ALA:HB1	1.89	0.55
2:W:141:SER:HB3	5:W:302:CIT:H22	1.88	0.55
1:A:9:MET:CE	1:B:116:LYS:HG3	2.37	0.54
1:C:28:LYS:H	1:C:28:LYS:CD	2.20	0.54
1:T:217:ARG:HD2	1:T:223:ARG:HD3	1.88	0.54
1:T:142:THR:OG1	1:T:146:SER:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:THR:HG22	1:C:233:LEU:CD1	2.36	0.54
2:M:47:GLY:HA2	5:M:302:CIT:H22	1.88	0.54
1:O:16:ARG:NH1	1:O:114:GLN:O	2.33	0.54
1:A:33:LEU:HD11	1:A:180:ALA:HB1	1.90	0.54
1:C:70:GLU:HB3	1:C:118:TYR:CD2	2.43	0.54
1:S:11:GLN:HG3	1:S:14:ARG:NH1	2.21	0.54
2:M:18:ARG:HD3	2:M:193:THR:HG23	1.89	0.54
1:U:98:GLN:O	1:U:102:VAL:HG13	2.07	0.54
1:B:74:LEU:HD13	1:B:122:LEU:HD11	1.90	0.54
1:E:179:ASP:O	1:E:183:ILE:HG13	2.07	0.54
1:Q:170:SER:CB	1:Q:183:ILE:HD11	2.38	0.54
2:M:112:SER:O	2:M:114:PRO:HD3	2.08	0.54
1:O:205:VAL:HG13	1:O:230:LEU:HD23	1.89	0.54
1:E:161:GLU:HB2	1:E:162:PRO:HD3	1.90	0.54
2:L:72:VAL:HG23	2:L:73:PRO:HD2	1.90	0.54
1:S:91:ARG:HD3	1:S:219:ARG:HH21	1.73	0.54
1:A:179:ASP:OD1	1:A:182:ARG:NH2	2.41	0.54
1:A:68:PHE:HA	1:A:71:PHE:CZ	2.43	0.54
1:O:28:LYS:HD2	1:O:28:LYS:H	1.72	0.54
1:F:89:TYR:CE1	2:N:82:ARG:HD3	2.43	0.53
2:L:99:LEU:HD11	2:L:101:LEU:HG	1.91	0.53
1:O:128:ALA:HB2	1:O:134:LYS:HB3	1.89	0.53
1:R:68:PHE:HA	1:R:71:PHE:CZ	2.44	0.53
1:Q:163:ILE:HD13	1:Q:188:LEU:HD23	1.89	0.53
2:V:72:VAL:HG23	2:V:73:PRO:HD2	1.89	0.53
1:E:33:LEU:HD11	1:E:40:LEU:HD23	1.91	0.53
1:B:87:TYR:CZ	2:I:58:LEU:HD13	2.43	0.53
1:U:68:PHE:HA	1:U:71:PHE:CE2	2.44	0.53
1:D:18:GLU:OE2	1:D:21:ARG:NH2	2.42	0.53
1:G:68:PHE:HA	1:G:71:PHE:CE2	2.43	0.53
1:T:56:LEU:HG	1:T:62:PHE:HB2	1.90	0.53
1:A:128:ALA:HB2	1:A:134:LYS:HB3	1.90	0.53
1:G:25:ALA:O	1:G:158:GLY:HA2	2.09	0.53
1:P:151:PRO:HD3	1:Q:48:ARG:HH12	1.72	0.53
1:P:54:SER:CB	1:P:75:ARG:HD2	2.38	0.53
2:V:107:TYR:CE1	2:V:117:ALA:HB3	2.43	0.53
2:M:131:ILE:HB	6:M:412:HOH:O	2.09	0.53
2:I:156:GLN:OE1	2:I:165:ARG:NH2	2.42	0.53
2:L:161:ASP:OD1	2:L:209:ARG:NH2	2.39	0.53
1:Q:11:GLN:HG2	1:Q:12:ALA:N	2.24	0.53
2:H:72:VAL:CG2	2:H:73:PRO:HD2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:33:LYS:O	2:M:44:GLY:HA2	2.09	0.53
1:O:181:LEU:CD2	1:O:233:LEU:HD23	2.39	0.53
1:P:164:ALA:O	1:P:168:LYS:HG3	2.09	0.53
1:C:219:ARG:NE	6:C:401:HOH:O	2.43	0.52
2:N:165:ARG:HG3	2:N:213:LEU:HD22	1.91	0.52
2:Z:194:ALA:HB3	2:Z:210:ILE:HD11	1.89	0.52
1:C:51:GLN:OE1	1:C:224:ARG:NH2	2.43	0.52
1:R:81:PHE:CE1	1:R:102:VAL:HG11	2.44	0.52
1:G:31:VAL:HG12	1:G:33:LEU:HD12	1.92	0.52
1:S:217:ARG:NH1	1:S:223:ARG:HG3	2.25	0.52
1:S:77:GLY:HA3	3:S:301:DMF:C1	2.38	0.52
1:A:55:GLU:HB2	1:A:222:PHE:CG	2.44	0.52
2:K:164:LEU:HD21	2:K:205:VAL:HG11	1.91	0.52
2:M:83:LEU:HD23	2:M:123:PHE:CZ	2.44	0.52
1:R:142:THR:OG1	1:R:146:SER:HB2	2.09	0.52
1:R:18:GLU:OE2	1:R:21:ARG:NH1	2.43	0.52
1:S:68:PHE:HA	1:S:71:PHE:CZ	2.45	0.52
1:O:76:ARG:HD3	6:O:401:HOH:O	2.09	0.52
1:R:77:GLY:HA3	3:R:301:DMF:C	2.39	0.52
2:Z:43:THR:HG22	2:Z:104:LEU:CD1	2.39	0.52
1:T:161:GLU:HB2	1:T:162:PRO:HD3	1.91	0.52
1:C:18:GLU:OE1	1:C:21:ARG:NH1	2.43	0.52
1:D:161:GLU:HB3	1:D:162:PRO:HD3	1.92	0.52
1:D:181:LEU:O	1:D:185:VAL:HG23	2.09	0.52
2:K:141:SER:HB3	5:K:302:CIT:H42	1.91	0.52
1:O:33:LEU:HD11	1:O:40:LEU:HD23	1.92	0.52
2:K:20:SER:HB3	2:K:28:GLY:HA3	1.91	0.51
1:O:100:ALA:HB1	1:O:147:ILE:HD11	1.92	0.51
1:Q:210:VAL:CG1	1:Q:225:ILE:HB	2.40	0.51
1:E:33:LEU:HD12	1:E:40:LEU:HB3	1.92	0.51
2:L:165:ARG:HG3	2:L:213:LEU:HD22	1.92	0.51
1:O:56:LEU:HG	1:O:62:PHE:HB2	1.92	0.51
1:B:25:ALA:O	1:B:158:GLY:HA2	2.09	0.51
1:E:182:ARG:HD2	6:E:415:HOH:O	2.10	0.51
2:J:132:GLU:CG	2:J:137:GLN:HE21	2.23	0.51
2:L:76:PHE:CE2	2:L:80:ILE:HD11	2.45	0.51
1:O:123:CYS:SG	1:O:154:VAL:HG21	2.50	0.51
2:X:84:ALA:HB1	2:X:127:GLY:O	2.11	0.51
1:F:40:LEU:HA	1:F:212:VAL:HG12	1.93	0.51
2:K:156:GLN:OE1	2:K:165:ARG:NH1	2.43	0.51
2:L:20:SER:HB3	2:L:28:GLY:HA3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:202:THR:O	1:O:203:LEU:HD12	2.11	0.51
1:E:32:ALA:HA	1:E:40:LEU:O	2.11	0.51
2:X:47:GLY:HA2	5:X:302:CIT:H41	1.92	0.51
1:E:54:SER:CB	1:E:75:ARG:HD2	2.41	0.51
2:J:47:GLY:HA2	5:J:302:CIT:H41	1.93	0.51
1:O:68:PHE:HA	1:O:71:PHE:CE2	2.46	0.51
1:Q:62:PHE:CE2	1:Q:122:LEU:HD22	2.46	0.51
2:Y:12:VAL:HG12	2:Y:197:ILE:HB	1.93	0.51
1:B:68:PHE:HA	1:B:71:PHE:CZ	2.46	0.51
1:G:70:GLU:HB3	1:G:118:TYR:CD2	2.45	0.51
1:F:89:TYR:CD1	2:N:82:ARG:HD3	2.46	0.51
1:D:181:LEU:HD23	1:D:233:LEU:HB3	1.93	0.50
1:G:54:SER:CB	1:G:75:ARG:HD2	2.41	0.50
2:M:123:PHE:HA	2:M:128:GLY:O	2.11	0.50
1:B:85:ARG:HD2	6:B:402:HOH:O	2.11	0.50
1:F:225:ILE:HG22	1:F:230:LEU:HB2	1.93	0.50
1:B:150:GLU:HG3	1:B:154:VAL:HG12	1.93	0.50
1:F:41:PHE:CB	1:F:53:ILE:HD13	2.41	0.50
2:H:76:PHE:CE2	2:H:80:ILE:HD11	2.47	0.50
2:V:72:VAL:CG2	2:V:73:PRO:HD2	2.42	0.50
2:W:205:VAL:HG11	2:W:210:ILE:HD11	1.92	0.50
1:A:9:MET:HE2	1:B:117:PRO:HD2	1.93	0.50
1:G:205:VAL:HG13	1:G:230:LEU:HD23	1.94	0.50
1:P:151:PRO:HD2	6:P:403:HOH:O	2.12	0.50
1:P:56:LEU:CD1	1:P:62:PHE:HB2	2.40	0.50
1:T:55:GLU:OE1	1:T:220:ARG:NH2	2.40	0.50
2:L:45:ILE:N	2:L:45:ILE:HD12	2.26	0.50
1:Q:210:VAL:HG12	1:Q:225:ILE:HB	1.93	0.50
1:Q:60:VAL:HG11	1:Q:99:LEU:HD12	1.91	0.50
2:X:37:THR:OG1	2:X:41:THR:HG22	2.11	0.50
2:Y:95:MET:CE	2:Y:95:MET:HA	2.41	0.50
1:B:30:VAL:HG22	1:B:43:ALA:CB	2.40	0.50
1:E:231:GLN:HA	1:E:234:LEU:HD12	1.94	0.50
2:X:112:SER:O	2:X:114:PRO:HD3	2.12	0.50
1:C:231:GLN:HA	1:C:234:LEU:HD12	1.94	0.50
2:L:62:GLU:OE2	2:L:82:ARG:HD3	2.12	0.50
1:O:97:ARG:HD3	1:P:49:SER:HB2	1.93	0.50
1:C:16:ARG:NH1	1:C:111:PHE:O	2.45	0.50
1:C:28:LYS:H	1:C:28:LYS:CE	2.25	0.50
1:E:89:TYR:CD1	2:M:82:ARG:HD3	2.47	0.50
1:R:181:LEU:O	1:R:185:VAL:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:107:LEU:HD12	1:P:141:ILE:HG22	1.94	0.49
1:P:133:THR:O	1:P:133:THR:HG23	2.12	0.49
1:P:54:SER:HB2	6:P:424:HOH:O	2.10	0.49
1:D:41:PHE:HB3	1:D:53:ILE:CD1	2.40	0.49
2:K:45:ILE:HB	2:K:52:ALA:HB1	1.93	0.49
2:L:156:GLN:OE1	2:L:165:ARG:NH1	2.31	0.49
1:U:30:VAL:HG22	1:U:43:ALA:HB1	1.94	0.49
1:A:141:ILE:N	1:A:141:ILE:HD12	2.27	0.49
2:J:107:TYR:CE2	2:J:117:ALA:HB3	2.47	0.49
1:T:189:ARG:NH2	1:T:202:THR:OG1	2.46	0.49
1:A:30:VAL:HG13	1:A:43:ALA:HB2	1.95	0.49
1:D:54:SER:CB	1:D:75:ARG:HD2	2.42	0.49
1:F:55:GLU:OE1	1:F:220:ARG:NH1	2.45	0.49
2:L:72:VAL:CG2	2:L:73:PRO:HD2	2.43	0.49
1:U:30:VAL:HG22	1:U:43:ALA:CB	2.41	0.49
2:W:150:MET:O	2:W:154:TYR:HB2	2.12	0.49
1:G:68:PHE:HA	1:G:71:PHE:CZ	2.47	0.49
2:Z:161:ASP:OD1	2:Z:209:ARG:NH1	2.45	0.49
1:A:18:GLU:OE2	1:A:21:ARG:NH1	2.46	0.49
1:C:54:SER:CB	1:C:75:ARG:HD2	2.42	0.49
2:J:197:ILE:HG12	2:J:202:ALA:HB2	1.94	0.49
1:Q:219:ARG:NH2	1:Q:220:ARG:HD2	2.28	0.49
1:A:41:PHE:HB3	1:A:53:ILE:HD13	1.94	0.49
2:X:81:ASN:O	2:X:85:ILE:HG13	2.13	0.49
2:I:45:ILE:HB	2:I:52:ALA:HB1	1.95	0.49
2:L:92:ALA:HA	2:L:95:MET:HE2	1.95	0.49
2:X:173:ASP:HB3	6:X:418:HOH:O	2.12	0.49
1:F:55:GLU:OE2	1:F:220:ARG:HD2	2.12	0.48
1:O:67:LYS:HE3	1:O:69:ASN:OD1	2.12	0.48
1:R:67:LYS:HD3	1:R:70:GLU:CD	2.34	0.48
1:Q:101:ASN:HD21	1:R:76:ARG:HH21	1.59	0.48
2:V:123:PHE:HA	2:V:128:GLY:O	2.13	0.48
2:Y:161:ASP:OD1	2:Y:209:ARG:NH2	2.46	0.48
1:A:161:GLU:HB3	1:A:162:PRO:HD3	1.95	0.48
1:F:10:GLU:OE2	1:G:22:LYS:HE2	2.12	0.48
2:K:45:ILE:N	2:K:45:ILE:HD12	2.28	0.48
1:O:152:HIS:HB3	1:O:171:TYR:CE2	2.48	0.48
1:R:76:ARG:HG2	2:Y:69:LEU:HD22	1.94	0.48
1:E:101:ASN:ND2	1:F:76:ARG:HH21	2.12	0.48
2:X:194:ALA:HB3	2:X:205:VAL:HB	1.96	0.48
1:E:205:VAL:CG2	1:E:231:GLN:HG2	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:41:PHE:HB3	1:G:53:ILE:CD1	2.41	0.48
2:Z:137:GLN:HG3	2:Z:138:ALA:N	2.27	0.48
1:B:210:VAL:HG23	1:B:225:ILE:HB	1.94	0.48
2:W:3:ILE:HB	2:W:139:VAL:HG12	1.93	0.48
2:W:99:LEU:HD12	2:W:100:ALA:N	2.28	0.48
1:E:70:GLU:HB3	1:E:118:TYR:CD2	2.49	0.48
1:F:178:THR:HG22	1:F:182:ARG:NH1	2.27	0.48
1:S:212:VAL:HG12	1:S:223:ARG:HB3	1.96	0.48
1:T:54:SER:CB	1:T:75:ARG:HD2	2.43	0.48
2:X:88:ARG:HD3	2:X:126:ALA:O	2.14	0.48
1:D:41:PHE:CB	1:D:53:ILE:HD13	2.41	0.48
1:Q:189:ARG:HH21	1:Q:203:LEU:N	2.10	0.48
1:T:33:LEU:CD2	1:T:153:PHE:HB3	2.38	0.48
1:T:41:PHE:HB3	1:T:53:ILE:HD13	1.95	0.48
1:A:62:PHE:CE2	1:A:122:LEU:HD22	2.49	0.48
2:H:156:GLN:O	2:H:162:SER:OG	2.29	0.48
2:K:6:LEU:CA	2:K:120:ILE:HD11	2.43	0.48
2:Y:18:ARG:HD3	2:Y:193:THR:HG23	1.94	0.48
1:E:163:ILE:HD13	1:E:188:LEU:HD23	1.96	0.48
2:Y:205:VAL:HG11	2:Y:210:ILE:HD11	1.95	0.48
1:A:121:GLU:OE1	1:A:140:ARG:HD2	2.14	0.48
1:D:232:ALA:O	1:D:233:LEU:HD23	2.14	0.47
2:I:137:GLN:OE1	2:I:147:LYS:HD3	2.14	0.47
1:C:93:ASP:OD1	2:K:75:THR:HG23	2.14	0.47
1:S:41:PHE:CB	1:S:53:ILE:HD13	2.44	0.47
1:T:55:GLU:HB2	1:T:222:PHE:CG	2.50	0.47
1:D:141:ILE:N	1:D:141:ILE:HD12	2.28	0.47
1:E:30:VAL:HG22	1:E:43:ALA:HB1	1.95	0.47
1:G:123:CYS:HA	1:G:139:TYR:O	2.15	0.47
1:P:32:ALA:HA	1:P:40:LEU:O	2.15	0.47
1:R:54:SER:HB2	1:R:75:ARG:HD2	1.97	0.47
2:Y:137:GLN:HG3	2:Y:138:ALA:N	2.29	0.47
1:B:123:CYS:HA	1:B:139:TYR:O	2.14	0.47
1:B:54:SER:HB2	1:B:75:ARG:HD2	1.96	0.47
1:S:150:GLU:HG3	1:S:154:VAL:HG22	1.95	0.47
2:I:33:LYS:O	2:I:44:GLY:HA2	2.14	0.47
2:L:99:LEU:HD12	2:L:100:ALA:N	2.29	0.47
2:Y:141:SER:HB3	5:Y:302:CIT:H41	1.96	0.47
6:C:425:HOH:O	1:D:115:ALA:HB3	2.14	0.47
1:F:25:ALA:O	1:F:158:GLY:HA2	2.14	0.47
1:P:74:LEU:HD11	1:P:107:LEU:HD21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:54:SER:CB	1:R:75:ARG:HD2	2.45	0.47
1:R:56:LEU:HD13	1:R:99:LEU:HG	1.95	0.47
1:R:56:LEU:HG	1:R:62:PHE:HB2	1.97	0.47
1:B:45:ASN:ND2	1:B:50:LEU:O	2.32	0.47
1:D:9:MET:HE2	1:E:19:LEU:HD13	1.96	0.47
2:H:123:PHE:HA	2:H:128:GLY:O	2.15	0.47
2:K:211:ALA:O	2:K:215:ARG:HG3	2.14	0.47
2:M:197:ILE:HG12	2:M:202:ALA:HB2	1.97	0.47
1:O:202:THR:HA	6:O:414:HOH:O	2.14	0.47
1:O:54:SER:CB	1:O:75:ARG:HD2	2.45	0.47
1:O:67:LYS:HG2	1:O:69:ASN:OD1	2.14	0.47
1:S:72:ASP:O	1:S:76:ARG:HG3	2.15	0.47
1:B:181:LEU:HD11	1:B:234:LEU:HD21	1.96	0.47
1:G:56:LEU:HG	1:G:62:PHE:HB2	1.97	0.47
2:H:20:SER:HB3	2:H:28:GLY:HA3	1.97	0.47
2:L:197:ILE:HG12	2:L:202:ALA:CB	2.45	0.47
1:O:25:ALA:O	1:O:158:GLY:HA2	2.14	0.47
2:Z:72:VAL:CG2	2:Z:73:PRO:HD2	2.45	0.47
2:H:45:ILE:HD12	2:H:52:ALA:O	2.15	0.47
1:R:22:LYS:O	1:R:26:ARG:HG3	2.15	0.47
1:U:39:VAL:HG23	1:U:127:VAL:HG12	1.96	0.47
1:U:123:CYS:HA	1:U:139:TYR:O	2.15	0.47
1:C:128:ALA:HB2	1:C:134:LYS:HB3	1.97	0.46
1:D:22:LYS:O	1:D:26:ARG:HG2	2.16	0.46
1:R:77:GLY:HA3	3:R:301:DMF:O	2.15	0.46
1:D:123:CYS:HB2	1:D:156:MET:SD	2.55	0.46
2:Z:18:ARG:HD3	2:Z:193:THR:HG23	1.96	0.46
1:G:10:GLU:O	1:G:14:ARG:HG3	2.15	0.46
2:K:7:LYS:HE2	2:K:118:GLY:O	2.15	0.46
2:V:42:ALA:HB2	2:V:195:VAL:HG11	1.97	0.46
1:E:99:LEU:HA	1:E:102:VAL:CG1	2.45	0.46
2:J:137:GLN:HG3	2:J:138:ALA:N	2.31	0.46
2:L:92:ALA:HA	2:L:95:MET:CE	2.46	0.46
2:M:173:ASP:OD1	2:M:221:ARG:NH1	2.46	0.46
1:O:30:VAL:HG22	1:O:43:ALA:CB	2.45	0.46
1:S:16:ARG:NH1	1:S:111:PHE:O	2.49	0.46
1:C:28:LYS:N	1:C:28:LYS:HD3	2.30	0.46
2:M:132:GLU:HG3	2:M:137:GLN:HB2	1.98	0.46
1:C:28:LYS:H	1:C:28:LYS:HD3	1.79	0.46
1:F:93:ASP:OD1	2:N:75:THR:HG23	2.16	0.46
2:X:1:THR:HG22	2:X:2:THR:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:219:ARG:NH2	2:X:64:GLU:OE1	2.47	0.46
1:B:99:LEU:HD12	1:B:100:ALA:H	5.46	0.46
2:X:41:THR:HG23	2:X:104:LEU:HD11	1.98	0.46
2:J:66:TYR:CD2	3:J:304:DMF:H13	2.50	0.46
1:T:118:TYR:HB3	1:T:120:VAL:HG22	1.98	0.46
1:A:56:LEU:HD13	1:A:99:LEU:HD13	1.97	0.46
1:D:35:TYR:CZ	1:D:177:LEU:HD13	2.50	0.46
1:F:62:PHE:CE2	1:F:122:LEU:HD22	2.50	0.46
1:F:54:SER:CB	1:F:75:ARG:HD2	2.46	0.46
2:N:14:MET:SD	2:N:34:VAL:HG13	2.56	0.46
1:O:189:ARG:HA	6:O:407:HOH:O	2.16	0.46
1:R:147:ILE:HG12	1:S:50:LEU:HD11	1.98	0.46
1:B:60:VAL:HG11	1:B:99:LEU:HD12	1.98	0.46
2:H:132:GLU:HG3	2:H:137:GLN:HB2	1.98	0.46
2:I:80:ILE:HB	3:I:303:DMF:H23	1.98	0.46
1:B:101:ASN:ND2	1:C:76:ARG:HH21	2.14	0.45
1:B:155:VAL:HG11	1:B:163:ILE:HB	1.99	0.45
1:C:32:ALA:HA	1:C:40:LEU:O	2.16	0.45
1:D:70:GLU:HB3	1:D:118:TYR:CD2	2.52	0.45
1:O:202:THR:HG22	1:O:202:THR:O	2.15	0.45
2:I:198:ASP:HB2	6:I:404:HOH:O	2.16	0.45
1:B:93:ASP:OD1	2:J:75:THR:HG23	2.16	0.45
1:O:42:VAL:HG22	1:O:210:VAL:HG12	1.97	0.45
1:U:28:LYS:HB3	1:U:44:GLU:HB2	1.98	0.45
1:C:217:ARG:HD3	1:C:218:PRO:HD2	1.98	0.45
1:G:89:TYR:CD1	2:H:82:ARG:HD3	2.52	0.45
2:X:141:SER:HB3	5:X:302:CIT:H22	1.97	0.45
2:Y:169:GLU:HA	2:Y:217:ILE:HD13	1.97	0.45
2:K:144:LEU:HD23	2:K:144:LEU:C	2.37	0.45
1:P:231:GLN:O	1:P:235:VAL:HG12	2.17	0.45
1:B:123:CYS:SG	1:B:154:VAL:HG21	2.56	0.45
1:E:181:LEU:O	1:E:185:VAL:HG23	2.16	0.45
2:M:18:ARG:NH1	2:M:191:PHE:O	2.48	0.45
1:F:40:LEU:HD21	1:F:181:LEU:HA	1.97	0.45
1:R:101:ASN:ND2	1:S:76:ARG:NH2	2.64	0.45
1:T:60:VAL:HG11	1:T:99:LEU:HD12	1.97	0.45
2:W:72:VAL:HG23	2:W:73:PRO:HD2	1.98	0.45
2:H:6:LEU:HG	2:H:13:VAL:HG13	1.99	0.45
1:R:45:ASN:ND2	1:R:209:GLU:OE1	2.45	0.45
1:T:181:LEU:O	1:T:185:VAL:HG23	2.17	0.45
1:A:179:ASP:O	1:A:183:ILE:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:VAL:HG13	1:C:230:LEU:HD23	1.98	0.45
1:C:39:VAL:HG23	1:C:127:VAL:HG12	1.97	0.45
2:J:81:ASN:O	2:J:85:ILE:HG12	2.17	0.45
2:N:113:ASP:OD1	2:N:115:GLN:HB2	2.17	0.45
2:M:25:MET:CE	2:N:144:LEU:HD21	2.44	0.45
1:Q:155:VAL:HG11	1:Q:164:ALA:HB2	1.99	0.45
2:I:14:MET:SD	2:I:34:VAL:HG13	2.57	0.45
1:O:181:LEU:HD22	1:O:233:LEU:HD23	1.99	0.45
1:P:107:LEU:HD12	1:P:141:ILE:CG2	2.47	0.45
1:R:229:ALA:O	1:R:233:LEU:HD13	2.17	0.45
2:W:20:SER:HB2	2:W:31:VAL:HG21	1.98	0.45
1:P:152:HIS:NE2	1:P:173:GLU:OE2	2.41	0.45
1:P:87:TYR:CZ	2:W:58:LEU:HD13	2.52	0.45
1:U:118:TYR:N	6:U:403:HOH:O	2.48	0.45
1:E:138:LEU:HB2	1:E:150:GLU:O	2.16	0.44
1:P:74:LEU:CD1	1:P:120:VAL:HG21	2.47	0.44
1:Q:235:VAL:O	1:Q:235:VAL:HG13	2.17	0.44
2:Y:62:GLU:OE2	2:Y:82:ARG:CD	2.64	0.44
1:A:56:LEU:HG	1:A:62:PHE:HB2	1.99	0.44
1:B:56:LEU:HG	1:B:62:PHE:HB2	1.99	0.44
2:L:6:LEU:HD12	2:L:6:LEU:C	2.37	0.44
2:V:208:SER:O	2:V:212:GLU:HG2	2.17	0.44
1:A:123:CYS:HA	1:A:139:TYR:O	2.16	0.44
2:L:38:ASP:OD1	2:L:38:ASP:C	2.56	0.44
2:L:62:GLU:OE2	2:L:82:ARG:CD	2.65	0.44
1:O:76:ARG:HH11	1:U:101:ASN:ND2	2.15	0.44
1:A:66:GLY:HA3	1:A:119:GLU:O	2.18	0.44
2:K:165:ARG:HG3	2:K:213:LEU:HD22	1.99	0.44
1:Q:110:ILE:HA	1:Q:114:GLN:HG3	2.00	0.44
1:C:28:LYS:CD	1:C:28:LYS:N	2.81	0.44
2:J:81:ASN:HB2	3:J:303:DMF:H23	2.00	0.44
1:C:99:LEU:HA	1:C:102:VAL:HG12	1.99	0.44
1:D:78:GLY:HA3	1:D:103:TYR:OH	2.18	0.44
1:E:140:ARG:NH2	1:E:155:VAL:O	2.50	0.44
2:H:45:ILE:HB	2:H:52:ALA:HB1	1.99	0.44
1:O:181:LEU:HD23	1:O:233:LEU:HD23	1.99	0.44
1:Q:24:ILE:HD13	6:Q:426:HOH:O	2.17	0.44
1:R:99:LEU:O	1:R:102:VAL:HG22	2.17	0.44
1:R:16:ARG:HB3	1:R:117:PRO:HG3	1.99	0.44
1:U:217:ARG:NH1	1:U:220:ARG:O	2.50	0.44
1:Q:152:HIS:HB3	1:Q:171:TYR:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:GLU:HG2	1:C:48:ARG:HH21	1.82	0.44
1:F:58:ASP:OD1	1:F:91:ARG:NH2	2.40	0.44
2:J:169:GLU:HA	2:J:217:ILE:HD13	2.00	0.44
1:Q:41:PHE:CB	1:Q:53:ILE:HD13	2.47	0.44
1:Q:54:SER:CB	1:Q:75:ARG:HD2	2.48	0.44
1:C:123:CYS:HA	1:C:139:TYR:O	2.18	0.43
1:C:140:ARG:NH1	1:C:155:VAL:O	2.44	0.43
1:A:54:SER:CB	1:A:75:ARG:HD2	2.48	0.43
2:L:12:VAL:HG12	2:L:197:ILE:HB	2.01	0.43
1:T:137:GLU:O	1:T:138:LEU:HD23	2.18	0.43
2:Z:213:LEU:O	2:Z:217:ILE:HG13	2.18	0.43
1:O:89:TYR:CD1	2:W:82:ARG:HD3	2.53	0.43
1:Q:141:ILE:N	1:Q:141:ILE:HD12	2.33	0.43
1:S:39:VAL:HG23	1:S:127:VAL:CG1	2.48	0.43
1:T:99:LEU:HA	1:T:102:VAL:HG22	2.00	0.43
2:W:122:SER:HB3	2:W:137:GLN:HG2	2.01	0.43
1:G:24:ILE:HD11	1:G:120:VAL:O	2.18	0.43
1:G:121:GLU:OE2	1:G:140:ARG:NH1	2.48	0.43
2:I:20:SER:O	2:I:27:SER:N	2.45	0.43
1:O:30:VAL:HG13	1:O:43:ALA:HB2	2.01	0.43
2:Y:20:SER:HB2	2:Y:31:VAL:HG21	1.99	0.43
1:C:55:GLU:HB2	1:C:222:PHE:CG	2.54	0.43
1:D:57:TYR:CD1	1:D:82:ALA:HB1	2.53	0.43
2:H:65:HIS:NE2	2:H:69:LEU:HD11	2.33	0.43
2:J:132:GLU:HG3	2:J:137:GLN:HE21	1.82	0.43
1:B:85:ARG:HB3	6:B:402:HOH:O	2.19	0.43
1:O:170:SER:OG	1:O:183:ILE:HB	2.18	0.43
1:A:140:ARG:HD3	1:A:154:VAL:HG13	2.01	0.43
1:A:92:ARG:HA	6:A:407:HOH:O	2.18	0.43
1:D:68:PHE:HA	1:D:71:PHE:CZ	2.54	0.43
1:F:185:VAL:HG13	1:F:203:LEU:HD12	2.01	0.43
2:L:43:THR:HG22	2:L:45:ILE:HD11	2.01	0.43
1:T:66:GLY:HA3	1:T:119:GLU:O	2.19	0.43
1:G:92:ARG:HG2	1:G:92:ARG:O	2.19	0.43
2:H:95:MET:HA	2:H:95:MET:CE	2.49	0.43
1:U:32:ALA:HA	1:U:40:LEU:O	2.18	0.43
1:F:123:CYS:HA	1:F:139:TYR:O	2.19	0.43
2:L:65:HIS:NE2	2:L:69:LEU:HD11	2.34	0.43
1:U:22:LYS:O	1:U:26:ARG:HG3	2.18	0.43
1:A:99:LEU:HA	1:A:102:VAL:HG12	2.01	0.43
1:F:217:ARG:HD2	1:F:223:ARG:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:70:GLU:HB3	1:F:118:TYR:CD2	2.54	0.43
1:P:205:VAL:HG22	1:P:230:LEU:HG	2.01	0.43
1:R:70:GLU:HB3	1:R:118:TYR:CD2	2.54	0.43
1:U:77:GLY:HA3	3:U:301:DMF:C1	2.49	0.43
1:B:210:VAL:CG2	1:B:230:LEU:HD13	2.49	0.42
1:F:150:GLU:HA	1:F:151:PRO:HD3	1.85	0.42
2:I:6:LEU:HD12	2:I:13:VAL:HG12	2.01	0.42
2:I:72:VAL:CG2	2:I:73:PRO:HD2	2.49	0.42
2:L:14:MET:SD	2:L:34:VAL:HG13	2.59	0.42
1:P:179:ASP:O	1:P:183:ILE:HG13	2.19	0.42
6:Q:427:HOH:O	1:R:67:LYS:HE2	2.19	0.42
1:A:9:MET:CE	1:B:117:PRO:HD2	2.49	0.42
1:G:31:VAL:HG12	1:G:33:LEU:CD1	2.48	0.42
2:N:99:LEU:HG	2:N:100:ALA:N	2.34	0.42
2:N:3:ILE:O	2:N:138:ALA:HA	2.19	0.42
2:N:72:VAL:HG23	2:N:73:PRO:HD2	2.01	0.42
1:R:16:ARG:NH2	1:R:114:GLN:O	2.36	0.42
2:X:41:THR:CG2	2:X:104:LEU:HD11	2.49	0.42
2:Y:12:VAL:CG2	2:Y:120:ILE:HD11	2.49	0.42
2:W:38:ASP:C	2:W:38:ASP:OD1	2.57	0.42
2:H:148:SER:HB3	2:Z:148:SER:HB3	2.00	0.42
1:A:25:ALA:O	1:A:158:GLY:HA2	2.20	0.42
1:B:9:MET:HB3	1:C:15:GLU:HB3	2.01	0.42
1:D:30:VAL:HG22	1:D:43:ALA:HB1	1.99	0.42
1:D:76:ARG:HD3	6:D:315:HOH:O	2.19	0.42
2:K:88:ARG:HD3	2:K:126:ALA:O	2.19	0.42
1:T:92:ARG:O	1:T:92:ARG:HG3	2.19	0.42
2:Z:88:ARG:HD3	2:Z:126:ALA:O	2.19	0.42
1:A:32:ALA:HA	1:A:40:LEU:O	2.18	0.42
2:H:22:GLN:HG3	4:H:301:M6Y:O09	2.20	0.42
2:I:38:ASP:C	2:I:38:ASP:OD1	2.57	0.42
1:S:110:ILE:HG23	1:S:114:GLN:HG3	2.01	0.42
1:A:217:ARG:NE	1:A:223:ARG:HH11	2.18	0.42
2:H:124:ASP:OD1	2:H:128:GLY:N	2.46	0.42
2:K:103:LEU:HD12	2:K:121:VAL:O	2.20	0.42
2:L:112:SER:O	2:L:114:PRO:HD3	2.19	0.42
1:O:202:THR:C	1:O:203:LEU:HD12	2.40	0.42
1:O:89:TYR:CE1	2:W:82:ARG:HD3	2.54	0.42
1:D:56:LEU:HG	1:D:62:PHE:HB2	2.00	0.42
2:L:32:ARG:NE	2:L:34:VAL:O	2.42	0.42
2:Y:76:PHE:CE2	2:Y:80:ILE:HD11	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:PHE:CB	1:B:53:ILE:HD13	2.48	0.42
2:L:20:SER:HB3	2:L:28:GLY:CA	2.50	0.42
1:O:26:ARG:O	1:O:26:ARG:CG	2.67	0.42
1:O:85:ARG:NH1	1:O:98:GLN:NE2	2.67	0.42
1:Q:183:ILE:HD12	1:Q:183:ILE:HA	1.82	0.42
1:U:48:ARG:O	1:U:48:ARG:HG3	2.19	0.42
2:Z:186:LEU:N	2:Z:186:LEU:HD12	2.35	0.42
1:D:217:ARG:CZ	1:D:223:ARG:HD3	2.50	0.42
1:G:32:ALA:HA	1:G:40:LEU:O	2.20	0.42
1:C:220:ARG:HH22	2:J:67:GLU:CD	2.22	0.42
2:K:141:SER:HB3	5:K:302:CIT:C4	2.49	0.42
2:N:136:TYR:OH	2:N:151:LYS:HA	2.20	0.42
1:R:164:ALA:O	1:R:168:LYS:HB2	2.20	0.42
1:U:235:VAL:HG23	1:U:235:VAL:O	2.20	0.42
2:W:137:GLN:HG3	2:W:138:ALA:N	2.35	0.42
2:Y:1:THR:OG1	5:Y:302:CIT:O2	2.28	0.42
1:E:189:ARG:HB2	1:E:203:LEU:HD12	2.02	0.42
2:I:88:ARG:HD3	2:I:126:ALA:O	2.20	0.42
2:K:6:LEU:HA	2:K:120:ILE:CD1	2.50	0.42
2:N:137:GLN:HG3	2:N:138:ALA:N	2.35	0.42
1:T:60:VAL:HG11	1:T:99:LEU:CD1	2.50	0.42
2:Y:107:TYR:CE1	2:Y:117:ALA:HB3	2.55	0.42
1:A:116:LYS:HE3	6:A:414:HOH:O	2.19	0.41
2:N:78:GLY:O	2:N:82:ARG:HG2	2.20	0.41
1:U:51:GLN:HG3	6:U:423:HOH:O	2.20	0.41
1:C:11:GLN:O	1:C:15:GLU:HB2	2.19	0.41
1:E:53:ILE:HD12	1:E:209:GLU:HG2	2.02	0.41
2:I:22:GLN:HG3	4:I:301:M6Y:O09	2.21	0.41
1:Q:180:ALA:HA	1:Q:183:ILE:HG22	2.03	0.41
1:R:19:LEU:HD23	1:R:19:LEU:C	2.40	0.41
1:T:52:LYS:HE3	1:T:64:ALA:O	2.20	0.41
1:U:17:SER:HG	1:U:143:TYR:HH	1.66	0.41
1:A:41:PHE:CB	1:A:53:ILE:HD13	2.51	0.41
1:G:225:ILE:HG21	1:G:233:LEU:HD22	2.02	0.41
2:I:64:GLU:HG2	2:I:68:LYS:HE2	2.02	0.41
2:J:5:ALA:HA	2:J:13:VAL:O	2.20	0.41
1:S:33:LEU:CD1	1:S:153:PHE:HB3	2.46	0.41
1:S:19:LEU:HD23	1:S:19:LEU:C	2.41	0.41
1:T:32:ALA:HA	1:T:40:LEU:O	2.20	0.41
1:U:232:ALA:C	1:U:234:LEU:H	2.23	0.41
2:W:6:LEU:HA	2:W:120:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:197:ILE:HA	2:W:201:GLY:O	2.19	0.41
2:Z:112:SER:O	2:Z:114:PRO:HD3	2.20	0.41
1:C:225:ILE:HG22	1:C:230:LEU:HB2	2.02	0.41
2:H:3:ILE:O	2:H:138:ALA:HA	2.19	0.41
1:O:33:LEU:HD12	1:O:40:LEU:HB3	2.02	0.41
1:S:213:LEU:HA	1:S:213:LEU:HD23	1.89	0.41
2:Y:152:LYS:HD3	6:Y:404:HOH:O	2.20	0.41
1:E:178:THR:HG23	1:E:233:LEU:O	2.21	0.41
1:D:28:LYS:HB3	1:D:44:GLU:HB2	2.03	0.41
1:E:106:THR:O	1:E:110:ILE:HG13	2.20	0.41
2:H:78:GLY:O	2:H:82:ARG:HG2	2.20	0.41
2:N:211:ALA:O	2:N:215:ARG:HG3	2.20	0.41
1:S:217:ARG:HH12	1:S:223:ARG:HG3	1.86	0.41
1:T:52:LYS:HB3	1:T:52:LYS:HE3	1.91	0.41
1:T:54:SER:HB2	1:T:75:ARG:HD2	2.02	0.41
2:W:51:VAL:HG21	2:W:98:LEU:HB3	2.03	0.41
1:A:64:ALA:HA	1:A:156:MET:CE	2.48	0.41
1:C:161:GLU:HB3	1:C:162:PRO:HD3	2.03	0.41
1:E:230:LEU:O	1:E:234:LEU:HG	2.21	0.41
2:I:50:ALA:HB2	2:J:128:GLY:N	2.36	0.41
1:O:181:LEU:O	1:O:185:VAL:HG23	2.20	0.41
1:S:10:GLU:HB3	6:S:411:HOH:O	2.20	0.41
1:S:54:SER:HB2	1:S:75:ARG:HD2	2.03	0.41
1:D:205:VAL:HG13	1:D:230:LEU:HD23	2.02	0.41
2:M:141:SER:HB3	5:M:302:CIT:O5	2.20	0.41
1:S:54:SER:CB	1:S:75:ARG:HD2	2.51	0.41
1:B:137:GLU:HG2	1:C:48:ARG:NH2	2.36	0.41
1:C:166:ALA:O	1:C:170:SER:OG	2.28	0.41
1:F:33:LEU:HD12	1:F:33:LEU:O	2.21	0.41
1:T:30:VAL:HG21	1:T:52:LYS:HE2	2.02	0.41
1:T:35:TYR:CZ	1:T:177:LEU:HD13	2.55	0.41
2:W:72:VAL:HG22	2:W:73:PRO:HD2	2.02	0.41
1:F:142:THR:OG1	1:F:146:SER:HB2	2.20	0.41
2:H:38:ASP:OD1	2:H:38:ASP:C	2.59	0.41
2:N:112:SER:O	2:N:114:PRO:HD3	2.21	0.41
1:P:68:PHE:HA	1:P:71:PHE:CZ	2.55	0.41
1:Q:205:VAL:HG12	1:Q:230:LEU:HG	2.03	0.41
2:W:137:GLN:OE1	2:W:147:LYS:HD3	2.20	0.41
2:W:16:GLY:O	2:W:192:PRO:HB3	2.21	0.41
1:E:140:ARG:O	1:E:147:ILE:HA	2.21	0.40
2:L:137:GLN:OE1	2:L:147:LYS:HD3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:38:ASP:C	2:N:38:ASP:OD1	2.60	0.40
1:S:210:VAL:HG21	1:S:230:LEU:HD11	2.02	0.40
1:B:10:GLU:OE2	1:C:15:GLU:HG2	2.21	0.40
1:E:33:LEU:O	1:E:33:LEU:HD12	2.21	0.40
2:J:12:VAL:HG12	2:J:197:ILE:HB	2.04	0.40
2:J:45:ILE:HD12	2:J:45:ILE:N	2.36	0.40
1:O:167:LEU:O	1:O:171:TYR:N	2.55	0.40
1:O:163:ILE:HD13	1:O:188:LEU:HD23	2.02	0.40
1:O:205:VAL:HG22	1:O:230:LEU:HG	2.02	0.40
1:S:99:LEU:O	1:S:102:VAL:HG12	2.21	0.40
1:S:167:LEU:O	1:S:171:TYR:HB2	2.21	0.40
6:S:420:HOH:O	1:T:67:LYS:HG3	2.21	0.40
2:Y:20:SER:HB3	2:Y:28:GLY:HA3	2.03	0.40
2:Z:6:LEU:HA	2:Z:135:GLY:O	2.21	0.40
1:A:85:ARG:NE	6:A:403:HOH:O	2.47	0.40
1:S:152:HIS:HB3	1:S:171:TYR:CZ	2.56	0.40
1:T:168:LYS:HB2	1:T:168:LYS:HE3	1.88	0.40
2:Z:156:GLN:OE1	2:Z:165:ARG:NH1	2.39	0.40
1:E:39:VAL:HG23	1:E:127:VAL:HG12	2.04	0.40
1:E:77:GLY:HA3	3:E:301:DMF:C2	2.48	0.40
2:K:123:PHE:HA	2:K:128:GLY:O	2.21	0.40
1:E:208:LEU:HD23	1:E:208:LEU:HA	1.86	0.40
2:H:132:GLU:CG	2:H:137:GLN:HE21	2.34	0.40
2:H:137:GLN:OE1	2:H:147:LYS:HD3	2.20	0.40
2:H:51:VAL:HG21	2:H:98:LEU:HB3	2.03	0.40
2:I:137:GLN:HG3	2:I:138:ALA:N	2.36	0.40
1:Q:68:PHE:HA	1:Q:71:PHE:CZ	2.56	0.40
2:H:148:SER:CB	2:Z:148:SER:HB3	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	214/240 (89%)	210 (98%)	4 (2%)	0	100	100
1	B	211/240 (88%)	201 (95%)	10 (5%)	0	100	100
1	C	213/240 (89%)	203 (95%)	10 (5%)	0	100	100
1	D	211/240 (88%)	203 (96%)	8 (4%)	0	100	100
1	E	213/240 (89%)	207 (97%)	6 (3%)	0	100	100
1	F	212/240 (88%)	205 (97%)	7 (3%)	0	100	100
1	G	211/240 (88%)	206 (98%)	5 (2%)	0	100	100
1	O	213/240 (89%)	207 (97%)	6 (3%)	0	100	100
1	P	215/240 (90%)	209 (97%)	6 (3%)	0	100	100
1	Q	212/240 (88%)	204 (96%)	8 (4%)	0	100	100
1	R	211/240 (88%)	205 (97%)	5 (2%)	1 (0%)	29	43
1	S	214/240 (89%)	206 (96%)	7 (3%)	1 (0%)	29	43
1	T	213/240 (89%)	205 (96%)	8 (4%)	0	100	100
1	U	212/240 (88%)	203 (96%)	9 (4%)	0	100	100
2	H	220/234 (94%)	215 (98%)	5 (2%)	0	100	100
2	I	220/234 (94%)	210 (96%)	10 (4%)	0	100	100
2	J	220/234 (94%)	213 (97%)	7 (3%)	0	100	100
2	K	221/234 (94%)	216 (98%)	5 (2%)	0	100	100
2	L	221/234 (94%)	215 (97%)	6 (3%)	0	100	100
2	M	220/234 (94%)	216 (98%)	4 (2%)	0	100	100
2	N	221/234 (94%)	212 (96%)	9 (4%)	0	100	100
2	V	221/234 (94%)	218 (99%)	3 (1%)	0	100	100
2	W	221/234 (94%)	217 (98%)	4 (2%)	0	100	100
2	X	220/234 (94%)	217 (99%)	3 (1%)	0	100	100
2	Y	221/234 (94%)	217 (98%)	4 (2%)	0	100	100
2	Z	220/234 (94%)	215 (98%)	5 (2%)	0	100	100
2	a	221/234 (94%)	215 (97%)	6 (3%)	0	100	100
2	b	221/234 (94%)	218 (99%)	3 (1%)	0	100	100
All	All	6063/6636 (91%)	5888 (97%)	173 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	151	PRO
1	R	151	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	167/184 (91%)	165 (99%)	2 (1%)	71 84
1	B	165/184 (90%)	164 (99%)	1 (1%)	86 92
1	C	166/184 (90%)	164 (99%)	2 (1%)	71 84
1	D	164/184 (89%)	162 (99%)	2 (1%)	71 84
1	E	166/184 (90%)	165 (99%)	1 (1%)	86 92
1	F	165/184 (90%)	165 (100%)	0	100 100
1	G	165/184 (90%)	165 (100%)	0	100 100
1	O	166/184 (90%)	165 (99%)	1 (1%)	86 92
1	P	168/184 (91%)	168 (100%)	0	100 100
1	Q	166/184 (90%)	163 (98%)	3 (2%)	59 75
1	R	164/184 (89%)	161 (98%)	3 (2%)	59 75
1	S	167/184 (91%)	163 (98%)	4 (2%)	49 67
1	T	166/184 (90%)	166 (100%)	0	100 100
1	U	165/184 (90%)	165 (100%)	0	100 100
2	H	165/172 (96%)	162 (98%)	3 (2%)	59 75
2	I	165/172 (96%)	165 (100%)	0	100 100
2	J	165/172 (96%)	163 (99%)	2 (1%)	71 84
2	K	165/172 (96%)	165 (100%)	0	100 100
2	L	165/172 (96%)	165 (100%)	0	100 100
2	M	165/172 (96%)	165 (100%)	0	100 100
2	N	165/172 (96%)	165 (100%)	0	100 100
2	V	165/172 (96%)	164 (99%)	1 (1%)	86 92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	W	165/172 (96%)	164 (99%)	1 (1%)	86 92
2	X	165/172 (96%)	163 (99%)	2 (1%)	71 84
2	Y	165/172 (96%)	164 (99%)	1 (1%)	86 92
2	Z	165/172 (96%)	163 (99%)	2 (1%)	71 84
2	a	165/172 (96%)	165 (100%)	0	100 100
2	b	165/172 (96%)	164 (99%)	1 (1%)	86 92
All	All	4630/4984 (93%)	4598 (99%)	32 (1%)	84 91

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	LYS
1	A	169	GLU
1	B	57	TYR
1	C	33	LEU
1	C	233	LEU
1	D	132	GLU
1	D	228	SER
1	E	33	LEU
2	H	57	ARG
2	H	161	ASP
2	H	203	VAL
2	J	208	SER
2	J	219	GLU
1	O	165	ASN
1	Q	159	THR
1	Q	183	ILE
1	Q	189	ARG
1	R	99	LEU
1	R	169	GLU
1	R	228	SER
1	S	114	GLN
1	S	179	ASP
1	S	212	VAL
1	S	228	SER
2	V	212	GLU
2	W	209	ARG
2	X	17	ASP
2	X	122	SER
2	Y	82	ARG

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Mol	Chain	Res	Type
2	Z	31	VAL
2	Z	144	LEU
2	b	122	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	101	ASN
1	E	101	ASN
2	M	22	GLN
1	O	98	GLN
1	Q	101	ASN
1	R	98	GLN
1	R	101	ASN
1	U	101	ASN
2	W	110	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry

48 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	DMF	B	301	-	4,4,4	0.38	0	4,4,4	0.39	0
3	DMF	S	301	-	4,4,4	0.40	0	4,4,4	0.43	0
3	DMF	J	303	-	4,4,4	0.38	0	4,4,4	0.45	0
4	M6Y	W	301	-	42,44,44	2.81	11 (26%)	54,61,61	1.63	13 (24%)
5	CIT	V	302	-	3,12,12	1.46	0	3,17,17	2.23	1 (33%)
3	DMF	P	301	-	4,4,4	0.36	0	4,4,4	0.31	0
5	CIT	J	302	-	3,12,12	1.37	0	3,17,17	2.41	2 (66%)
4	M6Y	X	301	-	42,44,44	2.82	12 (28%)	54,61,61	1.60	10 (18%)
3	DMF	T	301	-	4,4,4	0.38	0	4,4,4	0.50	0
3	DMF	J	304	-	4,4,4	0.45	0	4,4,4	0.45	0
5	CIT	b	302	-	3,12,12	1.22	0	3,17,17	1.73	1 (33%)
5	CIT	Y	302	-	3,12,12	1.42	0	3,17,17	2.60	2 (66%)
4	M6Y	J	301	-	42,44,44	2.84	12 (28%)	54,61,61	1.64	11 (20%)
3	DMF	R	302	-	4,4,4	0.36	0	4,4,4	0.44	0
5	CIT	W	302	-	3,12,12	1.32	0	3,17,17	1.81	1 (33%)
4	M6Y	a	301	-	42,44,44	2.83	11 (26%)	54,61,61	1.63	10 (18%)
5	CIT	a	302	-	3,12,12	1.42	0	3,17,17	2.26	2 (66%)
4	M6Y	V	301	-	42,44,44	2.87	11 (26%)	54,61,61	1.52	10 (18%)
5	CIT	N	302	-	3,12,12	1.37	0	3,17,17	2.62	2 (66%)
4	M6Y	M	301	-	42,44,44	2.85	10 (23%)	54,61,61	1.52	7 (12%)
4	M6Y	L	301	-	42,44,44	2.85	11 (26%)	54,61,61	1.54	10 (18%)
3	DMF	G	302	-	4,4,4	0.38	0	4,4,4	0.43	0
4	M6Y	b	301	-	42,44,44	3.48	26 (61%)	54,61,61	1.84	18 (33%)
3	DMF	S	302	-	4,4,4	0.41	0	4,4,4	0.37	0
3	DMF	O	301	-	4,4,4	0.32	0	4,4,4	0.31	0
5	CIT	M	302	-	3,12,12	1.20	0	3,17,17	1.81	1 (33%)
5	CIT	I	302	-	3,12,12	1.54	0	3,17,17	2.14	1 (33%)
5	CIT	X	302	-	3,12,12	1.42	0	3,17,17	1.71	0
4	M6Y	N	301	-	42,44,44	2.83	11 (26%)	54,61,61	1.51	11 (20%)
3	DMF	E	301	-	4,4,4	0.38	0	4,4,4	0.36	0
3	DMF	G	301	-	4,4,4	0.35	0	4,4,4	0.33	0
3	DMF	C	301	-	4,4,4	0.38	0	4,4,4	0.43	0
5	CIT	L	302	-	3,12,12	1.25	0	3,17,17	2.38	1 (33%)
4	M6Y	Z	301	-	42,44,44	2.82	11 (26%)	54,61,61	1.52	12 (22%)
3	DMF	I	303	-	4,4,4	0.41	0	4,4,4	0.36	0
3	DMF	Q	301	-	4,4,4	0.36	0	4,4,4	0.32	0
4	M6Y	Y	301	-	42,44,44	2.85	11 (26%)	54,61,61	1.56	12 (22%)
5	CIT	K	302	-	3,12,12	1.11	0	3,17,17	1.80	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	CIT	Z	302	-	3,12,12	1.33	0	3,17,17	1.86	1 (33%)
4	M6Y	H	301	-	42,44,44	2.85	11 (26%)	54,61,61	1.56	11 (20%)
3	DMF	R	301	-	4,4,4	0.35	0	4,4,4	0.42	0
3	DMF	A	301	-	4,4,4	0.37	0	4,4,4	0.38	0
4	M6Y	K	301	-	42,44,44	2.85	11 (26%)	54,61,61	1.59	11 (20%)
3	DMF	F	302	-	4,4,4	0.37	0	4,4,4	0.37	0
4	M6Y	I	301	-	42,44,44	2.85	11 (26%)	54,61,61	1.57	10 (18%)
5	CIT	H	302	-	3,12,12	1.25	0	3,17,17	1.98	1 (33%)
3	DMF	F	301	-	4,4,4	0.35	0	4,4,4	0.41	0
3	DMF	U	301	-	4,4,4	0.34	0	4,4,4	0.41	0

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
3	DMF	B	301	-	-	0/2/2/2	-
3	DMF	S	301	-	-	0/2/2/2	-
3	DMF	J	303	-	-	2/2/2/2	-
4	M6Y	W	301	-	-	2/34/47/47	0/4/4/4
5	CIT	V	302	-	-	1/6/16/16	-
3	DMF	P	301	-	-	0/2/2/2	-
5	CIT	J	302	-	-	1/6/16/16	-
4	M6Y	X	301	-	-	1/34/47/47	0/4/4/4
3	DMF	T	301	-	-	2/2/2/2	-
3	DMF	J	304	-	-	0/2/2/2	-
5	CIT	b	302	-	-	1/6/16/16	-
5	CIT	Y	302	-	-	1/6/16/16	-
4	M6Y	J	301	-	-	2/34/47/47	0/4/4/4
3	DMF	R	302	-	-	2/2/2/2	-
5	CIT	W	302	-	-	1/6/16/16	-
4	M6Y	a	301	-	-	1/34/47/47	0/4/4/4
5	CIT	a	302	-	-	1/6/16/16	-
4	M6Y	V	301	-	-	2/34/47/47	0/4/4/4
5	CIT	N	302	-	-	1/6/16/16	-
4	M6Y	M	301	-	-	1/34/47/47	0/4/4/4
4	M6Y	L	301	-	-	2/34/47/47	0/4/4/4
3	DMF	G	302	-	-	2/2/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	M6Y	b	301	-	-	3/34/47/47	0/4/4/4
3	DMF	S	302	-	-	0/2/2/2	-
3	DMF	O	301	-	-	2/2/2/2	-
5	CIT	M	302	-	-	6/6/16/16	-
5	CIT	I	302	-	-	1/6/16/16	-
5	CIT	X	302	-	-	1/6/16/16	-
4	M6Y	N	301	-	-	2/34/47/47	0/4/4/4
3	DMF	E	301	-	-	0/2/2/2	-
3	DMF	G	301	-	-	0/2/2/2	-
3	DMF	C	301	-	-	2/2/2/2	-
5	CIT	L	302	-	-	2/6/16/16	-
4	M6Y	Z	301	-	-	3/34/47/47	0/4/4/4
3	DMF	I	303	-	-	0/2/2/2	-
3	DMF	Q	301	-	-	0/2/2/2	-
4	M6Y	Y	301	-	-	2/34/47/47	0/4/4/4
5	CIT	K	302	-	-	3/6/16/16	-
5	CIT	Z	302	-	-	1/6/16/16	-
4	M6Y	H	301	-	-	1/34/47/47	0/4/4/4
3	DMF	R	301	-	-	2/2/2/2	-
3	DMF	A	301	-	-	0/2/2/2	-
4	M6Y	K	301	-	-	2/34/47/47	0/4/4/4
3	DMF	F	302	-	-	0/2/2/2	-
4	M6Y	I	301	-	-	1/34/47/47	0/4/4/4
5	CIT	H	302	-	-	1/6/16/16	-
3	DMF	F	301	-	-	0/2/2/2	-
3	DMF	U	301	-	-	2/2/2/2	-

All (170) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	b	301	M6Y	C11-N10	-10.15	1.28	1.47
4	V	301	M6Y	C14-N10	9.51	1.63	1.47
4	Y	301	M6Y	C14-N10	9.42	1.63	1.47
4	H	301	M6Y	C14-N10	9.40	1.63	1.47
4	K	301	M6Y	C14-N10	9.40	1.63	1.47
4	Z	301	M6Y	C14-N10	9.34	1.62	1.47
4	L	301	M6Y	C14-N10	9.34	1.62	1.47
4	I	301	M6Y	C14-N10	9.30	1.62	1.47
4	N	301	M6Y	C14-N10	9.25	1.62	1.47
4	a	301	M6Y	C14-N10	9.25	1.62	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	301	M6Y	C14-N10	9.24	1.62	1.47
4	W	301	M6Y	C14-N10	9.12	1.62	1.47
4	J	301	M6Y	C14-N10	9.11	1.62	1.47
4	X	301	M6Y	C14-N10	9.06	1.62	1.47
4	b	301	M6Y	C13-C14	-9.03	1.30	1.54
4	b	301	M6Y	C14-N10	7.85	1.60	1.47
4	X	301	M6Y	C11-N10	-7.74	1.32	1.47
4	J	301	M6Y	C11-N10	-7.64	1.32	1.47
4	I	301	M6Y	C11-N10	-7.64	1.32	1.47
4	M	301	M6Y	C11-N10	-7.61	1.33	1.47
4	N	301	M6Y	C11-N10	-7.60	1.33	1.47
4	a	301	M6Y	C11-N10	-7.60	1.33	1.47
4	H	301	M6Y	C11-N10	-7.60	1.33	1.47
4	L	301	M6Y	C11-N10	-7.57	1.33	1.47
4	V	301	M6Y	C11-N10	-7.55	1.33	1.47
4	K	301	M6Y	C11-N10	-7.54	1.33	1.47
4	Y	301	M6Y	C11-N10	-7.53	1.33	1.47
4	W	301	M6Y	C11-N10	-7.43	1.33	1.47
4	Z	301	M6Y	C11-N10	-7.40	1.33	1.47
4	J	301	M6Y	C13-C14	-7.14	1.35	1.54
4	I	301	M6Y	C13-C14	-7.13	1.35	1.54
4	H	301	M6Y	C13-C14	-7.13	1.35	1.54
4	Y	301	M6Y	C13-C14	-7.12	1.35	1.54
4	Z	301	M6Y	C13-C14	-7.11	1.35	1.54
4	X	301	M6Y	C13-C14	-7.09	1.35	1.54
4	V	301	M6Y	C13-C14	-7.07	1.35	1.54
4	W	301	M6Y	C13-C14	-7.03	1.35	1.54
4	L	301	M6Y	C13-C14	-7.01	1.35	1.54
4	M	301	M6Y	C13-C14	-7.00	1.35	1.54
4	K	301	M6Y	C13-C14	-6.98	1.35	1.54
4	a	301	M6Y	C13-C14	-6.93	1.36	1.54
4	N	301	M6Y	C13-C14	-6.92	1.36	1.54
4	L	301	M6Y	C04-N03	5.78	1.46	1.34
4	M	301	M6Y	C30-N32	5.76	1.46	1.33
4	V	301	M6Y	C30-N32	5.69	1.46	1.33
4	N	301	M6Y	C04-N03	5.67	1.46	1.34
4	J	301	M6Y	C30-N32	5.67	1.46	1.33
4	Y	301	M6Y	C04-N03	5.65	1.46	1.34
4	I	301	M6Y	C30-N32	5.64	1.45	1.33
4	I	301	M6Y	C04-N03	5.64	1.46	1.34
4	V	301	M6Y	C04-N03	5.63	1.46	1.34
4	Z	301	M6Y	C04-N03	5.62	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	b	301	M6Y	O05-C04	-5.62	1.12	1.23
4	M	301	M6Y	C04-N03	5.59	1.46	1.34
4	a	301	M6Y	C04-N03	5.57	1.46	1.34
4	X	301	M6Y	C04-N03	5.57	1.46	1.34
4	J	301	M6Y	C04-N03	5.54	1.46	1.34
4	W	301	M6Y	C04-N03	5.54	1.46	1.34
4	K	301	M6Y	C04-N03	5.52	1.46	1.34
4	H	301	M6Y	C30-N32	5.50	1.45	1.33
4	H	301	M6Y	C04-N03	5.46	1.46	1.34
4	L	301	M6Y	C30-N32	5.45	1.45	1.33
4	N	301	M6Y	C30-N32	5.43	1.45	1.33
4	Y	301	M6Y	C30-N32	5.42	1.45	1.33
4	W	301	M6Y	C30-N32	5.40	1.45	1.33
4	K	301	M6Y	C30-N32	5.39	1.45	1.33
4	X	301	M6Y	C30-N32	5.38	1.45	1.33
4	H	301	M6Y	C22-N21	5.38	1.45	1.34
4	Z	301	M6Y	C30-N32	5.35	1.45	1.33
4	K	301	M6Y	C22-N21	5.34	1.45	1.34
4	b	301	M6Y	O31-C30	-5.32	1.12	1.23
4	a	301	M6Y	C30-N32	5.32	1.45	1.33
4	a	301	M6Y	C22-N21	5.31	1.45	1.34
4	N	301	M6Y	C22-N21	5.23	1.45	1.34
4	J	301	M6Y	C22-N21	5.19	1.45	1.34
4	M	301	M6Y	C22-N21	5.18	1.45	1.34
4	W	301	M6Y	C22-N21	5.17	1.45	1.34
4	L	301	M6Y	C22-N21	5.16	1.45	1.34
4	b	301	M6Y	O23-C22	-5.15	1.12	1.23
4	Z	301	M6Y	C22-N21	5.11	1.45	1.34
4	Y	301	M6Y	C22-N21	5.06	1.45	1.34
4	V	301	M6Y	C22-N21	5.01	1.45	1.34
4	X	301	M6Y	C22-N21	4.97	1.45	1.34
4	I	301	M6Y	C22-N21	4.95	1.44	1.34
4	b	301	M6Y	O09-C08	-4.41	1.13	1.23
4	K	301	M6Y	C27-C26	4.12	1.53	1.48
4	M	301	M6Y	C27-C26	4.05	1.53	1.48
4	a	301	M6Y	C27-C26	4.05	1.53	1.48
4	Y	301	M6Y	C27-C26	4.01	1.53	1.48
4	I	301	M6Y	C27-C26	4.00	1.53	1.48
4	L	301	M6Y	C27-C26	3.99	1.53	1.48
4	J	301	M6Y	C27-C26	3.95	1.53	1.48
4	N	301	M6Y	C27-C26	3.94	1.53	1.48
4	W	301	M6Y	C27-C26	3.91	1.53	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	b	301	M6Y	C39-C37	-3.88	1.31	1.37
4	X	301	M6Y	C27-C26	3.87	1.53	1.48
4	V	301	M6Y	C27-C26	3.86	1.53	1.48
4	Z	301	M6Y	C27-C26	3.82	1.53	1.48
4	H	301	M6Y	C27-C26	3.75	1.53	1.48
4	b	301	M6Y	C24-N29	-3.70	1.26	1.33
4	Z	301	M6Y	C08-N10	3.62	1.46	1.35
4	Y	301	M6Y	C08-N10	3.58	1.46	1.35
4	K	301	M6Y	C08-N10	3.58	1.46	1.35
4	a	301	M6Y	C08-N10	3.54	1.46	1.35
4	b	301	M6Y	C30-N32	3.54	1.41	1.33
4	L	301	M6Y	C08-N10	3.53	1.46	1.35
4	J	301	M6Y	C08-N10	3.52	1.46	1.35
4	H	301	M6Y	C08-N10	3.52	1.46	1.35
4	W	301	M6Y	C08-N10	3.51	1.45	1.35
4	M	301	M6Y	C08-N10	3.51	1.45	1.35
4	V	301	M6Y	C08-N10	3.50	1.45	1.35
4	I	301	M6Y	C08-N10	3.48	1.45	1.35
4	N	301	M6Y	C08-N10	3.48	1.45	1.35
4	X	301	M6Y	C08-N10	3.41	1.45	1.35
4	b	301	M6Y	C25-C26	-3.08	1.35	1.39
4	b	301	M6Y	C04-N03	3.05	1.40	1.34
4	b	301	M6Y	C06-N21	-3.04	1.39	1.45
4	b	301	M6Y	F38-C37	-2.73	1.29	1.36
4	b	301	M6Y	C16-C15	-2.72	1.34	1.39
4	b	301	M6Y	C20-C15	-2.56	1.34	1.39
4	b	301	M6Y	C34-C40	-2.46	1.33	1.38
4	b	301	M6Y	C35-C34	-2.37	1.35	1.39
4	Y	301	M6Y	O23-C22	-2.35	1.18	1.23
4	L	301	M6Y	O23-C22	-2.35	1.18	1.23
4	X	301	M6Y	O31-C30	-2.35	1.18	1.23
4	L	301	M6Y	O31-C30	-2.31	1.18	1.23
4	X	301	M6Y	O23-C22	-2.31	1.18	1.23
4	V	301	M6Y	O23-C22	-2.29	1.18	1.23
4	N	301	M6Y	O23-C22	-2.29	1.18	1.23
4	b	301	M6Y	F41-C40	-2.28	1.29	1.35
4	Z	301	M6Y	O23-C22	-2.26	1.18	1.23
4	M	301	M6Y	O23-C22	-2.25	1.18	1.23
4	V	301	M6Y	O05-C04	-2.25	1.18	1.23
4	b	301	M6Y	C39-C40	-2.24	1.33	1.37
4	I	301	M6Y	O05-C04	-2.24	1.18	1.23
4	K	301	M6Y	O23-C22	-2.24	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	a	301	M6Y	O23-C22	-2.24	1.18	1.23
4	W	301	M6Y	O23-C22	-2.23	1.18	1.23
4	K	301	M6Y	O05-C04	-2.22	1.19	1.23
4	N	301	M6Y	O31-C30	-2.21	1.19	1.23
4	J	301	M6Y	O05-C04	-2.21	1.19	1.23
4	b	301	M6Y	C02-N03	-2.21	1.41	1.45
4	I	301	M6Y	O23-C22	-2.21	1.18	1.23
4	a	301	M6Y	O31-C30	-2.19	1.19	1.23
4	L	301	M6Y	O05-C04	-2.19	1.19	1.23
4	a	301	M6Y	O05-C04	-2.18	1.19	1.23
4	V	301	M6Y	O31-C30	-2.18	1.19	1.23
4	H	301	M6Y	O23-C22	-2.17	1.18	1.23
4	N	301	M6Y	O05-C04	-2.17	1.19	1.23
4	W	301	M6Y	O05-C04	-2.17	1.19	1.23
4	H	301	M6Y	O31-C30	-2.15	1.19	1.23
4	b	301	M6Y	C15-C14	-2.15	1.48	1.51
4	Y	301	M6Y	O05-C04	-2.15	1.19	1.23
4	b	301	M6Y	C08-N10	2.14	1.41	1.35
4	Z	301	M6Y	O31-C30	-2.13	1.19	1.23
4	Z	301	M6Y	O05-C04	-2.13	1.19	1.23
4	J	301	M6Y	O31-C30	-2.13	1.19	1.23
4	b	301	M6Y	C22-N21	2.12	1.38	1.34
4	b	301	M6Y	C19-C20	-2.12	1.34	1.38
4	W	301	M6Y	O31-C30	-2.11	1.19	1.23
4	K	301	M6Y	O31-C30	-2.10	1.19	1.23
4	M	301	M6Y	O05-C04	-2.10	1.19	1.23
4	I	301	M6Y	O31-C30	-2.09	1.19	1.23
4	H	301	M6Y	O05-C04	-2.09	1.19	1.23
4	b	301	M6Y	C25-C24	-2.08	1.36	1.39
4	X	301	M6Y	O09-C08	-2.08	1.18	1.23
4	J	301	M6Y	O09-C08	-2.07	1.18	1.23
4	J	301	M6Y	O23-C22	-2.05	1.19	1.23
4	Y	301	M6Y	O31-C30	-2.03	1.19	1.23
4	X	301	M6Y	O05-C04	-2.03	1.19	1.23

All (173) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	J	301	M6Y	C13-C14-N10	6.06	108.89	101.94
4	I	301	M6Y	C13-C14-N10	6.00	108.82	101.94
4	X	301	M6Y	C13-C14-N10	5.94	108.75	101.94
4	L	301	M6Y	C13-C14-N10	5.80	108.60	101.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	K	301	M6Y	C13-C14-N10	5.76	108.55	101.94
4	a	301	M6Y	C13-C14-N10	5.60	108.37	101.94
4	M	301	M6Y	C13-C14-N10	5.50	108.25	101.94
4	Y	301	M6Y	C13-C14-N10	5.32	108.04	101.94
4	W	301	M6Y	C13-C14-N10	5.22	107.93	101.94
4	N	301	M6Y	C13-C14-N10	5.03	107.71	101.94
4	Z	301	M6Y	C13-C14-N10	5.03	107.71	101.94
4	V	301	M6Y	C13-C14-N10	4.92	107.58	101.94
4	b	301	M6Y	C13-C14-N10	4.67	107.30	101.94
4	H	301	M6Y	C13-C14-N10	4.37	106.95	101.94
4	b	301	M6Y	C36-C35-C34	-4.35	115.65	121.39
4	b	301	M6Y	C07-C06-N21	-3.67	103.41	110.60
5	N	302	CIT	C3-C2-C1	-3.63	109.17	114.98
4	b	301	M6Y	C02-C30-N32	3.57	123.85	116.45
5	Y	302	CIT	C3-C4-C5	-3.50	109.38	114.98
4	b	301	M6Y	C06-C07-C08	3.42	119.02	112.25
4	H	301	M6Y	C06-C07-C08	3.26	118.70	112.25
4	H	301	M6Y	C11-N10-C14	-3.26	108.04	111.83
4	a	301	M6Y	C39-C40-C34	-3.26	119.70	123.98
5	L	302	CIT	C3-C2-C1	-3.21	109.85	114.98
4	N	301	M6Y	C11-N10-C14	-3.16	108.16	111.83
4	V	301	M6Y	C40-C39-C37	3.16	119.94	116.62
5	V	302	CIT	C3-C4-C5	-3.16	109.92	114.98
4	b	301	M6Y	C24-C22-N21	3.15	121.05	115.20
4	Y	301	M6Y	C24-C22-N21	3.13	121.00	115.20
4	a	301	M6Y	C40-C39-C37	3.11	119.89	116.62
4	a	301	M6Y	C11-N10-C14	-3.08	108.26	111.83
4	K	301	M6Y	C39-C40-C34	-3.07	119.95	123.98
5	a	302	CIT	C3-C4-C5	-3.06	110.08	114.98
4	Y	301	M6Y	C40-C39-C37	3.06	119.83	116.62
4	W	301	M6Y	C30-C02-N03	-3.06	104.03	111.60
4	N	301	M6Y	C39-C40-C34	-3.03	120.01	123.98
4	Y	301	M6Y	C39-C40-C34	-3.01	120.03	123.98
4	Z	301	M6Y	C39-C40-C34	-3.01	120.03	123.98
4	I	301	M6Y	C40-C39-C37	3.00	119.78	116.62
4	M	301	M6Y	C40-C39-C37	3.00	119.78	116.62
4	W	301	M6Y	C40-C39-C37	3.00	119.77	116.62
4	K	301	M6Y	C40-C39-C37	3.00	119.77	116.62
4	b	301	M6Y	C11-N10-C14	-2.95	108.41	111.83
4	W	301	M6Y	C39-C40-C34	-2.94	120.12	123.98
4	X	301	M6Y	C40-C39-C37	2.94	119.71	116.62
4	J	301	M6Y	C15-C14-N10	-2.93	107.72	112.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	301	M6Y	C40-C39-C37	2.91	119.68	116.62
4	N	301	M6Y	C40-C39-C37	2.90	119.67	116.62
4	J	301	M6Y	C11-N10-C14	-2.90	108.47	111.83
4	X	301	M6Y	C15-C14-N10	-2.90	107.79	112.99
4	X	301	M6Y	C39-C40-C34	-2.89	120.19	123.98
4	J	301	M6Y	C40-C39-C37	2.89	119.65	116.62
4	H	301	M6Y	C13-C14-C15	-2.88	108.03	113.61
4	M	301	M6Y	C39-C40-C34	-2.87	120.22	123.98
4	J	301	M6Y	C39-C40-C34	-2.86	120.24	123.98
5	K	302	CIT	C4-C3-C2	2.84	116.92	109.33
5	b	302	CIT	C4-C3-C2	2.82	116.87	109.33
4	a	301	M6Y	C34-C33-N32	-2.82	107.08	113.03
5	J	302	CIT	C3-C4-C5	-2.81	110.48	114.98
4	V	301	M6Y	C24-C22-N21	2.80	120.40	115.20
4	V	301	M6Y	C39-C40-C34	-2.79	120.32	123.98
4	L	301	M6Y	C11-N10-C14	-2.79	108.59	111.83
4	I	301	M6Y	C39-C40-C34	-2.78	120.33	123.98
4	W	301	M6Y	C11-N10-C14	-2.78	108.60	111.83
5	I	302	CIT	C3-C2-C1	-2.78	110.53	114.98
4	b	301	M6Y	C35-C34-C40	2.77	121.46	116.61
4	H	301	M6Y	C39-C40-C34	-2.77	120.35	123.98
4	K	301	M6Y	C11-N10-C14	-2.77	108.62	111.83
4	W	301	M6Y	C24-C22-N21	2.75	120.30	115.20
5	J	302	CIT	C3-C2-C1	-2.73	110.61	114.98
4	b	301	M6Y	O05-C04-N03	-2.72	117.89	122.93
4	L	301	M6Y	C39-C40-C34	-2.70	120.43	123.98
4	b	301	M6Y	O31-C30-N32	-2.70	117.19	122.99
4	a	301	M6Y	C06-C07-C08	2.70	117.58	112.25
4	Z	301	M6Y	C40-C39-C37	2.68	119.44	116.62
4	X	301	M6Y	C30-C02-N03	-2.67	104.99	111.60
4	N	301	M6Y	C24-C22-N21	2.64	120.11	115.20
4	Z	301	M6Y	C11-N10-C14	-2.63	108.77	111.83
5	Y	302	CIT	C3-C2-C1	-2.60	110.82	114.98
4	M	301	M6Y	C06-C07-C08	2.59	117.37	112.25
4	V	301	M6Y	C36-C37-C39	-2.57	119.96	123.29
4	b	301	M6Y	C35-C36-C37	2.54	120.99	118.36
4	X	301	M6Y	C11-N10-C14	-2.53	108.90	111.83
4	L	301	M6Y	C24-C22-N21	2.52	119.89	115.20
5	N	302	CIT	C3-C4-C5	-2.52	110.96	114.98
4	K	301	M6Y	C12-C11-N10	2.51	107.66	103.25
4	Y	301	M6Y	C11-N10-C14	-2.51	108.92	111.83
4	K	301	M6Y	C06-C07-C08	2.51	117.21	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	Y	301	M6Y	C30-C02-N03	-2.50	105.42	111.60
4	Z	301	M6Y	C34-C33-N32	-2.48	107.79	113.03
4	V	301	M6Y	C11-N10-C14	-2.48	108.95	111.83
4	L	301	M6Y	C40-C39-C37	2.47	119.21	116.62
4	I	301	M6Y	C11-N10-C14	-2.47	108.97	111.83
4	W	301	M6Y	C12-C11-N10	2.47	107.58	103.25
4	b	301	M6Y	C33-N32-C30	-2.46	118.80	122.34
4	M	301	M6Y	C36-C37-C39	-2.45	120.11	123.29
4	L	301	M6Y	C12-C11-N10	2.44	107.52	103.25
4	H	301	M6Y	C24-C22-N21	2.43	119.72	115.20
4	W	301	M6Y	C36-C37-C39	-2.43	120.14	123.29
4	Z	301	M6Y	C30-C02-N03	-2.42	105.60	111.60
4	a	301	M6Y	C24-C22-N21	2.42	119.69	115.20
4	H	301	M6Y	C36-C37-C39	-2.41	120.16	123.29
4	N	301	M6Y	C33-N32-C30	-2.39	118.89	122.34
5	a	302	CIT	C3-C2-C1	-2.39	111.15	114.98
4	a	301	M6Y	C30-C02-N03	-2.39	105.68	111.60
5	H	302	CIT	C3-C2-C1	-2.39	111.16	114.98
4	Y	301	M6Y	C36-C37-C39	-2.38	120.20	123.29
4	Z	301	M6Y	C33-N32-C30	-2.36	118.94	122.34
4	I	301	M6Y	C36-C37-C39	-2.35	120.23	123.29
4	L	301	M6Y	C06-C07-C08	2.34	116.88	112.25
4	b	301	M6Y	O09-C08-N10	-2.33	116.49	121.54
4	L	301	M6Y	C13-C14-C15	-2.32	109.11	113.61
4	M	301	M6Y	C11-N10-C14	-2.32	109.13	111.83
4	K	301	M6Y	C24-C22-N21	2.32	119.51	115.20
4	X	301	M6Y	C33-N32-C30	-2.31	119.02	122.34
4	J	301	M6Y	C36-C37-C39	-2.31	120.29	123.29
4	M	301	M6Y	C12-C11-N10	2.31	107.29	103.25
4	H	301	M6Y	C33-N32-C30	-2.30	119.02	122.34
4	X	301	M6Y	C36-C37-C39	-2.30	120.31	123.29
4	Y	301	M6Y	C12-C11-N10	2.30	107.28	103.25
4	N	301	M6Y	C30-C02-N03	-2.29	105.93	111.60
4	W	301	M6Y	C06-C07-C08	2.29	116.77	112.25
4	X	301	M6Y	C02-C30-N32	2.28	121.18	116.45
4	W	301	M6Y	C15-C14-N10	-2.28	108.90	112.99
5	Z	302	CIT	C3-C4-C5	-2.27	111.35	114.98
4	b	301	M6Y	F38-C37-C36	2.26	122.38	118.54
4	Z	301	M6Y	C12-C11-N10	2.26	107.21	103.25
4	Z	301	M6Y	C24-C22-N21	2.24	119.36	115.20
4	b	301	M6Y	F38-C37-C39	-2.23	115.07	118.25
4	V	301	M6Y	C13-C14-C15	-2.22	109.31	113.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	V	301	M6Y	C02-C30-N32	2.20	121.01	116.45
4	Y	301	M6Y	C06-N21-C22	-2.20	116.22	121.60
4	a	301	M6Y	C36-C37-C39	-2.20	120.43	123.29
4	Y	301	M6Y	C34-C33-N32	-2.20	108.39	113.03
4	H	301	M6Y	C02-C30-N32	2.20	121.00	116.45
4	I	301	M6Y	C30-C02-N03	-2.19	106.17	111.60
4	b	301	M6Y	C14-N10-C08	2.19	127.40	120.83
4	N	301	M6Y	C36-C37-C39	-2.19	120.45	123.29
4	J	301	M6Y	C24-C22-N21	2.17	119.24	115.20
4	Z	301	M6Y	C06-C07-C08	2.17	116.55	112.25
4	J	301	M6Y	C06-C07-C08	2.17	116.54	112.25
5	M	302	CIT	C4-C3-C2	2.17	115.12	109.33
4	I	301	M6Y	C06-C07-C08	2.16	116.53	112.25
4	I	301	M6Y	C24-C22-N21	2.16	119.22	115.20
4	K	301	M6Y	C36-C37-C39	-2.15	120.50	123.29
4	V	301	M6Y	C30-C02-N03	-2.15	106.28	111.60
4	J	301	M6Y	C30-C02-N03	-2.13	106.33	111.60
4	L	301	M6Y	C34-C33-N32	-2.13	108.53	113.03
4	a	301	M6Y	C35-C34-C40	2.13	120.33	116.61
4	Y	301	M6Y	C06-C07-C08	2.12	116.44	112.25
4	I	301	M6Y	C13-C14-C15	-2.12	109.51	113.61
4	Z	301	M6Y	C35-C34-C40	2.12	120.31	116.61
4	K	301	M6Y	C30-C02-N03	-2.11	106.38	111.60
4	J	301	M6Y	C12-C11-N10	2.10	106.94	103.25
5	W	302	CIT	C4-C3-C2	2.07	114.86	109.33
4	L	301	M6Y	C35-C34-C40	2.06	120.22	116.61
4	H	301	M6Y	O31-C30-N32	-2.06	118.57	122.99
4	Y	301	M6Y	C35-C34-C40	2.06	120.22	116.61
4	V	301	M6Y	C12-C11-N10	2.06	106.86	103.25
4	b	301	M6Y	C33-C34-C40	-2.06	116.88	120.88
4	Z	301	M6Y	C13-C14-C15	-2.05	109.63	113.61
4	W	301	M6Y	C35-C34-C40	2.05	120.20	116.61
4	N	301	M6Y	C02-C30-N32	2.05	120.69	116.45
4	X	301	M6Y	C13-C14-C15	-2.04	109.65	113.61
4	K	301	M6Y	C33-N32-C30	-2.04	119.41	122.34
4	J	301	M6Y	C13-C14-C15	-2.03	109.67	113.61
4	K	301	M6Y	C35-C34-C40	2.03	120.15	116.61
4	b	301	M6Y	C30-C02-N03	-2.02	106.59	111.60
4	W	301	M6Y	C34-C33-N32	-2.02	108.76	113.03
4	N	301	M6Y	C35-C34-C40	2.02	120.14	116.61
4	N	301	M6Y	C06-C07-C08	2.01	116.23	112.25
4	W	301	M6Y	C33-N32-C30	-2.01	119.44	122.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	301	M6Y	C02-C30-N32	2.01	120.61	116.45

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	W	301	M6Y	O23-C22-C24-C25
4	X	301	M6Y	O23-C22-C24-C25
4	J	301	M6Y	O23-C22-C24-C25
4	a	301	M6Y	O23-C22-C24-C25
4	L	301	M6Y	O23-C22-C24-C25
4	b	301	M6Y	O23-C22-C24-C25
5	M	302	CIT	C1-C2-C3-O7
5	M	302	CIT	C1-C2-C3-C4
5	M	302	CIT	C1-C2-C3-C6
5	M	302	CIT	C6-C3-C4-C5
4	Z	301	M6Y	O23-C22-C24-C25
4	Y	301	M6Y	O23-C22-C24-C25
5	K	302	CIT	C2-C3-C4-C5
4	K	301	M6Y	O23-C22-C24-C25
4	I	301	M6Y	O23-C22-C24-C25
4	N	301	M6Y	C04-C06-N21-C22
5	M	302	CIT	C2-C3-C4-C5
5	M	302	CIT	O7-C3-C4-C5
5	K	302	CIT	O7-C3-C4-C5
3	R	302	DMF	O-C-N-C1
5	K	302	CIT	C1-C2-C3-O7
3	R	302	DMF	O-C-N-C2
5	L	302	CIT	C2-C3-C4-C5
3	T	301	DMF	O-C-N-C1
4	b	301	M6Y	N21-C06-C07-C08
5	J	302	CIT	O7-C3-C4-C5
3	J	303	DMF	O-C-N-C1
3	T	301	DMF	O-C-N-C2
3	U	301	DMF	O-C-N-C1
5	V	302	CIT	O7-C3-C4-C5
5	Y	302	CIT	C1-C2-C3-O7
5	W	302	CIT	O7-C3-C4-C5
5	a	302	CIT	C1-C2-C3-O7
5	N	302	CIT	C1-C2-C3-O7
5	X	302	CIT	O7-C3-C4-C5
5	Z	302	CIT	C1-C2-C3-O7

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Mol	Chain	Res	Type	Atoms
3	G	302	DMF	O-C-N-C1
3	R	301	DMF	O-C-N-C1
5	b	302	CIT	O7-C3-C4-C5
5	H	302	CIT	C1-C2-C3-O7
3	U	301	DMF	O-C-N-C2
3	J	303	DMF	O-C-N-C2
3	C	301	DMF	O-C-N-C1
5	I	302	CIT	O7-C3-C4-C5
5	L	302	CIT	C1-C2-C3-O7
3	G	302	DMF	O-C-N-C2
3	R	301	DMF	O-C-N-C2
4	L	301	M6Y	C30-C02-N03-C04
3	C	301	DMF	O-C-N-C2
4	Z	301	M6Y	C30-C02-N03-C04
4	Y	301	M6Y	C30-C02-N03-C04
4	Z	301	M6Y	N03-C02-C30-N32
3	O	301	DMF	O-C-N-C1
4	V	301	M6Y	O23-C22-C24-C25
4	W	301	M6Y	C30-C02-N03-C04
4	b	301	M6Y	C30-C02-N03-C04
4	V	301	M6Y	N03-C02-C30-N32
4	J	301	M6Y	C30-C02-N03-C04
4	M	301	M6Y	C30-C02-N03-C04
4	K	301	M6Y	N21-C06-C07-C08
4	H	301	M6Y	C30-C02-N03-C04
4	N	301	M6Y	C30-C02-N03-C04
3	O	301	DMF	O-C-N-C2

There are no ring outliers.

22 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	S	301	DMF	2	0
3	J	303	DMF	1	0
5	J	302	CIT	1	0
3	J	304	DMF	1	0
5	Y	302	CIT	2	0
5	W	302	CIT	1	0
5	N	302	CIT	1	0
3	O	301	DMF	1	0
5	M	302	CIT	2	0
5	I	302	CIT	2	0

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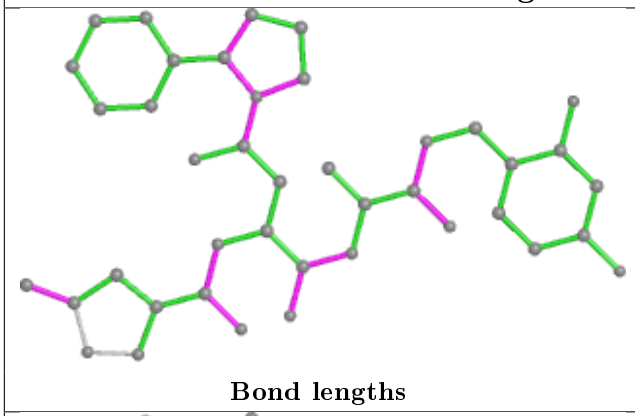
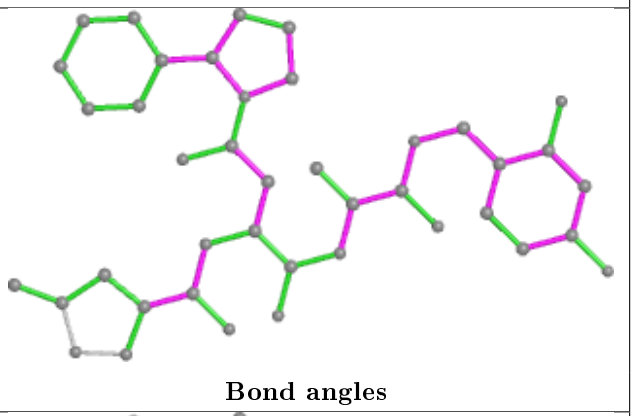
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	X	302	CIT	2	0
3	E	301	DMF	2	0
3	C	301	DMF	1	0
3	I	303	DMF	1	0
3	Q	301	DMF	1	0
5	K	302	CIT	2	0
5	Z	302	CIT	1	0
4	H	301	M6Y	1	0
3	R	301	DMF	2	0
4	I	301	M6Y	1	0
3	F	301	DMF	1	0
3	U	301	DMF	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

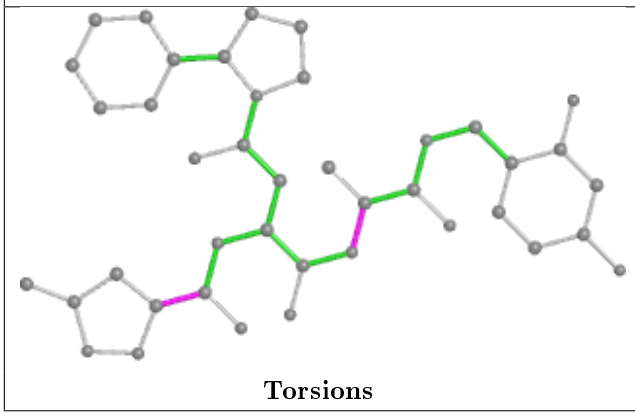
Ligand M6Y W 301



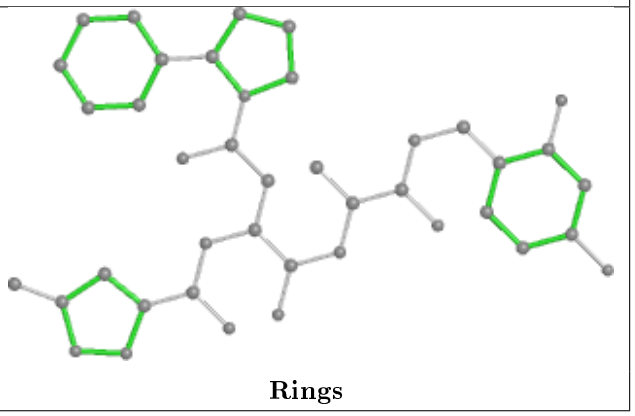
Bond lengths



Bond angles

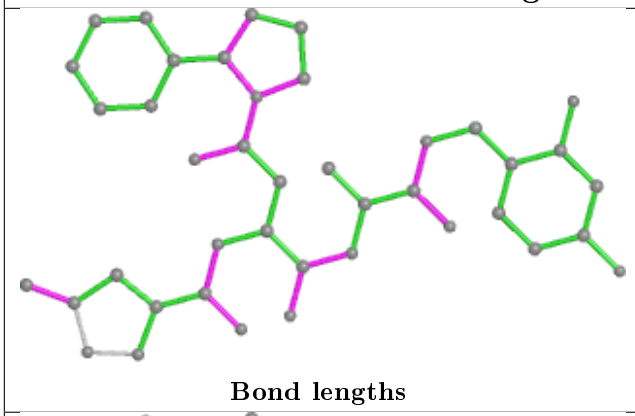


Torsions



Rings

Ligand M6Y X 301



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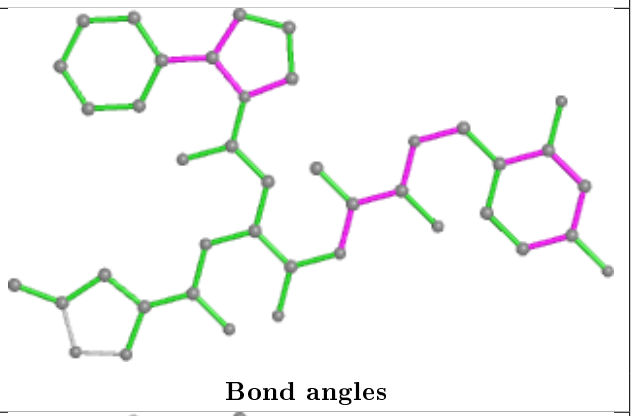

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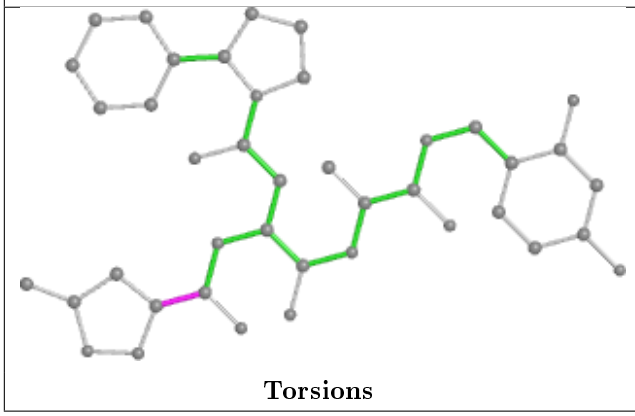

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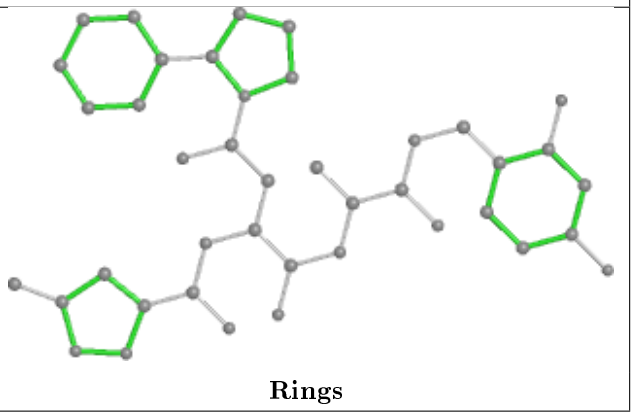
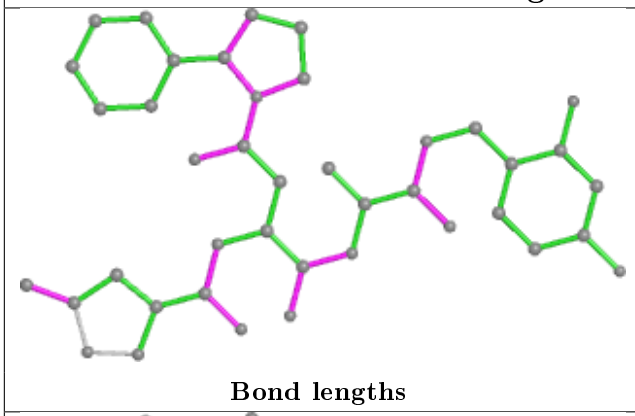


Rings

Ligand M6Y J 301



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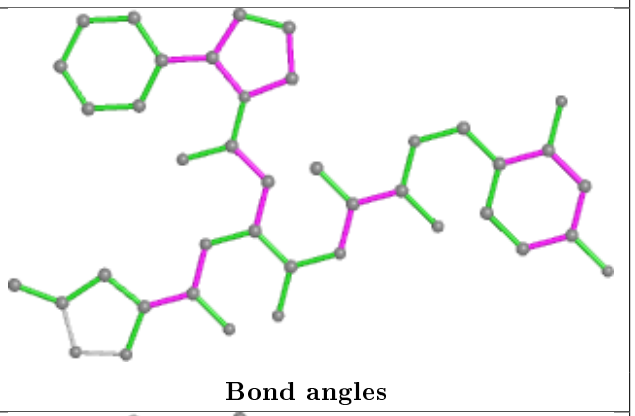
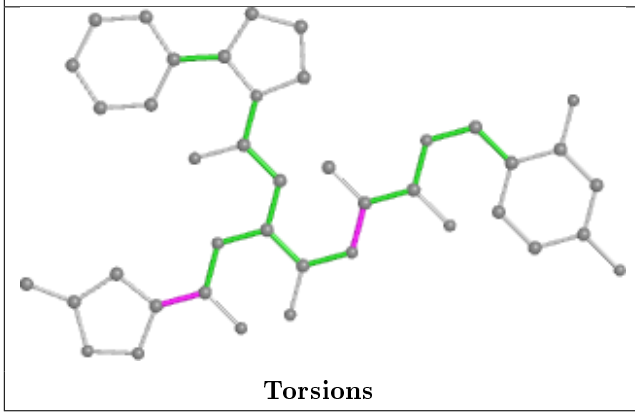
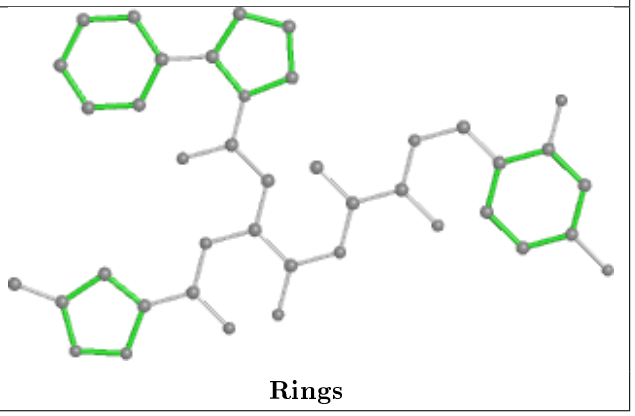


Bond angles

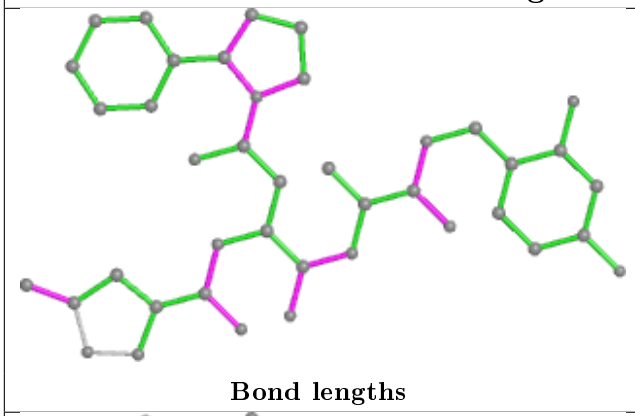


Torsions



Rings

Ligand M6Y a 301



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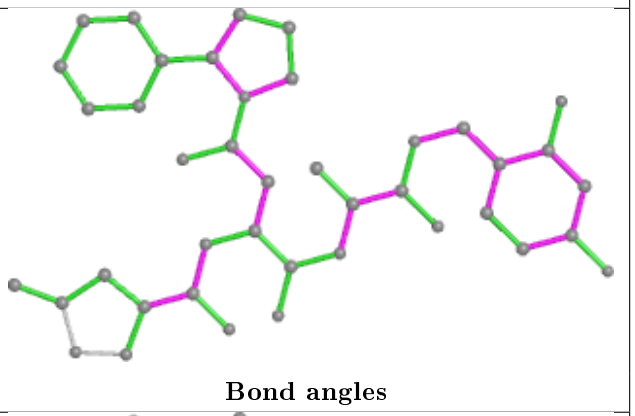
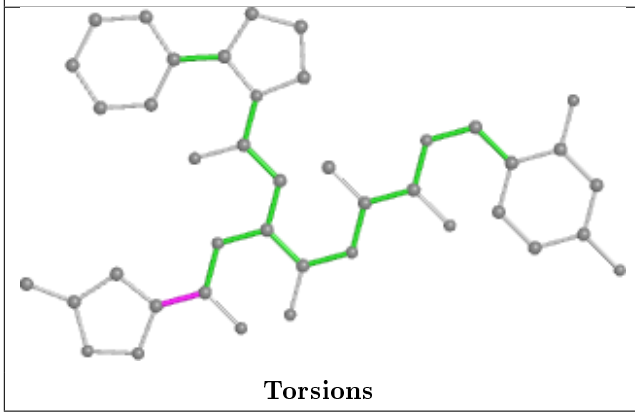


Bond angles



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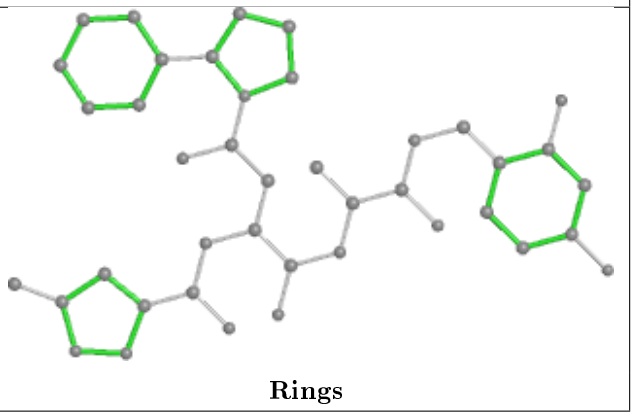
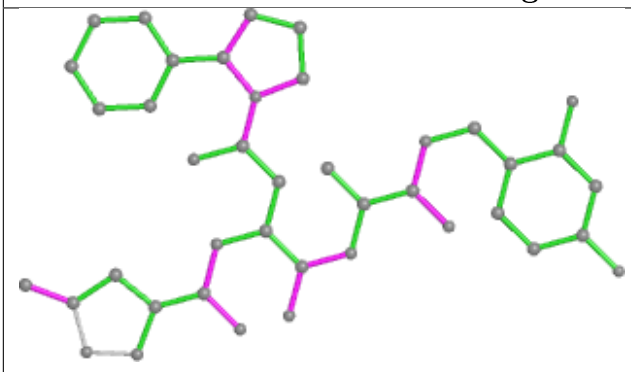


Rings

Ligand M6Y V 301



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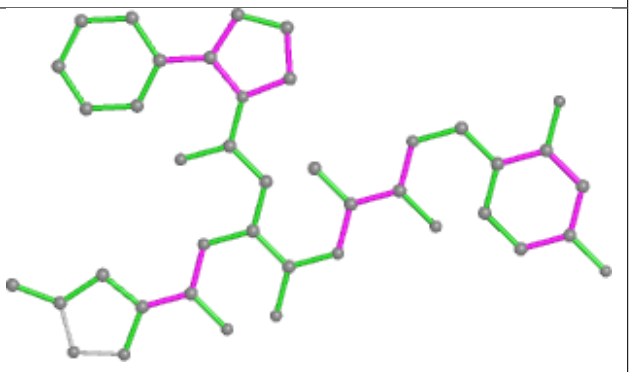

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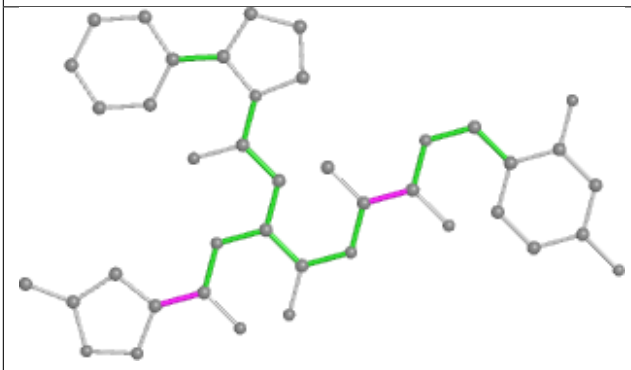

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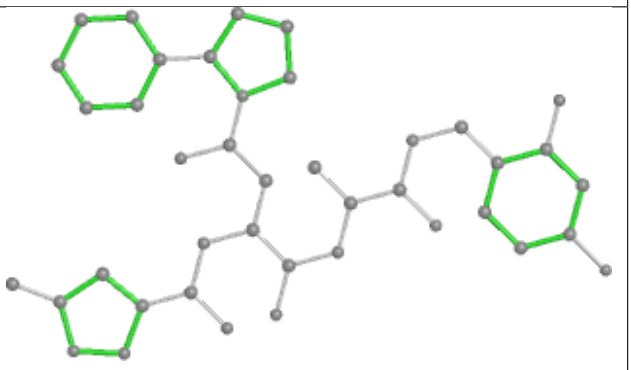
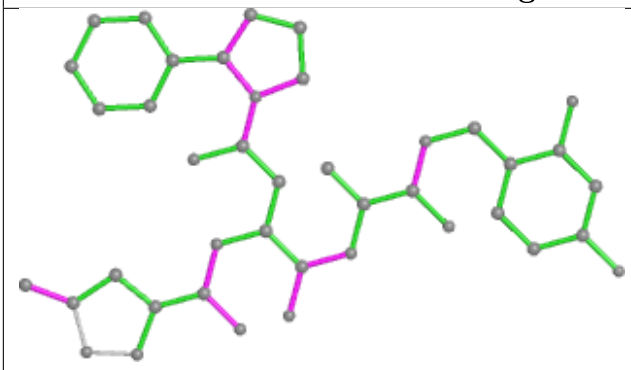


Rings

Ligand M6Y M 301



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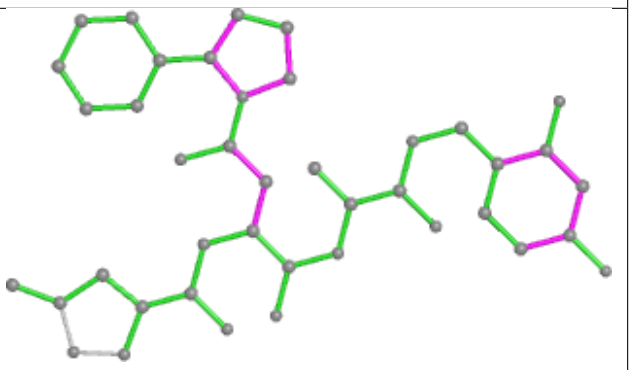

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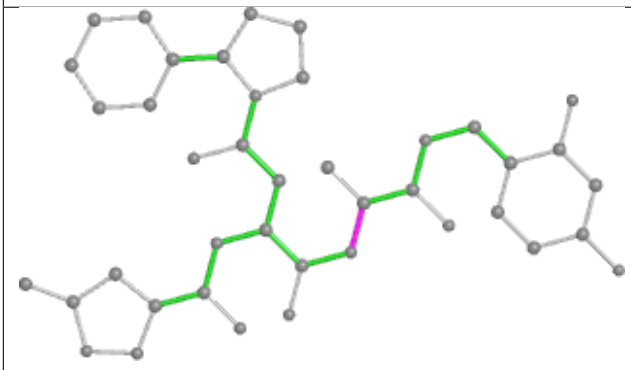

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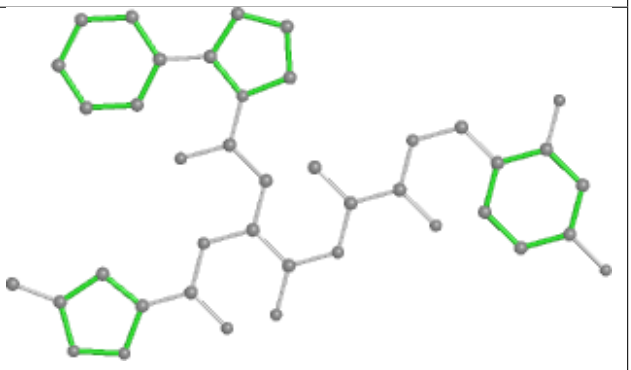
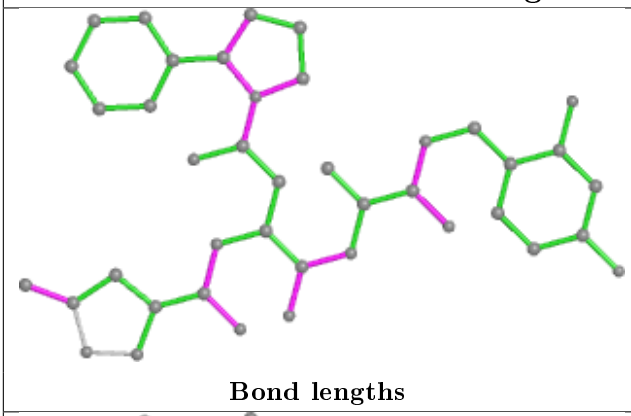


Rings

Ligand M6Y L 301



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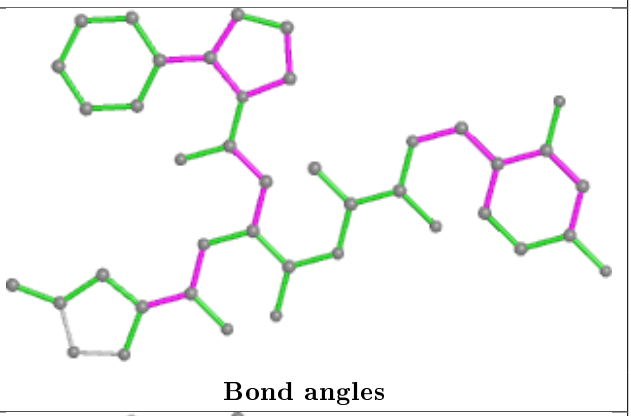

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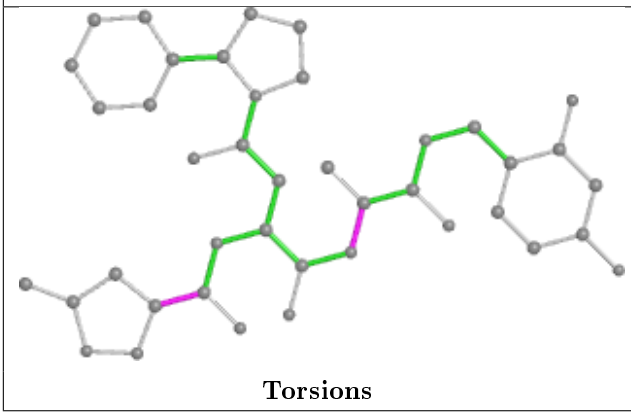

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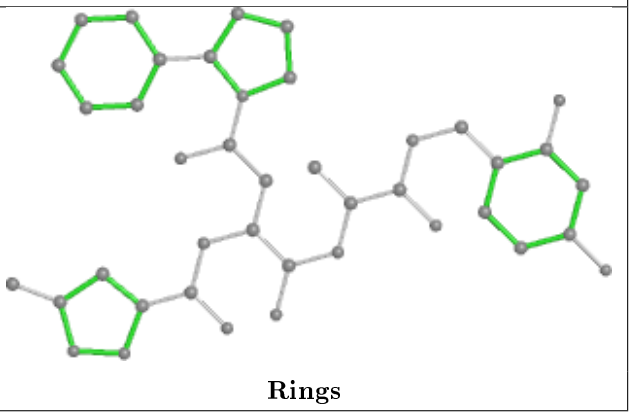
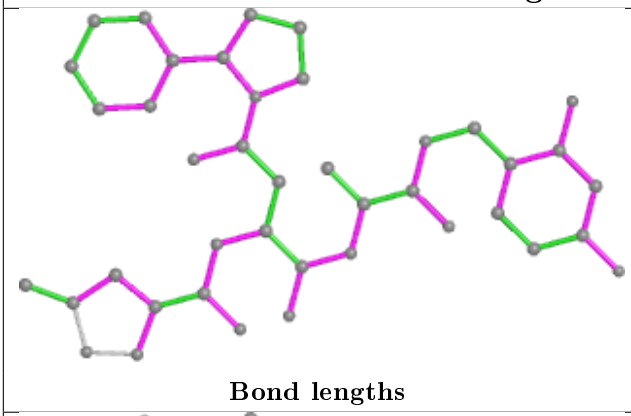


Rings

Ligand M6Y b 301



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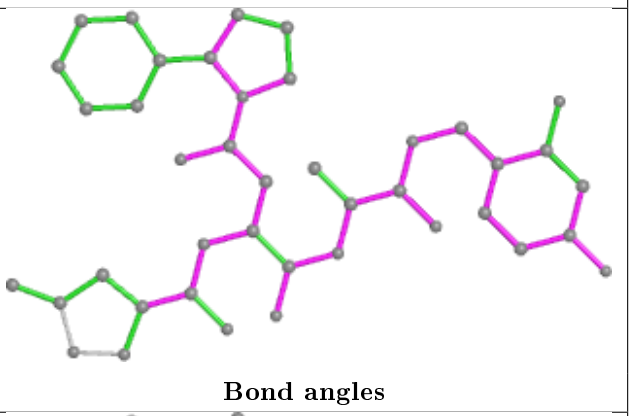

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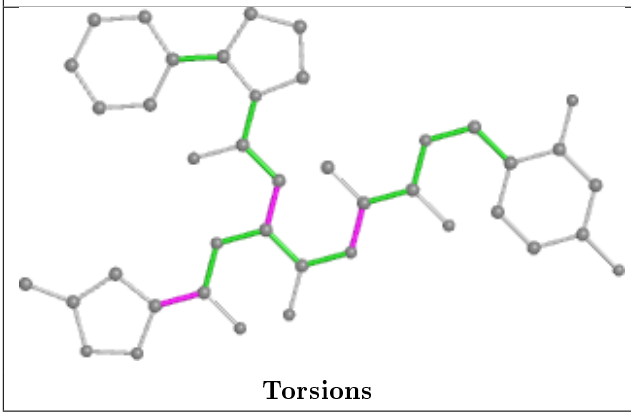

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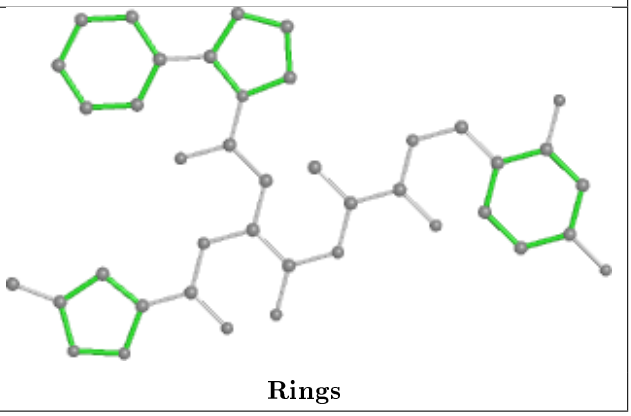
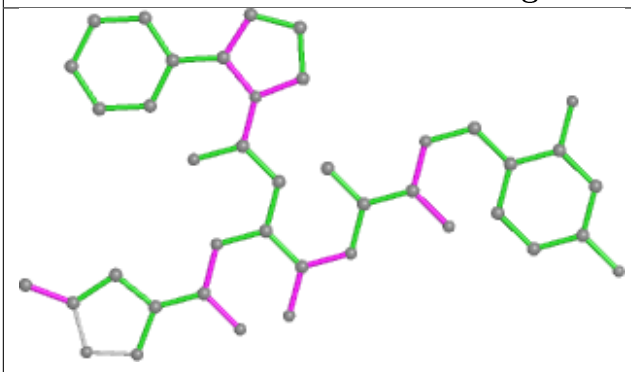


Rings

Ligand M6Y N 301



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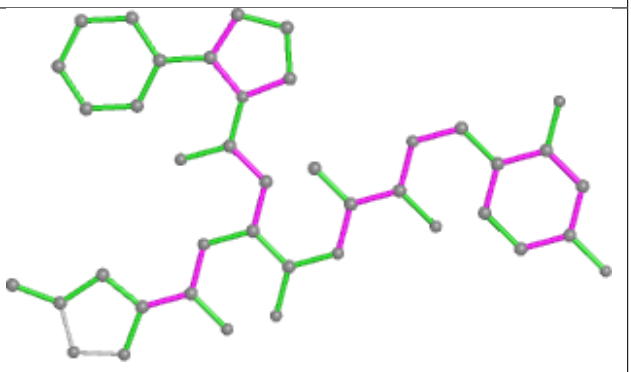
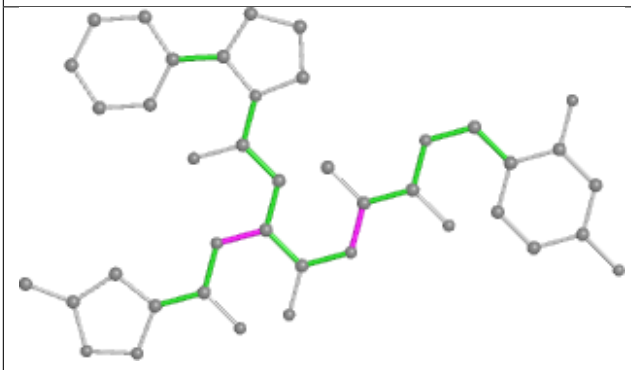


Bond angles



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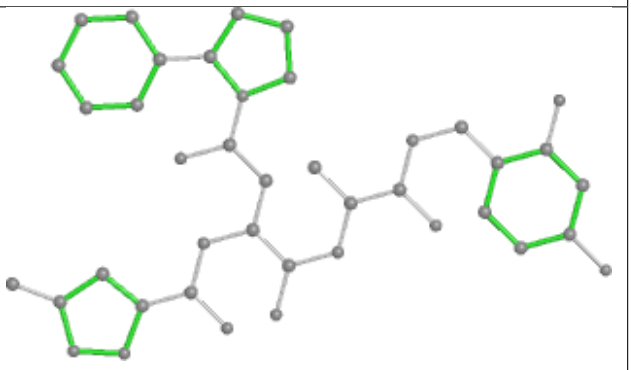
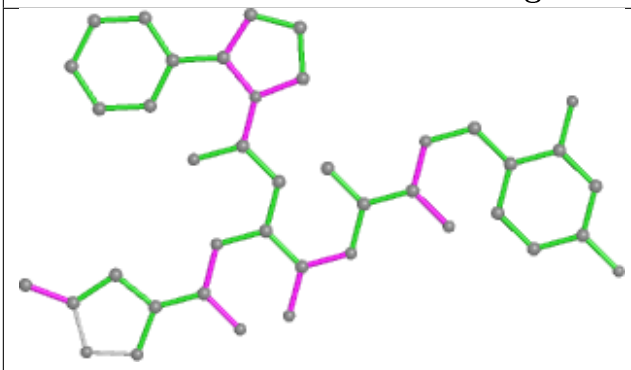


Rings

Ligand M6Y Z 301



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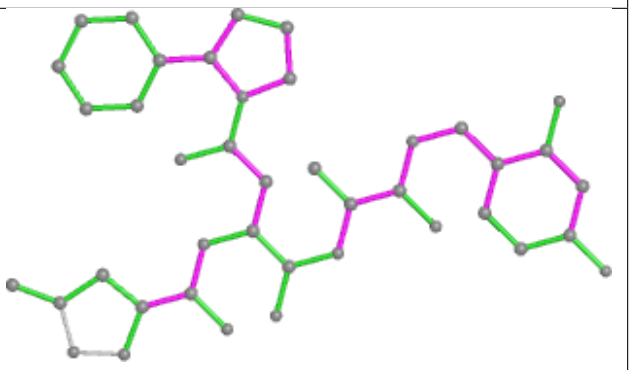

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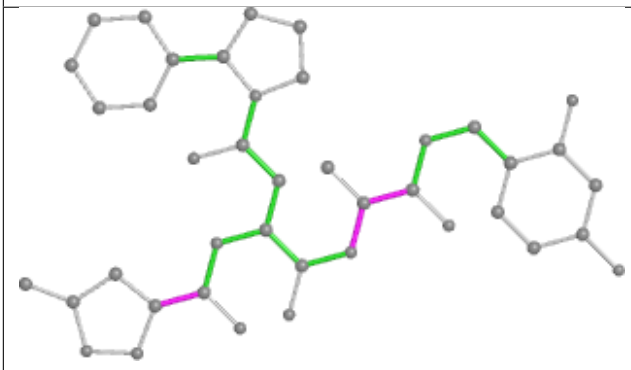

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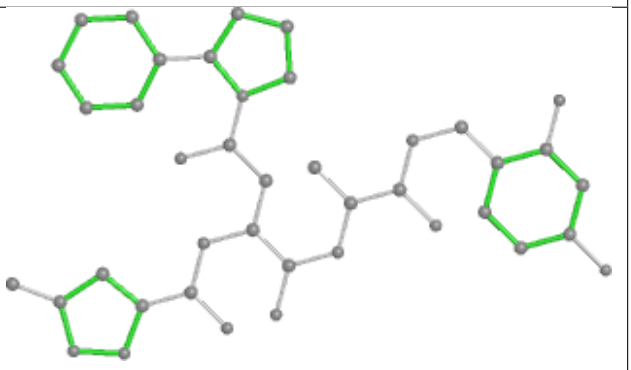
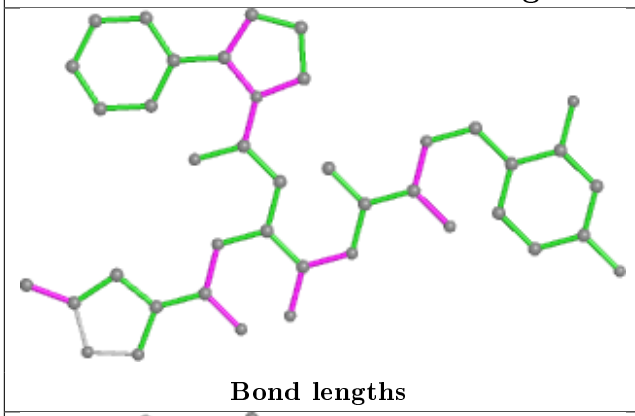


Rings

Ligand M6Y Y 301



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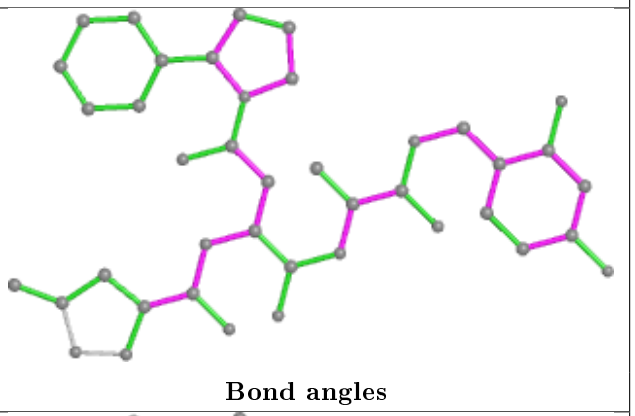

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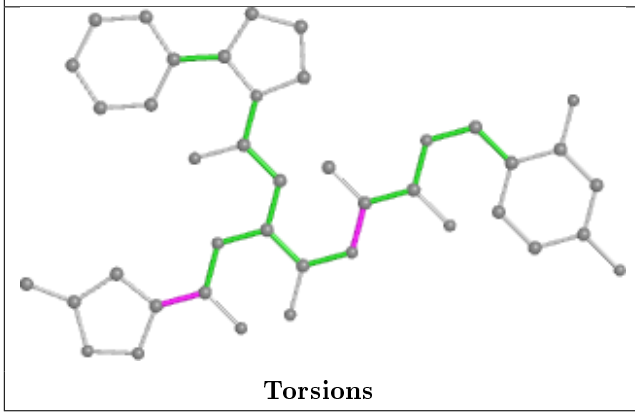

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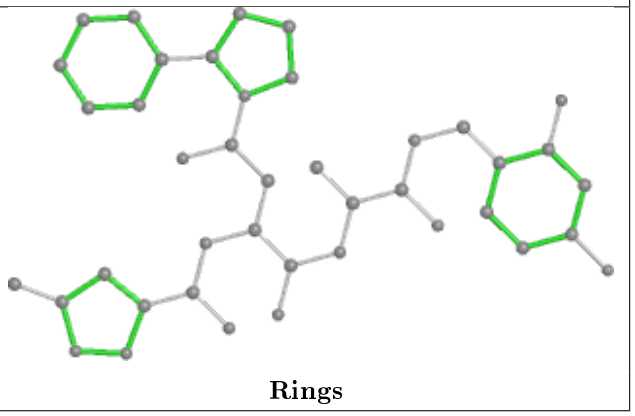
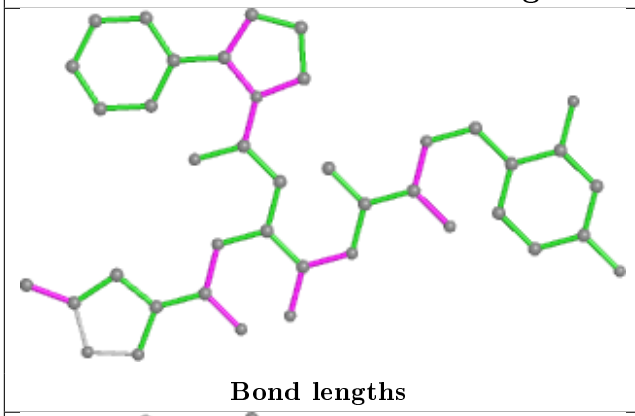
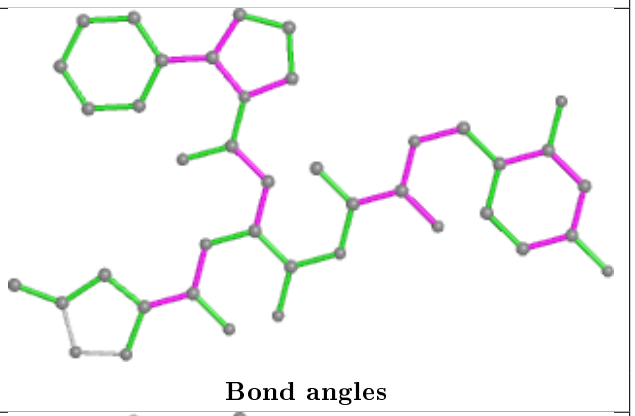


Rings

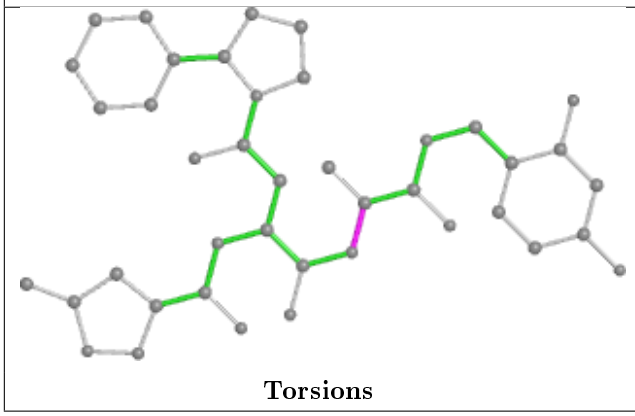
Ligand M6Y H 301



Bond lengths



Bond angles



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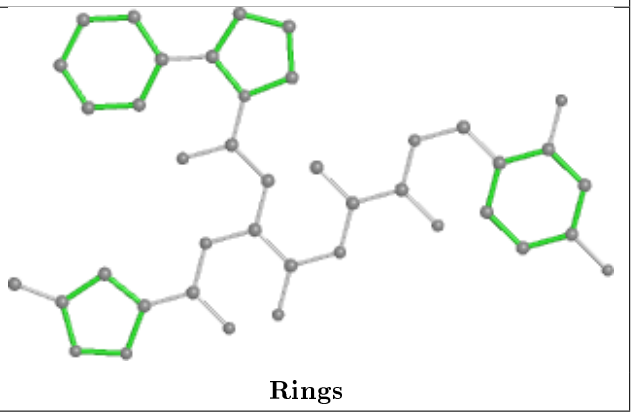
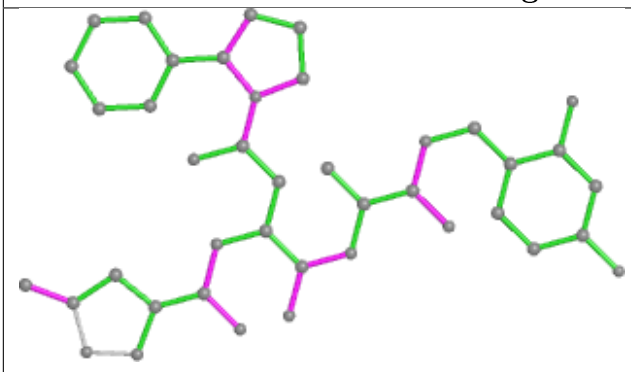
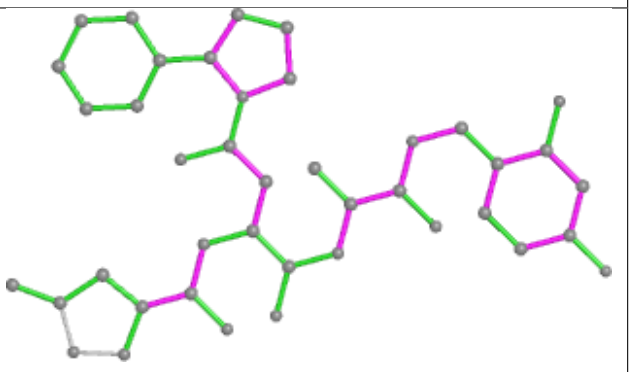


Rings

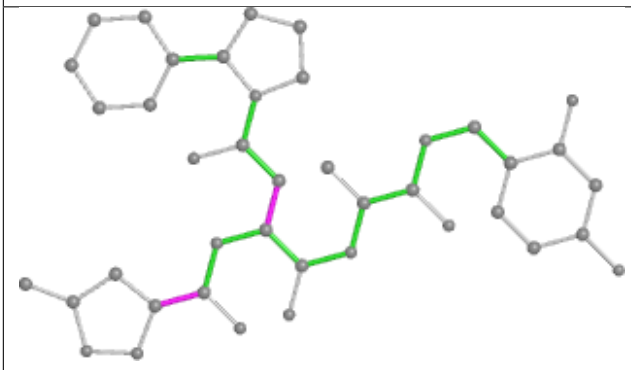
Ligand M6Y K 301



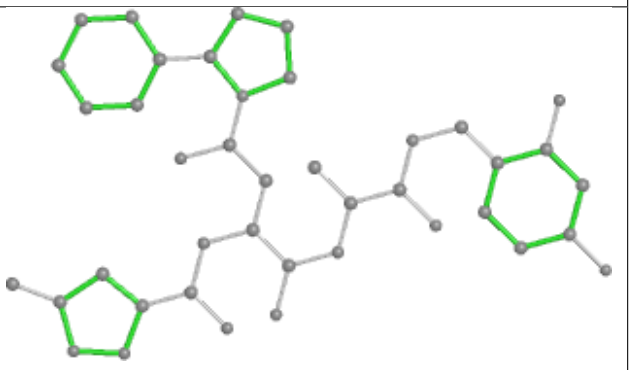
Bond lengths



Bond angles

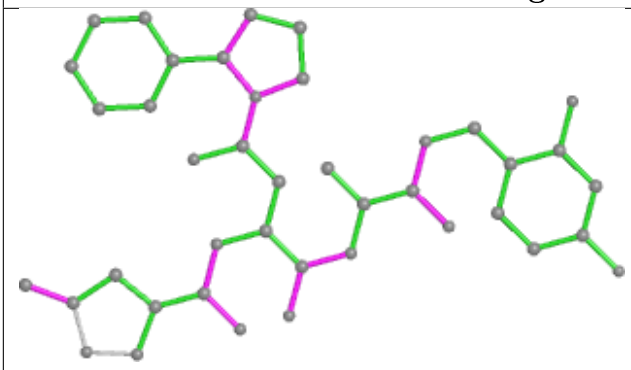


Torsions

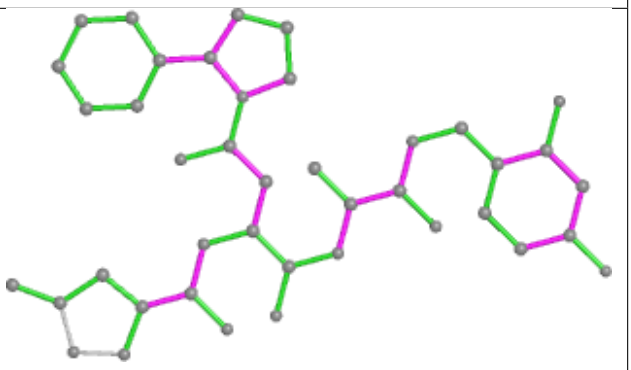


Rings

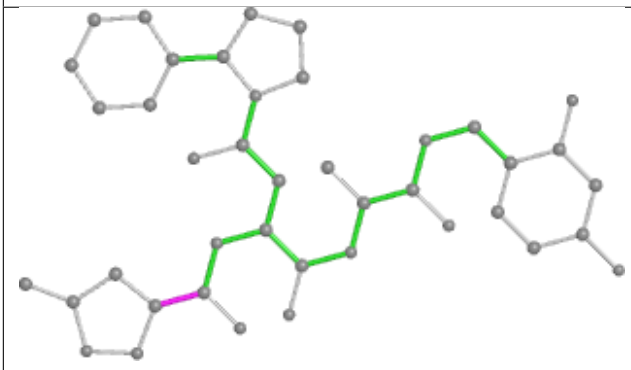
Ligand M6Y I 301



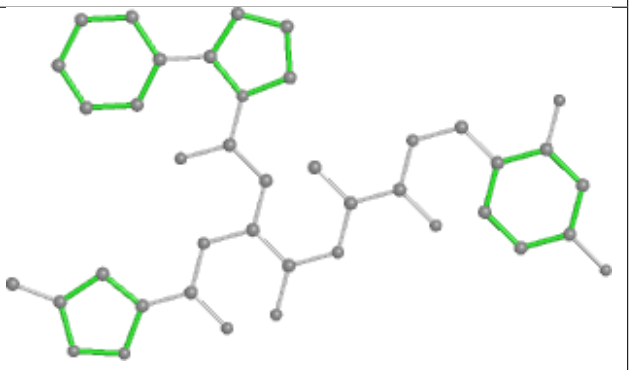
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	218/240 (90%)	-0.35	3 (1%) 75 73	19, 33, 55, 83	0
1	B	215/240 (89%)	-0.05	11 (5%) 28 25	23, 44, 73, 89	0
1	C	217/240 (90%)	-0.06	11 (5%) 28 25	21, 42, 73, 86	0
1	D	215/240 (89%)	-0.07	6 (2%) 53 49	20, 40, 66, 80	0
1	E	217/240 (90%)	-0.06	8 (3%) 41 38	22, 41, 69, 83	0
1	F	216/240 (90%)	-0.04	10 (4%) 32 29	21, 45, 70, 87	0
1	G	216/240 (90%)	-0.32	2 (0%) 84 83	21, 35, 62, 71	0
1	O	217/240 (90%)	-0.07	10 (4%) 32 29	23, 42, 74, 89	0
1	P	219/240 (91%)	-0.24	3 (1%) 75 73	20, 37, 64, 93	0
1	Q	216/240 (90%)	-0.31	2 (0%) 84 83	19, 35, 60, 99	0
1	R	215/240 (89%)	-0.20	3 (1%) 75 73	19, 34, 59, 68	0
1	S	218/240 (90%)	-0.35	5 (2%) 60 56	19, 32, 60, 87	0
1	T	217/240 (90%)	-0.17	5 (2%) 60 56	22, 43, 65, 93	0
1	U	216/240 (90%)	-0.16	9 (4%) 36 33	20, 36, 62, 79	0
2	H	222/234 (94%)	-0.54	0 100 100	18, 26, 44, 64	0
2	I	222/234 (94%)	-0.63	0 100 100	17, 25, 42, 58	0
2	J	222/234 (94%)	-0.58	1 (0%) 91 91	17, 25, 42, 80	0
2	K	223/234 (95%)	-0.66	0 100 100	14, 25, 42, 53	0
2	L	223/234 (95%)	-0.62	1 (0%) 92 93	17, 26, 42, 63	0
2	M	222/234 (94%)	-0.60	0 100 100	15, 27, 47, 69	0
2	N	223/234 (95%)	-0.54	2 (0%) 84 83	18, 29, 51, 68	0
2	V	223/234 (95%)	-0.66	0 100 100	15, 24, 41, 53	0
2	W	223/234 (95%)	-0.70	1 (0%) 92 93	17, 25, 41, 58	0
2	X	222/234 (94%)	-0.57	1 (0%) 91 91	18, 25, 40, 62	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
2	Y	223/234 (95%)	-0.66	0 100 100	16, 24, 41, 68	0
2	Z	222/234 (94%)	-0.61	1 (0%) 91 91	17, 26, 44, 61	0
2	a	223/234 (95%)	-0.60	0 100 100	19, 28, 48, 66	0
2	b	223/234 (95%)	-0.52	1 (0%) 92 93	17, 27, 44, 67	0
All	All	6148/6636 (92%)	-0.39	96 (1%) 72 69	14, 30, 63, 99	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	236	ASP	6.6
2	J	115	GLN	5.5
1	F	191	GLY	4.3
1	T	202	THR	4.3
1	B	235	VAL	4.1
1	O	202	THR	4.0
1	Q	236	ASP	4.0
1	C	9	MET	3.9
1	G	9	MET	3.7
1	U	9	MET	3.6
1	C	235	VAL	3.5
1	S	236	ASP	3.5
1	O	192	SER	3.4
1	F	189	ARG	3.4
1	F	192	SER	3.3
1	D	203	LEU	3.3
1	Q	235	VAL	3.2
1	C	203	LEU	3.2
1	U	203	LEU	3.2
1	U	232	ALA	3.2
2	N	223	GLY	3.1
1	B	233	LEU	3.1
1	F	203	LEU	3.1
1	D	188	LEU	3.0
1	A	9	MET	3.0
1	B	234	LEU	3.0
1	P	192	SER	2.9
1	E	235	VAL	2.9
1	O	189	ARG	2.9
1	T	203	LEU	2.9
1	F	166	ALA	2.9
1	B	231	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	S	192	SER	2.8
1	S	235	VAL	2.8
1	C	169	GLU	2.8
1	D	192	SER	2.8
1	B	182	ARG	2.8
1	R	234	LEU	2.7
1	O	182	ARG	2.7
1	O	169	GLU	2.7
1	F	9	MET	2.7
1	B	189	ARG	2.6
1	F	167	LEU	2.6
1	U	234	LEU	2.6
1	O	170	SER	2.5
1	O	188	LEU	2.5
1	E	182	ARG	2.5
1	E	189	ARG	2.5
1	U	182	ARG	2.5
2	W	114	PRO	2.5
2	X	115	GLN	2.5
2	L	115	GLN	2.5
1	D	164	ALA	2.4
1	C	182	ARG	2.4
1	E	205	VAL	2.4
1	B	203	LEU	2.4
2	N	114	PRO	2.4
1	U	189	ARG	2.4
1	D	189	ARG	2.4
1	P	169	GLU	2.3
2	Z	114	PRO	2.3
1	B	190	ALA	2.3
1	O	11	GLN	2.3
1	P	170	SER	2.3
1	B	169	GLU	2.3
1	E	14	ARG	2.3
1	D	184	ALA	2.3
1	F	10	GLU	2.3
1	E	172	ALA	2.3
1	A	10	GLU	2.3
1	T	189	ARG	2.3
1	U	11	GLN	2.3
1	T	169	GLU	2.3
1	A	182	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	9	MET	2.2
1	R	186	ALA	2.2
1	U	235	VAL	2.2
1	C	189	ARG	2.2
1	B	167	LEU	2.2
1	C	231	GLN	2.2
1	R	171	TYR	2.2
1	U	10	GLU	2.1
1	F	11	GLN	2.1
1	S	191	GLY	2.1
1	S	9	MET	2.1
1	F	158	GLY	2.1
1	G	233	LEU	2.1
1	C	10	GLU	2.1
1	C	232	ALA	2.1
1	E	192	SER	2.1
1	T	182	ARG	2.1
1	C	12	ALA	2.1
1	O	172	ALA	2.0
1	O	191	GLY	2.0
1	B	170	SER	2.0
2	b	115	GLN	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 carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CIT	N	302	13/13	0.90	0.19	31,47,61,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	DMF	S	302	5/5	0.90	0.27	34,47,56,57	0
5	CIT	Z	302	13/13	0.90	0.21	32,42,51,67	0
5	CIT	a	302	13/13	0.91	0.15	29,35,48,52	0
5	CIT	L	302	13/13	0.91	0.17	31,40,52,55	0
5	CIT	b	302	13/13	0.91	0.17	31,40,56,58	0
5	CIT	M	302	13/13	0.92	0.17	30,47,57,63	0
3	DMF	B	301	5/5	0.92	0.25	27,39,47,47	0
3	DMF	J	303	5/5	0.92	0.23	30,37,47,50	0
3	DMF	F	302	5/5	0.92	0.23	27,34,56,56	0
5	CIT	K	302	13/13	0.93	0.13	27,36,42,46	0
5	CIT	V	302	13/13	0.93	0.16	28,35,54,57	0
3	DMF	Q	301	5/5	0.93	0.21	21,33,40,46	0
5	CIT	H	302	13/13	0.93	0.15	26,39,50,56	0
3	DMF	F	301	5/5	0.93	0.21	25,34,44,46	0
3	DMF	S	301	5/5	0.94	0.20	22,28,35,36	0
3	DMF	I	303	5/5	0.94	0.24	24,35,42,44	0
5	CIT	W	302	13/13	0.94	0.16	26,38,47,52	0
5	CIT	J	302	13/13	0.94	0.17	31,39,47,47	0
3	DMF	J	304	5/5	0.95	0.26	26,41,50,54	0
5	CIT	I	302	13/13	0.95	0.13	33,38,49,52	0
5	CIT	X	302	13/13	0.95	0.21	27,36,44,55	0
3	DMF	A	301	5/5	0.95	0.22	35,42,47,47	0
3	DMF	E	301	5/5	0.95	0.15	26,34,45,45	0
3	DMF	G	302	5/5	0.95	0.20	34,41,51,51	0
5	CIT	Y	302	13/13	0.95	0.18	29,38,45,53	0
3	DMF	U	301	5/5	0.95	0.22	33,39,50,50	0
4	M6Y	M	301	41/41	0.96	0.14	20,26,36,48	0
4	M6Y	Y	301	41/41	0.96	0.14	18,24,35,47	0
3	DMF	R	302	5/5	0.96	0.18	36,43,52,52	0
4	M6Y	N	301	41/41	0.96	0.14	19,26,37,44	0
4	M6Y	H	301	41/41	0.96	0.14	17,24,38,47	0
4	M6Y	V	301	41/41	0.96	0.15	16,25,33,39	0
3	DMF	G	301	5/5	0.96	0.15	22,30,37,37	0
4	M6Y	I	301	41/41	0.96	0.15	17,27,38,46	0
3	DMF	O	301	5/5	0.96	0.24	27,33,39,42	0
4	M6Y	Z	301	41/41	0.96	0.14	14,24,33,43	0
4	M6Y	a	301	41/41	0.96	0.14	17,24,35,39	0
3	DMF	R	301	5/5	0.97	0.19	26,31,38,38	0
4	M6Y	J	301	41/41	0.97	0.14	17,23,31,31	0
4	M6Y	K	301	41/41	0.97	0.13	17,24,36,41	0
4	M6Y	X	301	41/41	0.97	0.15	20,26,35,47	0
4	M6Y	L	301	41/41	0.97	0.15	15,25,34,42	0

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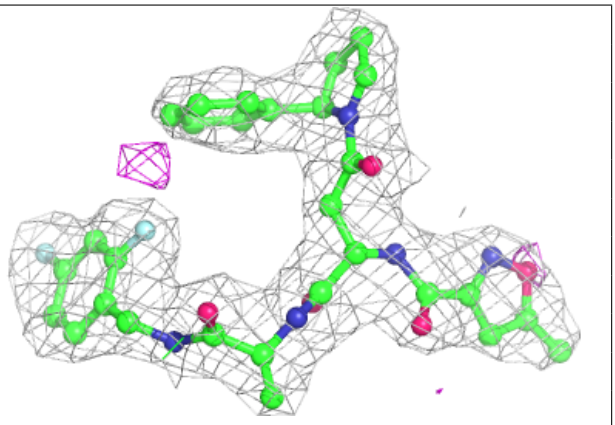
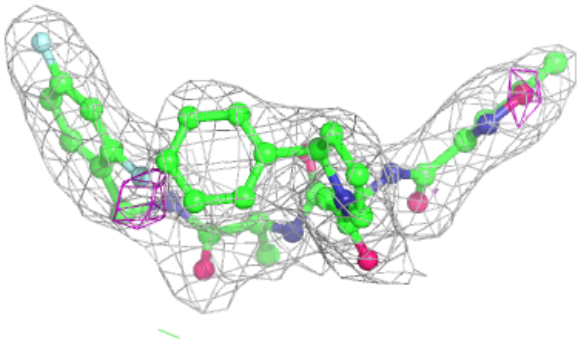
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	DMF	C	301	5/5	0.97	0.16	21,37,41,48	0
4	M6Y	W	301	41/41	0.97	0.14	19,25,34,42	0
4	M6Y	b	301	41/41	0.97	0.12	20,27,37,47	0
3	DMF	T	301	5/5	0.98	0.23	27,37,44,45	0
3	DMF	P	301	5/5	0.99	0.13	30,36,41,41	0

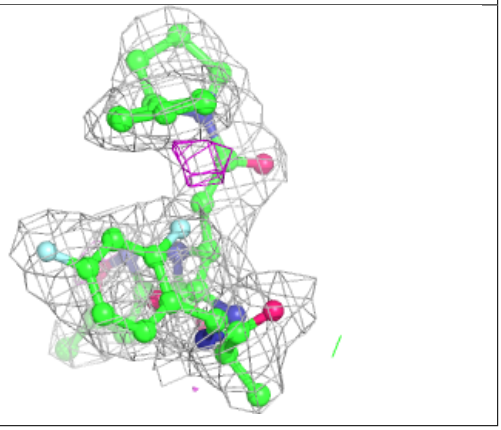
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around M6Y M 301:

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

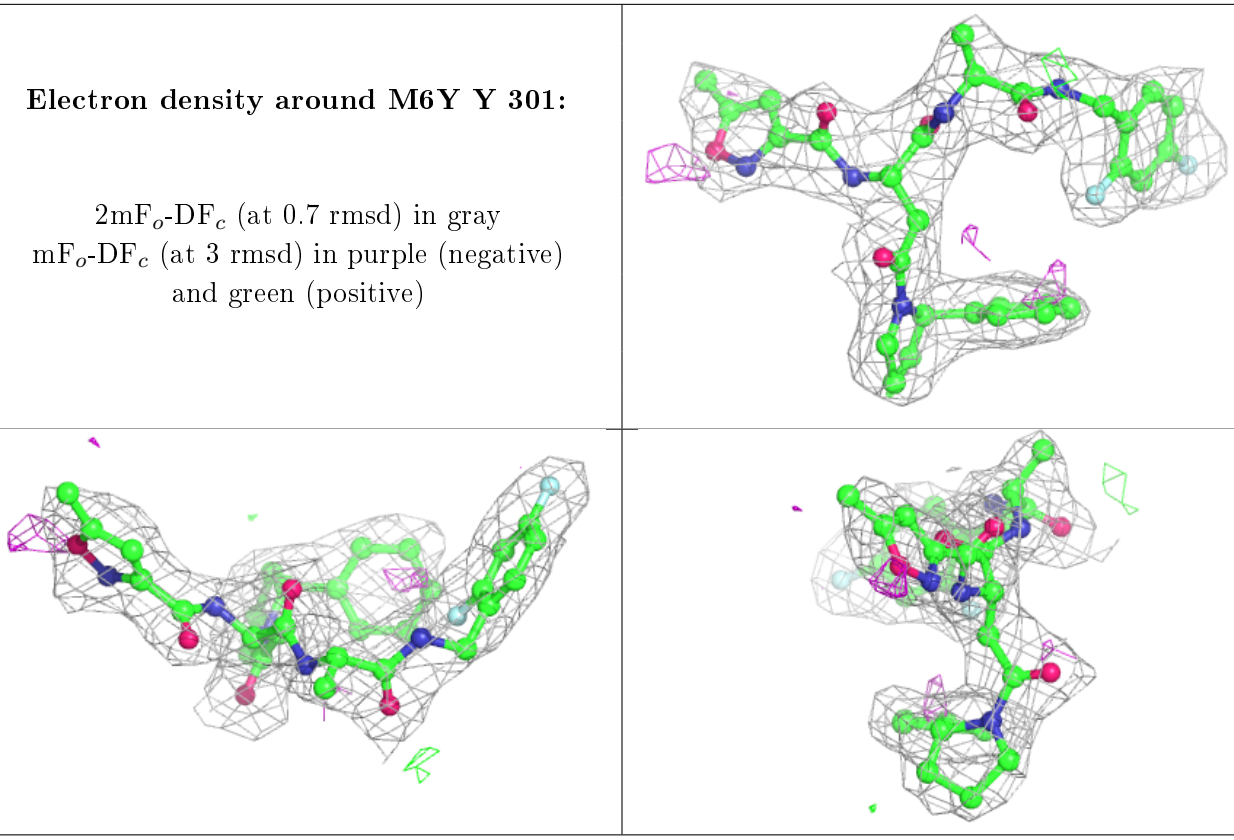






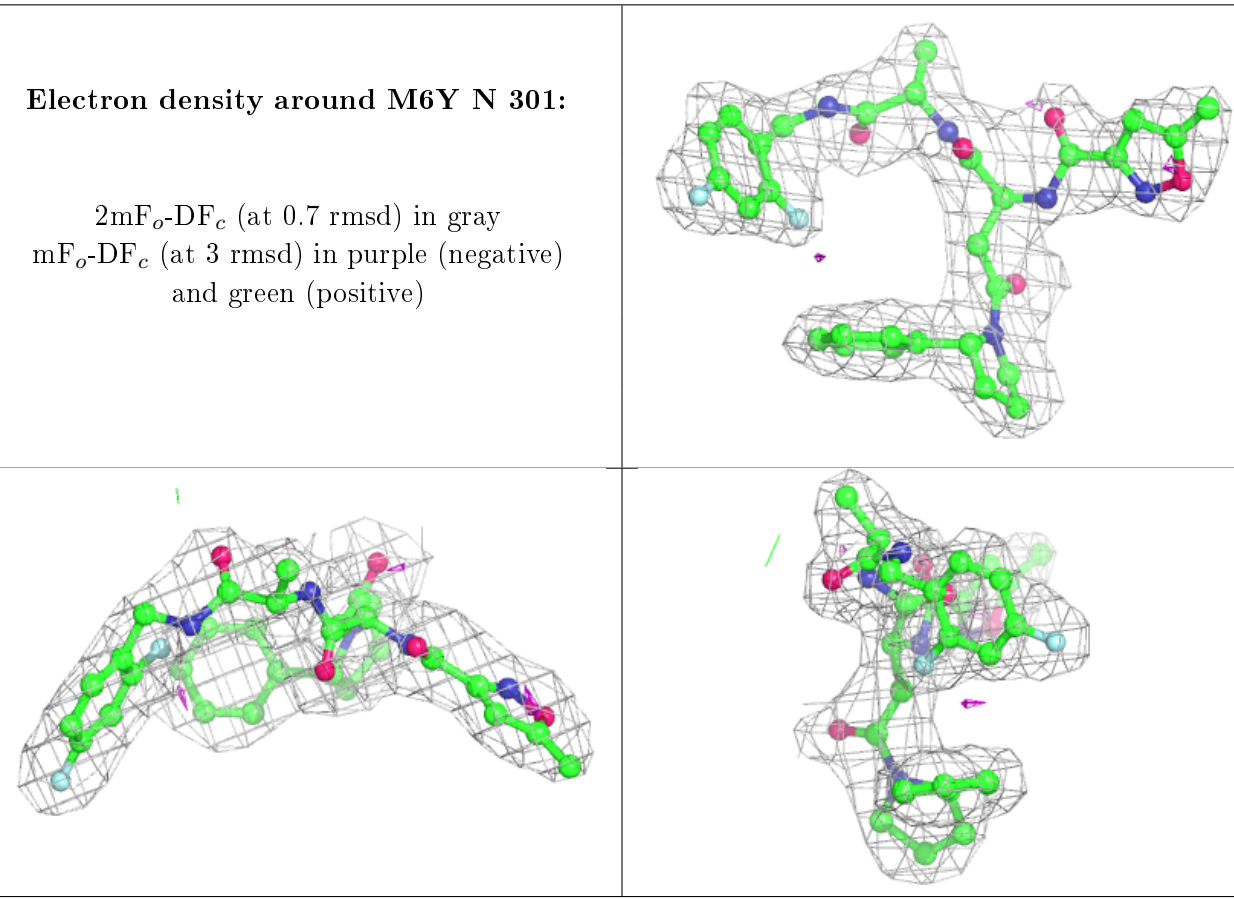
Electron density around M6Y Y 301:

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



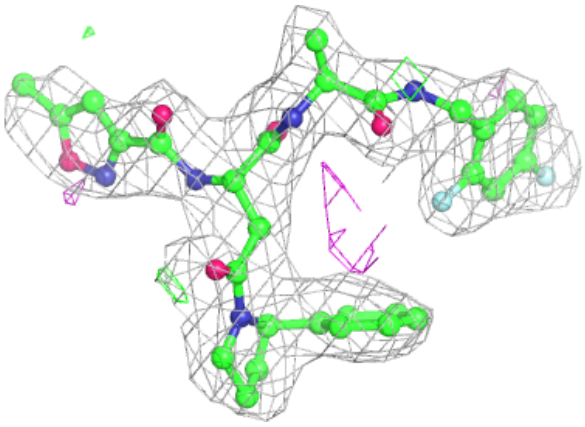
Electron density around M6Y N 301:

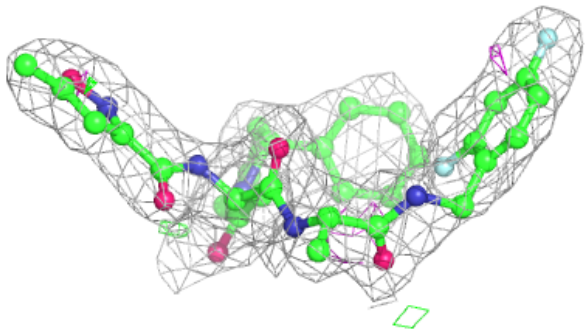
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

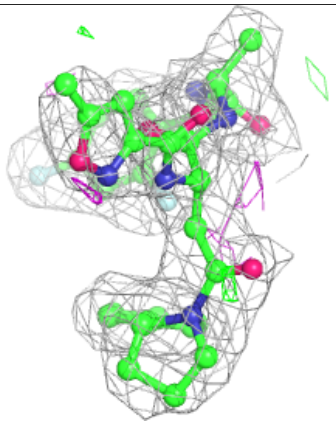


Electron density around M6Y H 301:

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

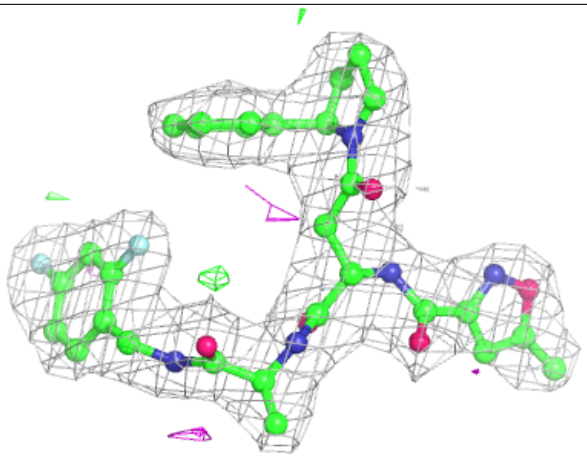


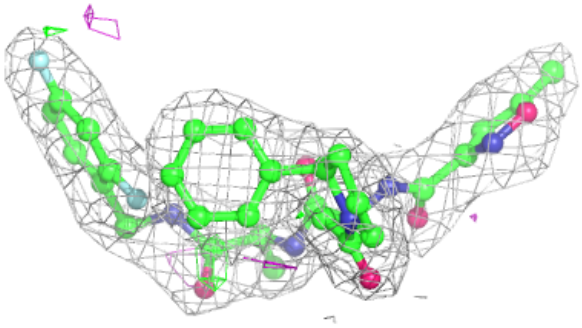


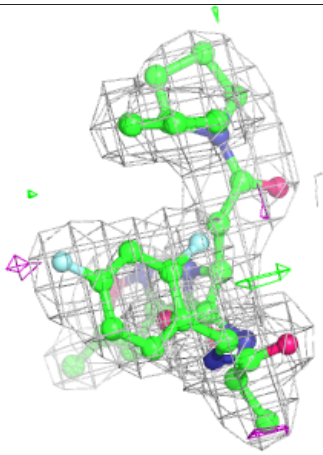


Electron density around M6Y V 301:

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

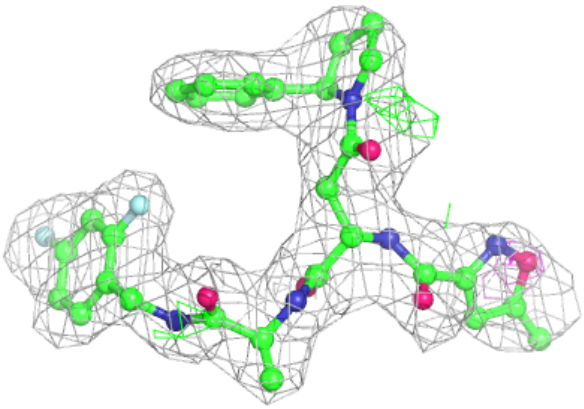


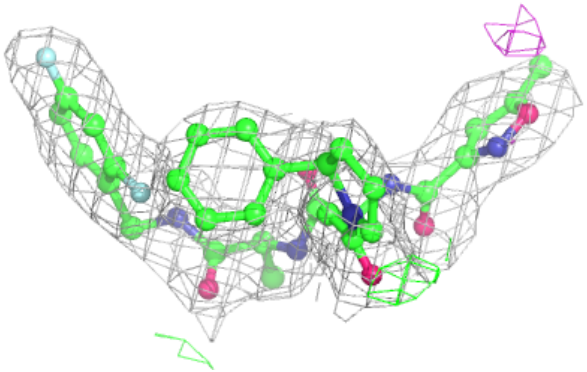


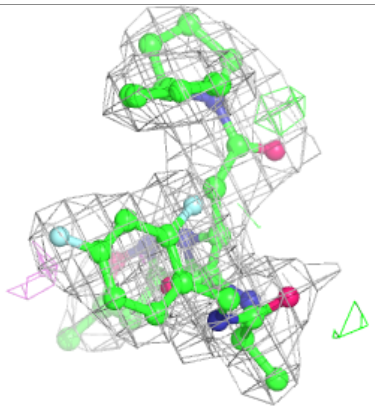


Electron density around M6Y I 301:

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

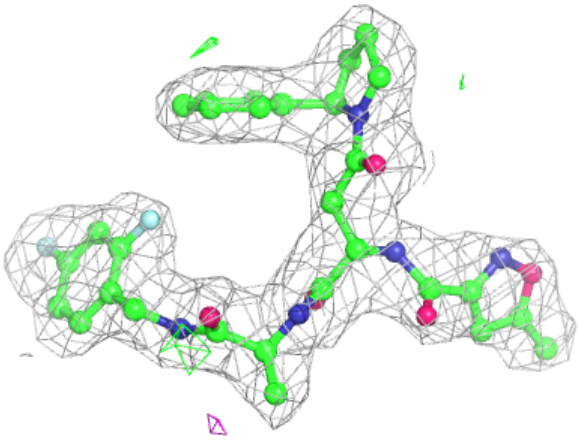


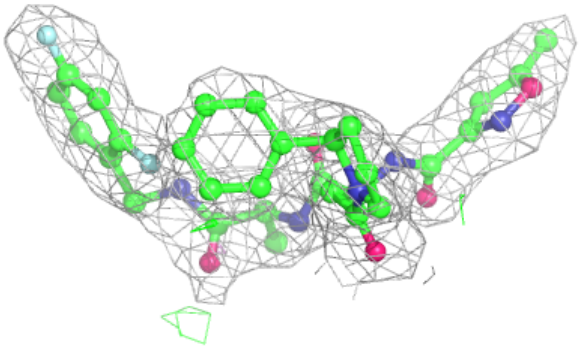


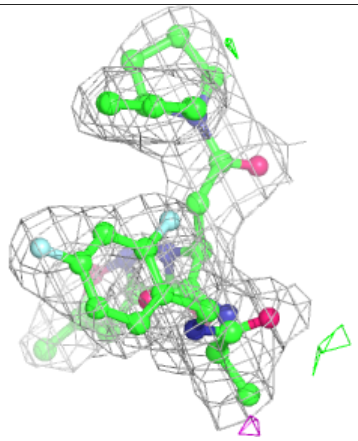


Electron density around M6Y Z 301:

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

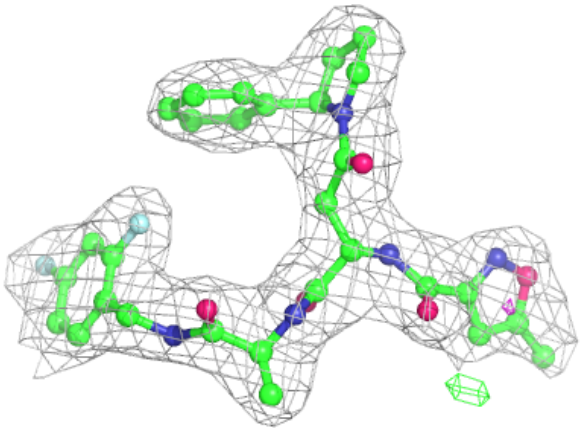


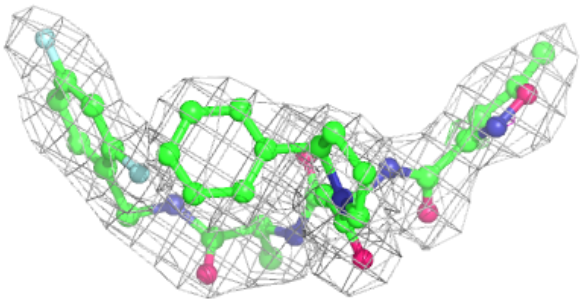


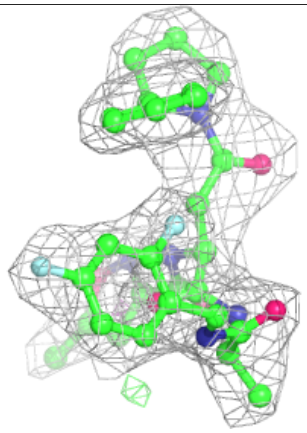


Electron density around M6Y a 301:

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

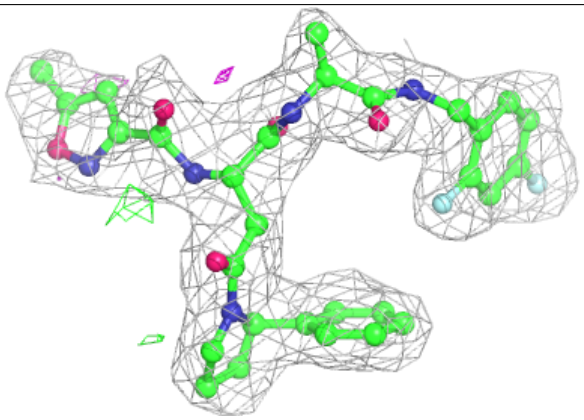


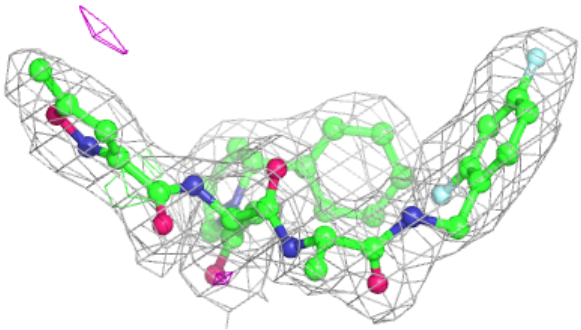


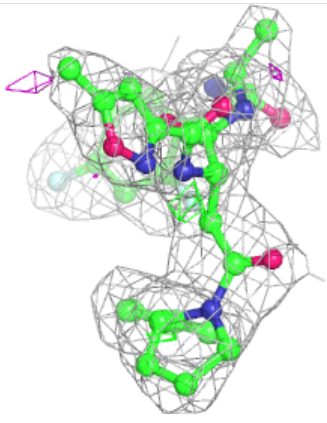


Electron density around M6Y J 301:

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

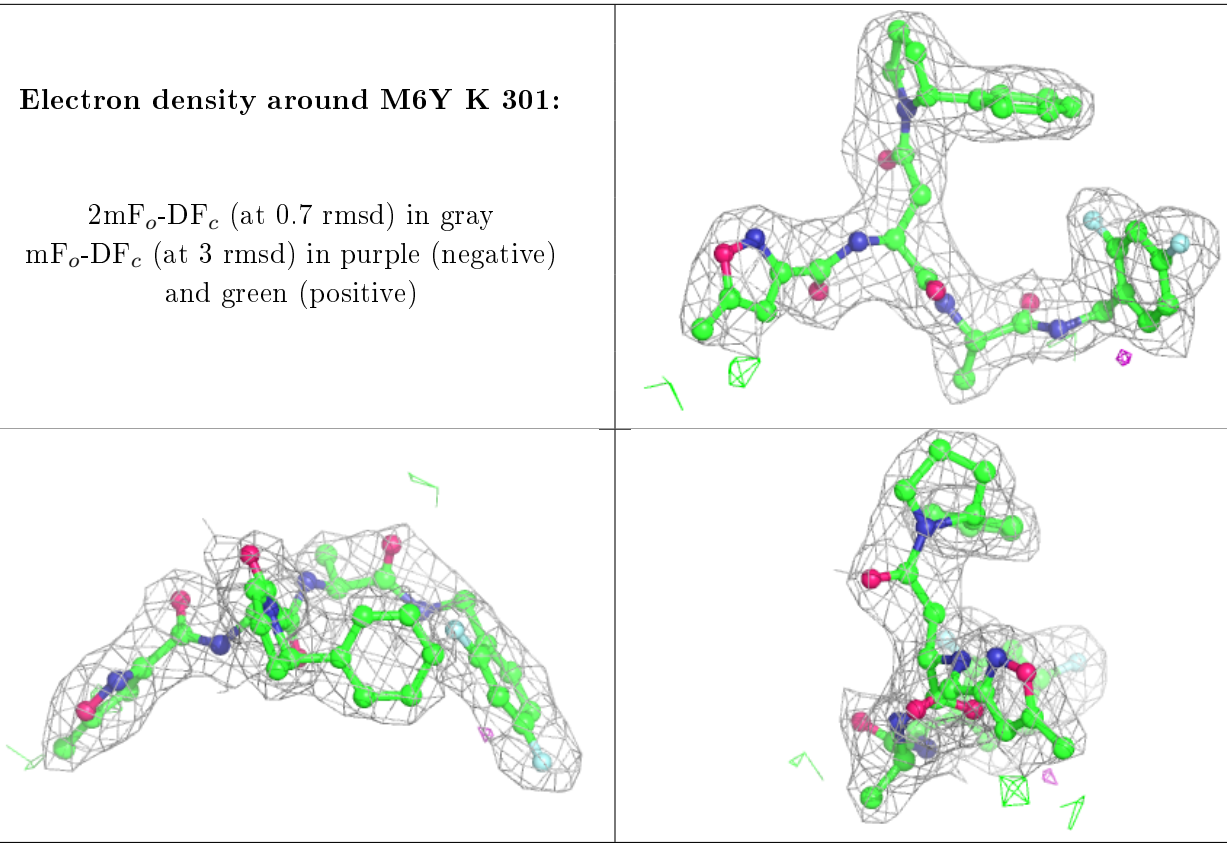






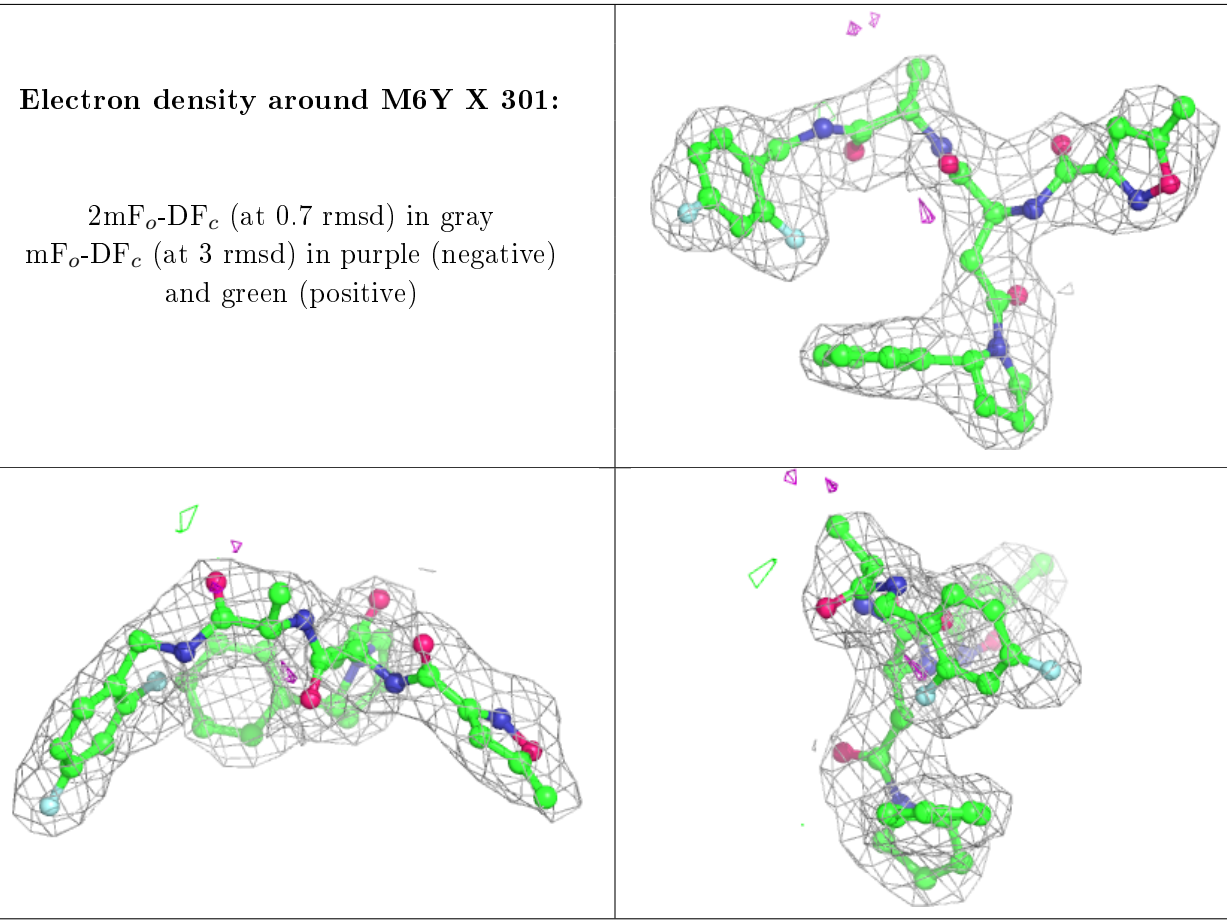
Electron density around M6Y K 301:

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



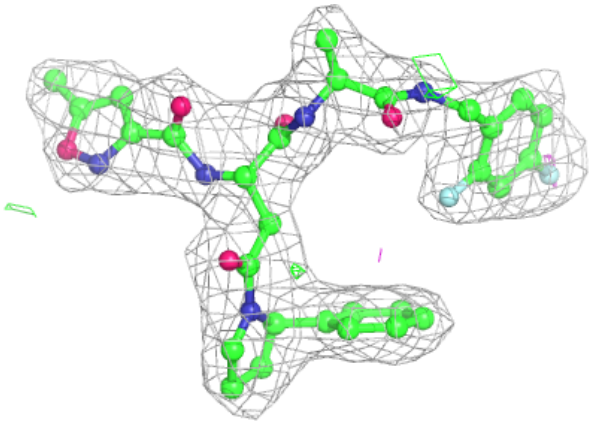
Electron density around M6Y X 301:

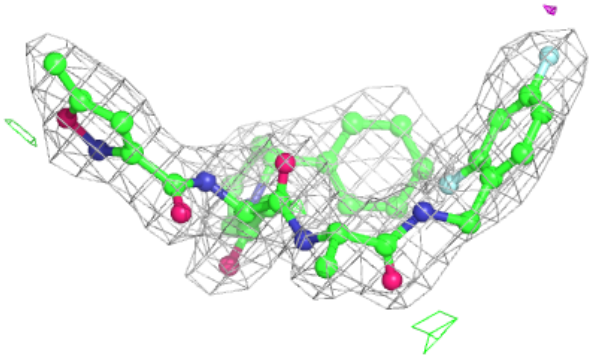
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

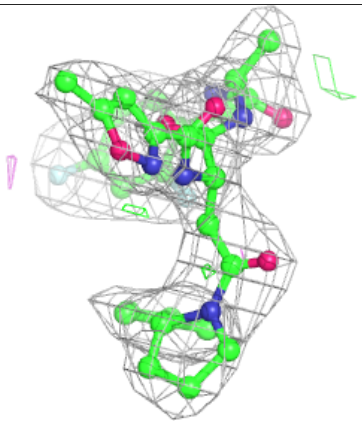


Electron density around M6Y L 301:

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

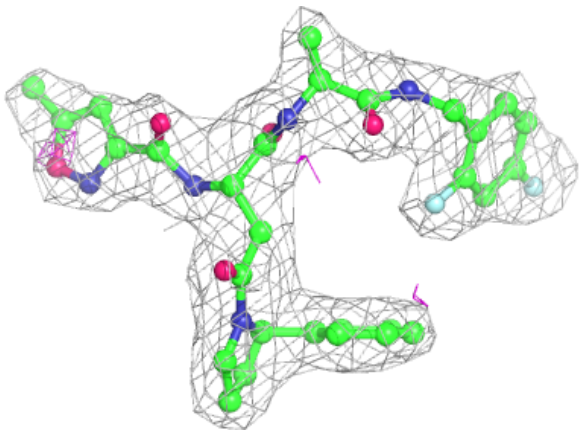


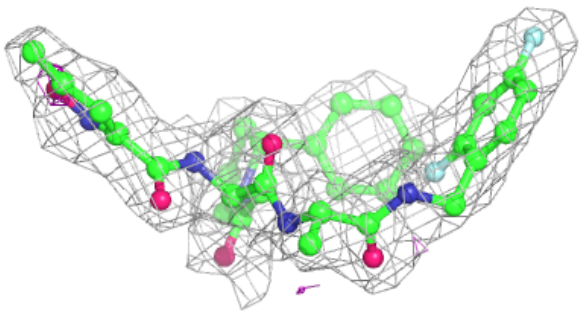


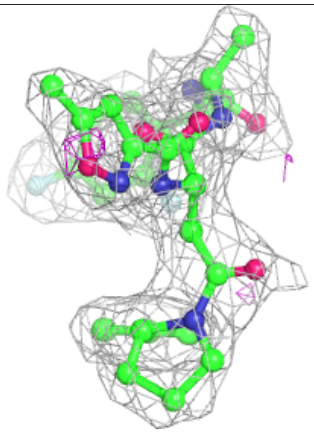


Electron density around M6Y W 301:

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

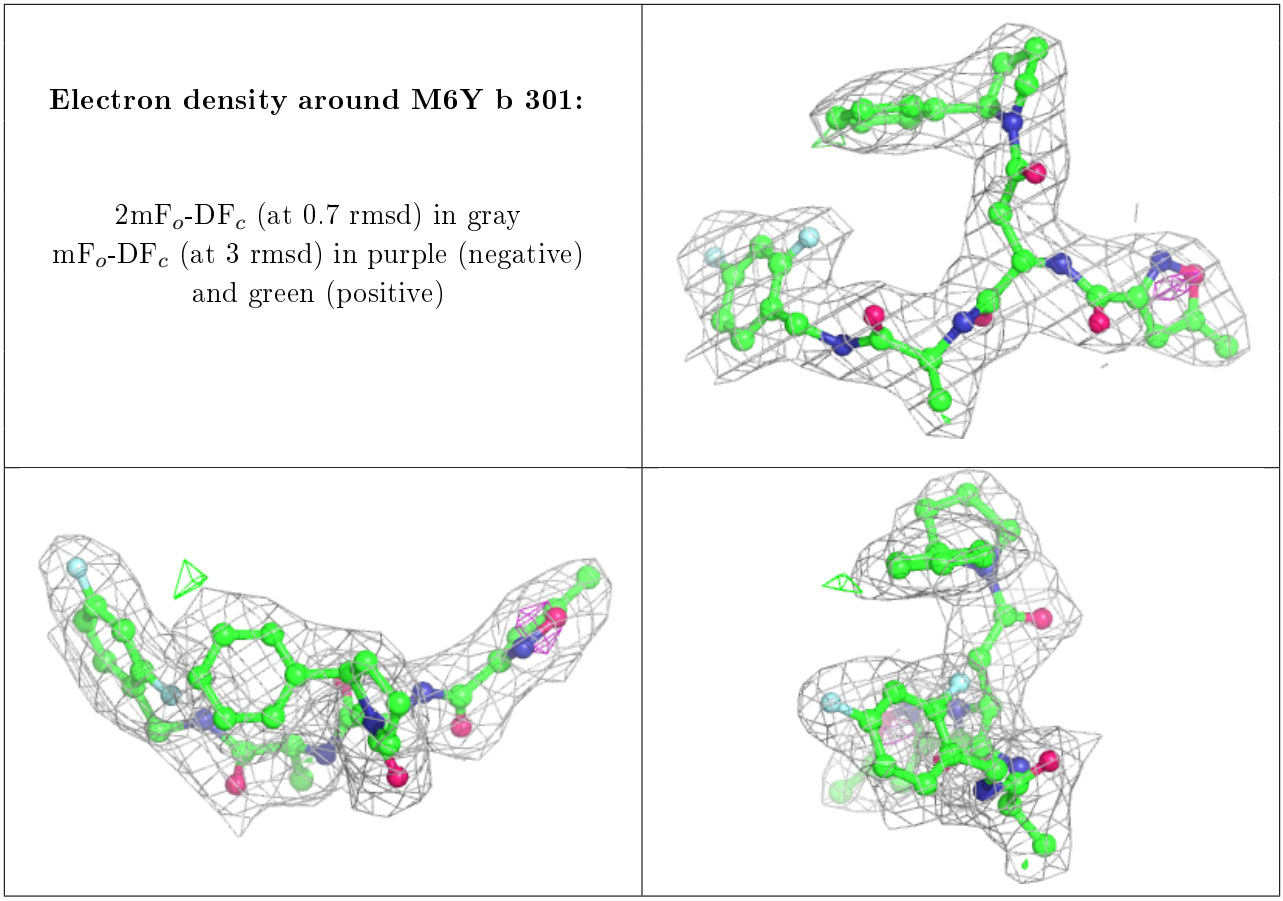






Electron density around M6Y b 301:

$2mF_o$-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.