Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2020 – 08:44 PM BST

PDB ID	:	5TRG
Title	:	Structure of Mycobacterium tuberculosis proteasome in complex with N,C-capped dipeptide DPLG-2
Authors	:	Hsu, H.-C.; Fan, H.; Singh, R.K.; Wang, R.; Sukenick, G.; Nathan, C.; Lin, G.; Li, H.
Deposited on	:	2016-10-26
Resolution	:	2.80 Å(reported)

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

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

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

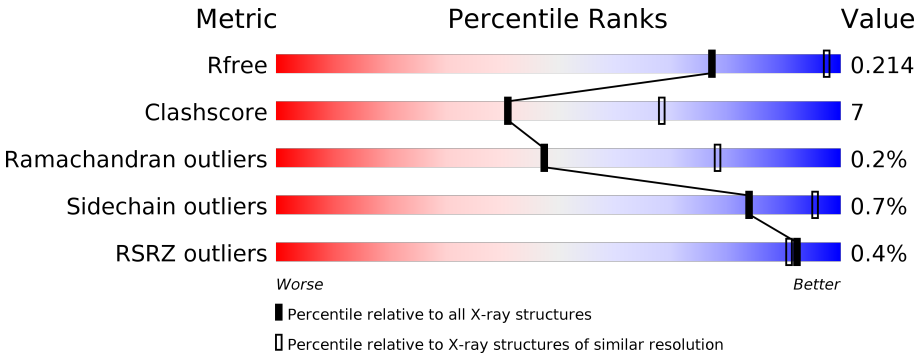
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance

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

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	75% 16% 9%
1	B	240	4% 62% 27% • 10%
1	C	240	2% 70% 18% •• 10%
1	D	240	73% 20% 7%
1	E	240	84% 7% 9%
1	F	240	% 65% 23% • 10%

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Mol	Chain	Length	Quality of chain
1	G	240	71% 19% 10%
1	O	240	72% 18% 9%
1	P	240	69% 22% 9%
1	Q	240	73% 18% 10%
1	R	240	75% 15% 10%
1	S	240	79% 11% 9%
1	T	240	75% 15% 10%
1	U	240	68% 21% 10%
2	H	240	79% 13% 8%
2	I	240	85% 8% 8%
2	J	240	83% 10% 8%
2	K	240	82% 11% 7%
2	L	240	84% 9% 7%
2	M	240	85% 7% 8%
2	N	240	84% 8% 7%
2	V	240	85% 8% 7%
2	W	240	79% 13% 7%
2	X	240	83% 9% 8%
2	Y	240	84% 9% 7%
2	Z	240	81% 11% 8%
2	a	240	92% 7%
2	b	240	92% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 47357 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Proteasome subunit alpha.

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	216	Total	C	N	O	S	0	0	0
			1664	1043	304	313	4			
1	D	223	Total	C	N	O	S	0	0	0
			1716	1070	313	329	4			
1	E	218	Total	C	N	O	S	0	0	0
			1677	1050	306	317	4			
1	F	215	Total	C	N	O	S	0	0	0
			1655	1035	303	313	4			
1	G	216	Total	C	N	O	S	0	0	0
			1662	1040	304	314	4			
1	O	218	Total	C	N	O	S	0	0	0
			1677	1050	306	317	4			
1	P	219	Total	C	N	O	S	0	0	0
			1685	1054	307	320	4			
1	Q	217	Total	C	N	O	S	0	0	0
			1677	1050	306	317	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 A5U4D5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	9	MET	-	initiating methionine	UNP A5U4D5
C	9	MET	-	initiating methionine	UNP A5U4D5
D	9	MET	-	initiating methionine	UNP A5U4D5
E	9	MET	-	initiating methionine	UNP A5U4D5
F	9	MET	-	initiating methionine	UNP A5U4D5
G	9	MET	-	initiating methionine	UNP A5U4D5
O	9	MET	-	initiating methionine	UNP A5U4D5
P	9	MET	-	initiating methionine	UNP A5U4D5
Q	9	MET	-	initiating methionine	UNP A5U4D5
R	9	MET	-	initiating methionine	UNP A5U4D5
S	9	MET	-	initiating methionine	UNP A5U4D5
T	9	MET	-	initiating methionine	UNP A5U4D5
U	9	MET	-	initiating methionine	UNP A5U4D5

- 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			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	235	HIS	-	expression tag	UNP A5U4D6
H	236	HIS	-	expression tag	UNP A5U4D6
H	237	HIS	-	expression tag	UNP A5U4D6
H	238	HIS	-	expression tag	UNP A5U4D6
H	239	HIS	-	expression tag	UNP A5U4D6
H	240	HIS	-	expression tag	UNP A5U4D6
I	235	HIS	-	expression tag	UNP A5U4D6
I	236	HIS	-	expression tag	UNP A5U4D6
I	237	HIS	-	expression tag	UNP A5U4D6
I	238	HIS	-	expression tag	UNP A5U4D6
I	239	HIS	-	expression tag	UNP A5U4D6
I	240	HIS	-	expression tag	UNP A5U4D6
J	235	HIS	-	expression tag	UNP A5U4D6
J	236	HIS	-	expression tag	UNP A5U4D6
J	237	HIS	-	expression tag	UNP A5U4D6
J	238	HIS	-	expression tag	UNP A5U4D6
J	239	HIS	-	expression tag	UNP A5U4D6
J	240	HIS	-	expression tag	UNP A5U4D6
K	235	HIS	-	expression tag	UNP A5U4D6
K	236	HIS	-	expression tag	UNP A5U4D6
K	237	HIS	-	expression tag	UNP A5U4D6
K	238	HIS	-	expression tag	UNP A5U4D6
K	239	HIS	-	expression tag	UNP A5U4D6
K	240	HIS	-	expression tag	UNP A5U4D6
L	235	HIS	-	expression tag	UNP A5U4D6
L	236	HIS	-	expression tag	UNP A5U4D6
L	237	HIS	-	expression tag	UNP A5U4D6
L	238	HIS	-	expression tag	UNP A5U4D6
L	239	HIS	-	expression tag	UNP A5U4D6
L	240	HIS	-	expression tag	UNP A5U4D6
M	235	HIS	-	expression tag	UNP A5U4D6
M	236	HIS	-	expression tag	UNP A5U4D6
M	237	HIS	-	expression tag	UNP A5U4D6
M	238	HIS	-	expression tag	UNP A5U4D6
M	239	HIS	-	expression tag	UNP A5U4D6
M	240	HIS	-	expression tag	UNP A5U4D6

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Chain	Residue	Modelled	Actual	Comment	Reference
N	235	HIS	-	expression tag	UNP A5U4D6
N	236	HIS	-	expression tag	UNP A5U4D6
N	237	HIS	-	expression tag	UNP A5U4D6
N	238	HIS	-	expression tag	UNP A5U4D6
N	239	HIS	-	expression tag	UNP A5U4D6
N	240	HIS	-	expression tag	UNP A5U4D6
V	235	HIS	-	expression tag	UNP A5U4D6
V	236	HIS	-	expression tag	UNP A5U4D6
V	237	HIS	-	expression tag	UNP A5U4D6
V	238	HIS	-	expression tag	UNP A5U4D6
V	239	HIS	-	expression tag	UNP A5U4D6
V	240	HIS	-	expression tag	UNP A5U4D6
W	235	HIS	-	expression tag	UNP A5U4D6
W	236	HIS	-	expression tag	UNP A5U4D6
W	237	HIS	-	expression tag	UNP A5U4D6
W	238	HIS	-	expression tag	UNP A5U4D6
W	239	HIS	-	expression tag	UNP A5U4D6
W	240	HIS	-	expression tag	UNP A5U4D6
X	235	HIS	-	expression tag	UNP A5U4D6
X	236	HIS	-	expression tag	UNP A5U4D6
X	237	HIS	-	expression tag	UNP A5U4D6
X	238	HIS	-	expression tag	UNP A5U4D6
X	239	HIS	-	expression tag	UNP A5U4D6
X	240	HIS	-	expression tag	UNP A5U4D6
Y	235	HIS	-	expression tag	UNP A5U4D6
Y	236	HIS	-	expression tag	UNP A5U4D6
Y	237	HIS	-	expression tag	UNP A5U4D6
Y	238	HIS	-	expression tag	UNP A5U4D6
Y	239	HIS	-	expression tag	UNP A5U4D6
Y	240	HIS	-	expression tag	UNP A5U4D6
Z	235	HIS	-	expression tag	UNP A5U4D6
Z	236	HIS	-	expression tag	UNP A5U4D6
Z	237	HIS	-	expression tag	UNP A5U4D6
Z	238	HIS	-	expression tag	UNP A5U4D6
Z	239	HIS	-	expression tag	UNP A5U4D6
Z	240	HIS	-	expression tag	UNP A5U4D6
a	235	HIS	-	expression tag	UNP A5U4D6
a	236	HIS	-	expression tag	UNP A5U4D6
a	237	HIS	-	expression tag	UNP A5U4D6
a	238	HIS	-	expression tag	UNP A5U4D6
a	239	HIS	-	expression tag	UNP A5U4D6
a	240	HIS	-	expression tag	UNP A5U4D6

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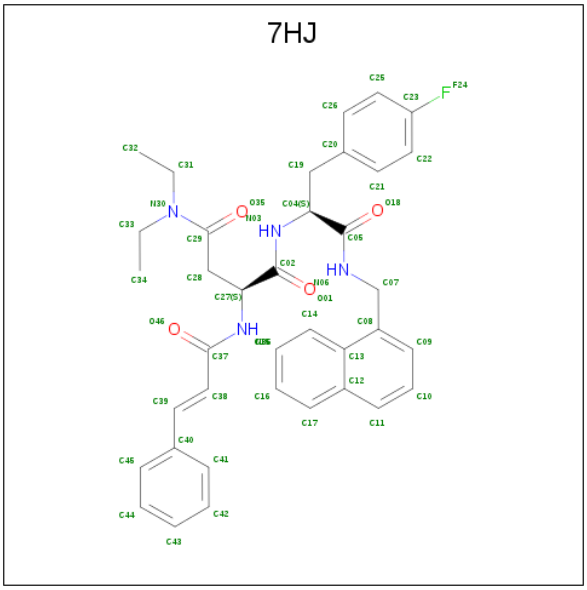
Chain	Residue	Modelled	Actual	Comment	Reference
b	235	HIS	-	expression tag	UNP A5U4D6
b	236	HIS	-	expression tag	UNP A5U4D6
b	237	HIS	-	expression tag	UNP A5U4D6
b	238	HIS	-	expression tag	UNP A5U4D6
b	239	HIS	-	expression tag	UNP A5U4D6
b	240	HIS	-	expression tag	UNP A5U4D6

- Molecule 3 is N,N-diethyl-N 2 -[(2E)-3-phenylprop-2-enoyl]-L-asparaginyl-4-fluoro-N-[(naphthalen-1-yl)methyl]-L-phenylalaninamide (three-letter code: 7HJ) (formula: $C_{37}H_{39}FN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	H	1	Total	C	F	N	O	0	0
			46	37	1	4	4		
3	I	1	Total	C	F	N	O	0	0
			46	37	1	4	4		
3	J	1	Total	C	F	N	O	0	0
			46	37	1	4	4		
3	K	1	Total	C	F	N	O	0	0
			46	37	1	4	4		
3	L	1	Total	C	F	N	O	0	0
			46	37	1	4	4		
3	M	1	Total	C	F	N	O	0	0
			46	37	1	4	4		
3	N	1	Total	C	F	N	O	0	0
			46	37	1	4	4		
3	V	1	Total	C	F	N	O	0	0
			46	37	1	4	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	W	1	Total	C	F	N	O	0	0
			46	37	1	4	4		
3	X	1	Total	C	F	N	O	0	0
			46	37	1	4	4		
3	Y	1	Total	C	F	N	O	0	0
			46	37	1	4	4		
3	Z	1	Total	C	F	N	O	0	0
			46	37	1	4	4		
3	a	1	Total	C	F	N	O	0	0
			46	37	1	4	4		
3	b	1	Total	C	F	N	O	0	0
			46	37	1	4	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total	O	0	0
			10	10		
4	B	1	Total	O	0	0
			1	1		
4	C	4	Total	O	0	0
			4	4		
4	D	7	Total	O	0	0
			7	7		
4	E	16	Total	O	0	0
			16	16		
4	F	5	Total	O	0	0
			5	5		
4	G	14	Total	O	0	0
			14	14		
4	H	11	Total	O	0	0
			11	11		
4	I	19	Total	O	0	0
			19	19		
4	J	14	Total	O	0	0
			14	14		
4	K	14	Total	O	0	0
			14	14		
4	L	16	Total	O	0	0
			16	16		
4	M	14	Total	O	0	0
			14	14		

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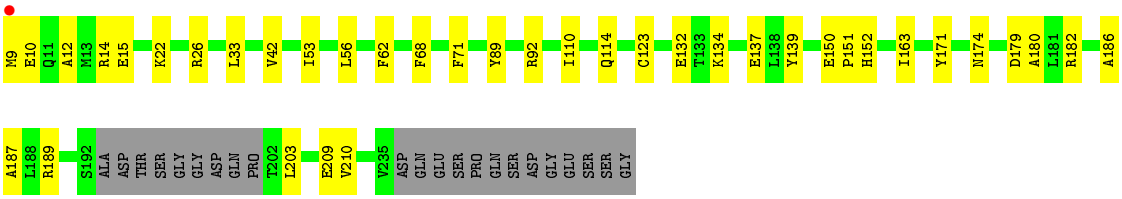
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	N	9	Total O 9 9	0	0
4	O	8	Total O 8 8	0	0
4	P	9	Total O 9 9	0	0
4	Q	8	Total O 8 8	0	0
4	R	9	Total O 9 9	0	0
4	S	15	Total O 15 15	0	0
4	T	11	Total O 11 11	0	0
4	U	13	Total O 13 13	0	0
4	V	14	Total O 14 14	0	0
4	W	17	Total O 17 17	0	0
4	X	15	Total O 15 15	0	0
4	Y	15	Total O 15 15	0	0
4	Z	16	Total O 16 16	0	0
4	a	7	Total O 7 7	0	0
4	b	18	Total O 18 18	0	0

3 Residue-property plots (i)

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

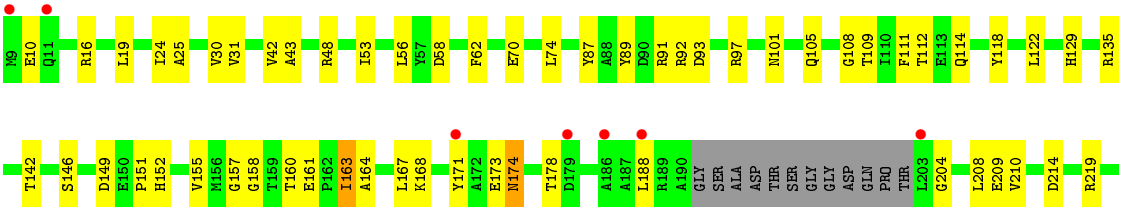
- Molecule 1: Proteasome subunit alpha

Chain A:



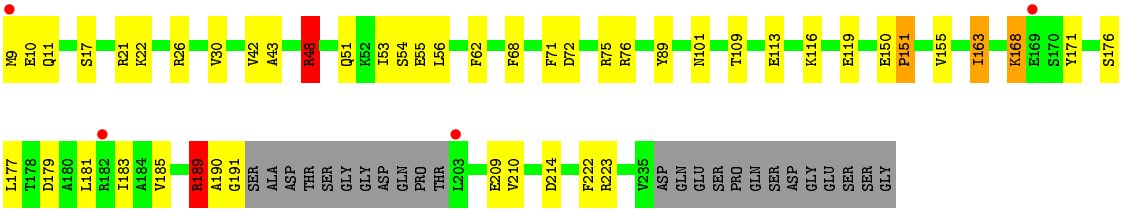
- Molecule 1: Proteasome subunit alpha

Chain B:



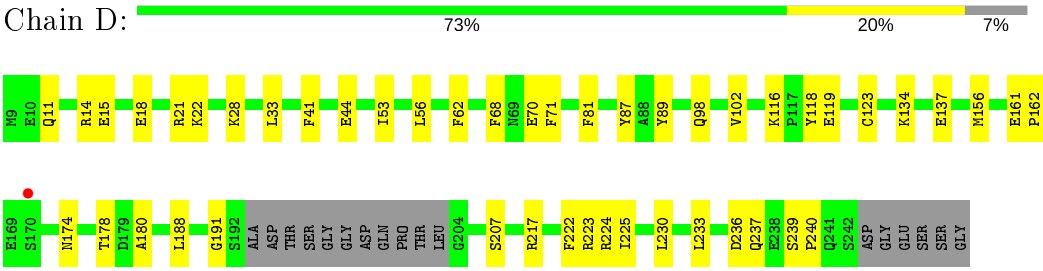
- Molecule 1: Proteasome subunit alpha

Chain C:



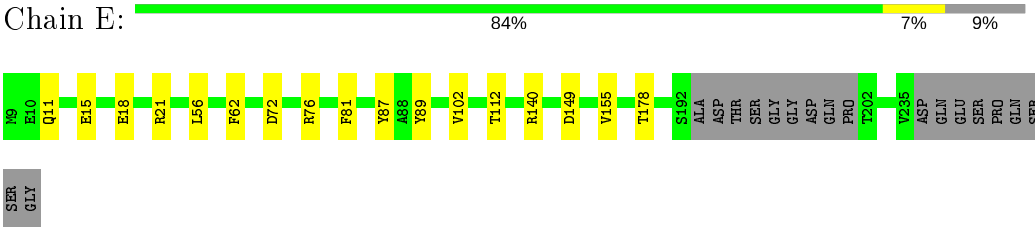
- Molecule 1: Proteasome subunit alpha

Chain D:



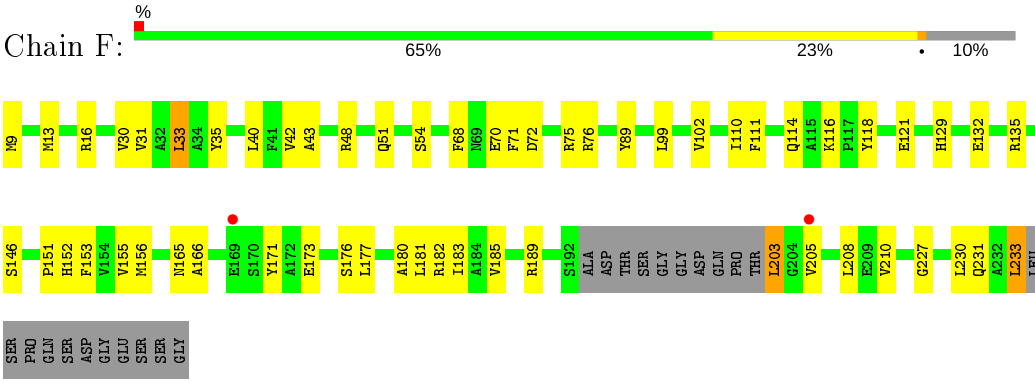
• Molecule 1: Proteasome subunit alpha

Chain E:



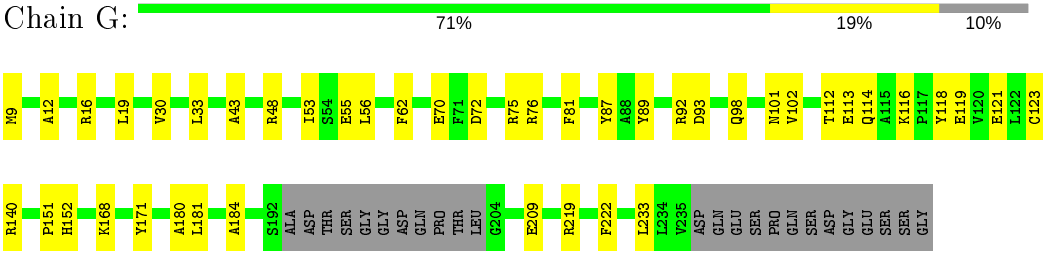
• Molecule 1: Proteasome subunit alpha

Chain F:



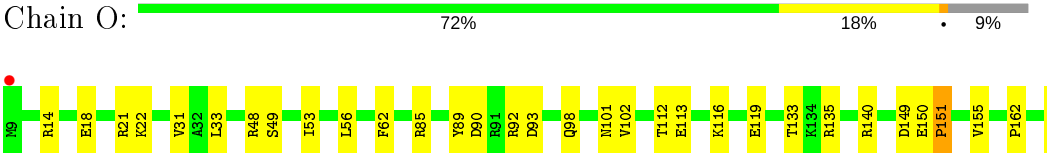
• Molecule 1: Proteasome subunit alpha

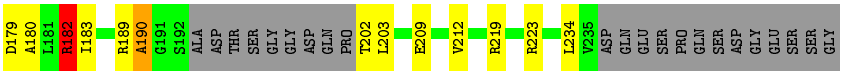
Chain G:



• Molecule 1: Proteasome subunit alpha

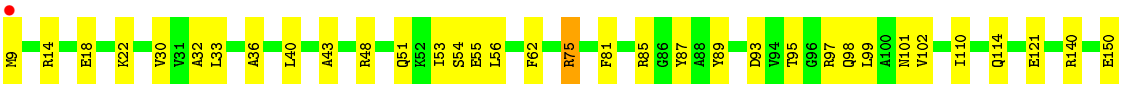
Chain O:

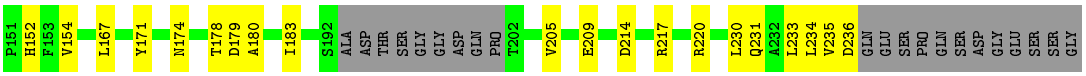




• Molecule 1: Proteasome subunit alpha

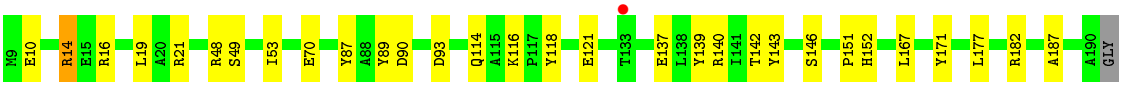
Chain P:





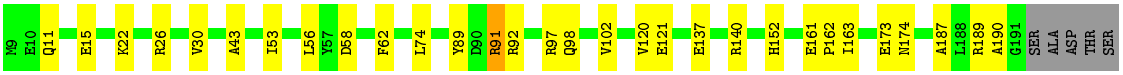
• Molecule 1: Proteasome subunit alpha

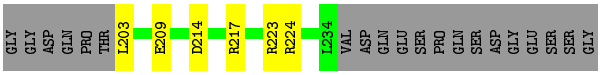
Chain Q:



• Molecule 1: Proteasome subunit alpha

Chain R:



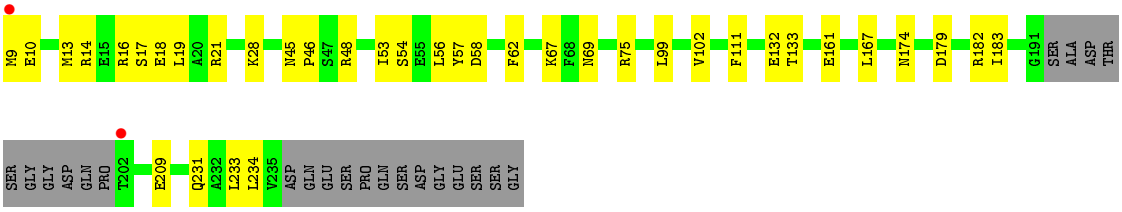


• Molecule 1: Proteasome subunit alpha

Chain S:

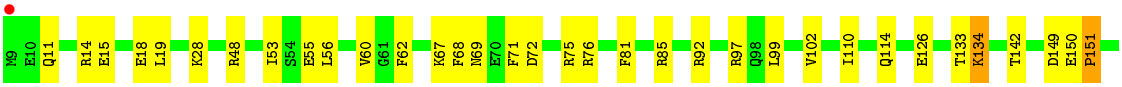
• Molecule 1: Proteasome subunit alpha

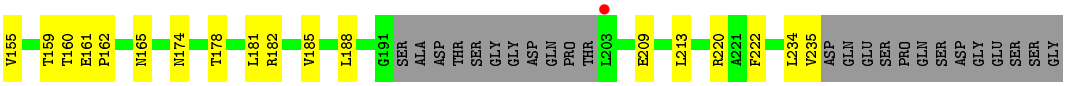
Chain T:



• Molecule 1: Proteasome subunit alpha

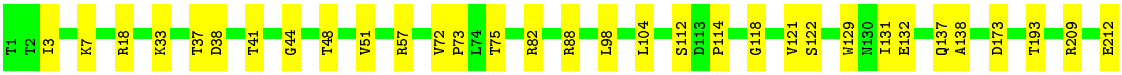
Chain U:





• Molecule 2: Proteasome subunit beta

Chain H:

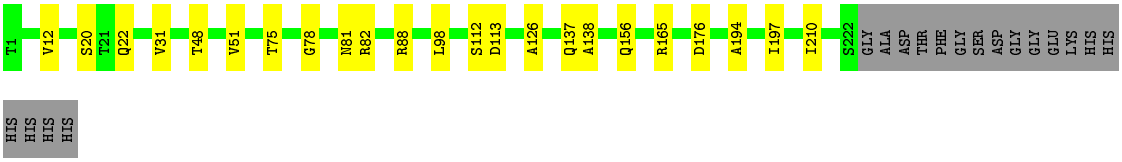


• Molecule 2: Proteasome subunit beta

Chain I:

• Molecule 2: Proteasome subunit beta

Chain J:

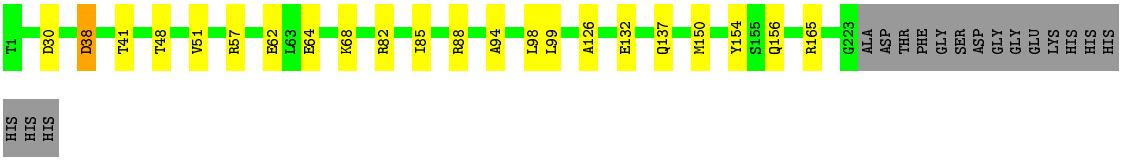


• Molecule 2: Proteasome subunit beta

Chain K:

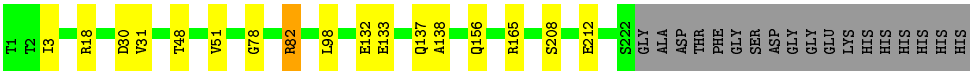
- Molecule 2: Proteasome subunit beta

Chain L:



- Molecule 2: Proteasome subunit beta

Chain M:



- Molecule 2: Proteasome subunit beta

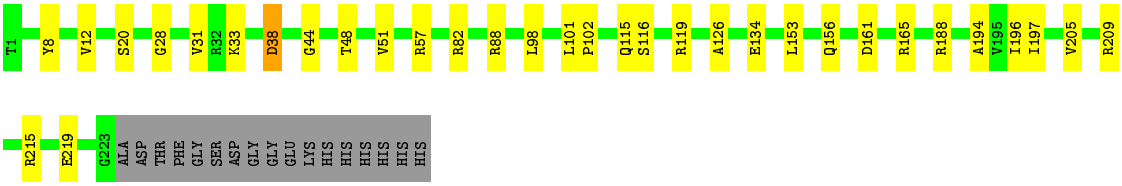
Chain N:

- Molecule 2: Proteasome subunit beta

Chain V:

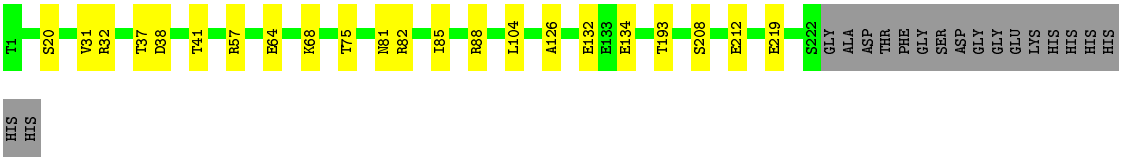
- Molecule 2: Proteasome subunit beta

Chain W:



- Molecule 2: Proteasome subunit beta

Chain X:

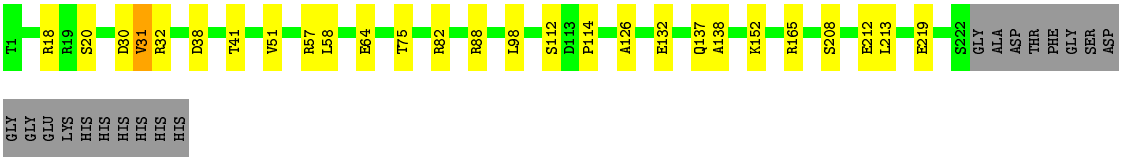


- Molecule 2: Proteasome subunit beta

Chain Y:

- Molecule 2: Proteasome subunit beta

Chain Z:



- Molecule 2: Proteasome subunit beta

Chain a:

- Molecule 2: Proteasome subunit beta

Chain b:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	120.05Å 219.09Å 137.89Å 90.00° 104.87° 90.00°	Depositor
Resolution (Å)	49.53 – 2.80 49.53 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.53-2.80) 99.4 (49.53-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.160 , 0.216 0.160 , 0.214	Depositor DCC
R_{free} test set	8302 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	48.5	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 48.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	47357	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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: 7HJ

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	0.66	0/1701	0.76	0/2297
1	B	0.64	0/1684	0.80	1/2274 (0.0%)
1	C	0.66	0/1688	0.78	4/2279 (0.2%)
1	D	0.64	0/1741	0.74	0/2351
1	E	0.67	0/1701	0.75	0/2297
1	F	0.65	0/1679	0.81	3/2266 (0.1%)
1	G	0.67	0/1686	0.73	0/2276
1	O	0.66	0/1701	0.77	2/2297 (0.1%)
1	P	0.65	0/1709	0.76	2/2308 (0.1%)
1	Q	0.65	0/1701	0.75	2/2297 (0.1%)
1	R	0.70	1/1681 (0.1%)	0.75	0/2269
1	S	0.67	0/1702	0.73	0/2298
1	T	0.72	0/1695	0.78	0/2289
1	U	0.76	1/1688 (0.1%)	0.81	1/2279 (0.0%)
2	H	0.63	0/1662	0.76	1/2254 (0.0%)
2	I	0.63	0/1662	0.74	0/2254
2	J	0.60	0/1662	0.71	0/2254
2	K	0.65	0/1666	0.79	2/2259 (0.1%)
2	L	0.65	0/1666	0.77	1/2259 (0.0%)
2	M	0.64	0/1662	0.78	1/2254 (0.0%)
2	N	0.58	0/1666	0.74	1/2259 (0.0%)
2	V	0.66	0/1666	0.79	1/2259 (0.0%)
2	W	0.64	0/1666	0.75	1/2259 (0.0%)
2	X	0.66	2/1662 (0.1%)	0.74	0/2254
2	Y	0.64	0/1666	0.75	0/2259
2	Z	0.67	1/1662 (0.1%)	0.76	1/2254 (0.0%)
2	a	0.66	0/1666	0.79	2/2259 (0.1%)
2	b	0.63	0/1666	0.71	1/2259 (0.0%)
All	All	0.66	5/47057 (0.0%)	0.76	27/63673 (0.0%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	U	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	219	GLU	CD-OE1	-7.73	1.17	1.25
2	Z	31	VAL	CB-CG1	-7.60	1.36	1.52
2	X	219	GLU	CD-OE2	-6.91	1.18	1.25
1	R	120	VAL	CB-CG1	-5.45	1.41	1.52
1	U	134	LYS	CB-CG	5.17	1.66	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	a	82	ARG	NE-CZ-NH2	7.94	124.27	120.30
1	Q	48	ARG	NE-CZ-NH2	7.48	124.04	120.30
1	F	208	LEU	CA-CB-CG	7.19	131.84	115.30
2	M	82	ARG	NE-CZ-NH2	7.09	123.85	120.30
2	L	38	ASP	CB-CG-OD1	6.70	124.33	118.30
1	F	203	LEU	CB-CG-CD2	-6.51	99.94	111.00
1	C	48	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	U	76	ARG	NE-CZ-NH2	-6.33	117.14	120.30
2	H	57	ARG	NE-CZ-NH1	-6.26	117.17	120.30
1	B	163	ILE	CG1-CB-CG2	-6.19	97.78	111.40
1	O	182	ARG	NE-CZ-NH2	-5.99	117.31	120.30
2	K	209	ARG	NE-CZ-NH1	5.98	123.29	120.30
2	W	38	ASP	CB-CG-OD1	5.77	123.50	118.30
2	b	38	ASP	CB-CG-OD1	5.54	123.28	118.30
1	Q	14	ARG	NE-CZ-NH2	5.50	123.05	120.30
2	N	38	ASP	CB-CG-OD1	5.46	123.21	118.30
1	O	14	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	C	189	ARG	NE-CZ-NH1	5.40	123.00	120.30
2	V	57	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	C	191	GLY	N-CA-C	5.34	126.45	113.10
2	a	38	ASP	CB-CG-OD1	5.31	123.08	118.30
1	F	33	LEU	CB-CG-CD1	-5.30	101.99	111.00
2	K	38	ASP	CB-CG-OD1	5.29	123.06	118.30
2	Z	58	LEU	CB-CG-CD2	-5.27	102.04	111.00
1	P	14	ARG	NE-CZ-NH2	5.17	122.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	75	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	C	48	ARG	NE-CZ-NH2	-5.07	117.77	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	U	133	THR	Peptide

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	29	0
1	B	1660	0	1665	63	0
1	C	1664	0	1668	45	0
1	D	1716	0	1705	38	2
1	E	1677	0	1680	11	0
1	F	1655	0	1653	56	0
1	G	1662	0	1662	33	0
1	O	1677	0	1680	41	0
1	P	1685	0	1684	39	0
1	Q	1677	0	1677	28	0
1	R	1657	0	1659	29	0
1	S	1678	0	1677	21	0
1	T	1671	0	1675	30	0
1	U	1664	0	1668	33	0
2	H	1638	0	1633	22	0
2	I	1638	0	1633	14	0
2	J	1638	0	1633	18	0
2	K	1642	0	1636	16	0
2	L	1642	0	1636	15	0
2	M	1638	0	1633	14	0
2	N	1642	0	1636	19	0
2	V	1642	0	1636	14	0
2	W	1642	0	1636	20	0
2	X	1638	0	1633	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Y	1642	0	1636	14	0
2	Z	1638	0	1633	18	2
2	a	1642	0	1636	0	0
2	b	1642	0	1636	0	0
3	H	46	0	0	1	0
3	I	46	0	0	0	0
3	J	46	0	0	2	0
3	K	46	0	0	0	0
3	L	46	0	0	1	0
3	M	46	0	0	1	0
3	N	46	0	0	3	0
3	V	46	0	0	1	0
3	W	46	0	0	1	0
3	X	46	0	0	0	0
3	Y	46	0	0	0	0
3	Z	46	0	0	1	0
3	a	46	0	0	0	0
3	b	46	0	0	0	0
4	A	10	0	0	0	0
4	B	1	0	0	0	0
4	C	4	0	0	0	0
4	D	7	0	0	0	0
4	E	16	0	0	0	0
4	F	5	0	0	0	0
4	G	14	0	0	0	0
4	H	11	0	0	0	0
4	I	19	0	0	0	0
4	J	14	0	0	2	0
4	K	14	0	0	0	0
4	L	16	0	0	0	0
4	M	14	0	0	0	0
4	N	9	0	0	0	0
4	O	8	0	0	0	0
4	P	9	0	0	0	0
4	Q	8	0	0	0	0
4	R	9	0	0	0	0
4	S	15	0	0	1	0
4	T	11	0	0	0	0
4	U	13	0	0	2	0
4	V	14	0	0	0	0
4	W	17	0	0	1	0
4	X	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Y	15	0	0	0	0
4	Z	16	0	0	0	0
4	a	7	0	0	0	0
4	b	18	0	0	0	0
All	All	47357	0	46319	618	2

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 7.

All (618) 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:T:10:GLU:O	1:T:14:ARG:HG3	1.45	1.15
1:S:92:ARG:NH1	1:S:132:GLU:OE2	1.82	1.12
1:T:182:ARG:NH2	1:T:233:LEU:O	1.91	1.02
1:R:58:ASP:OD1	1:R:91:ARG:NH1	1.95	0.99
1:O:182:ARG:HH22	1:O:234:LEU:HA	1.25	0.99
1:F:189:ARG:HE	1:F:203:LEU:HD11	1.25	0.99
1:F:189:ARG:HG2	1:F:203:LEU:HD21	1.45	0.94
1:R:92:ARG:HG3	1:R:92:ARG:HH21	1.35	0.92
1:F:233:LEU:HD13	1:F:233:LEU:H	1.36	0.91
1:F:16:ARG:NH1	1:F:114:GLN:O	2.03	0.90
1:B:160:THR:O	1:B:163:ILE:HG22	1.72	0.90
1:B:87:TYR:O	2:I:57:ARG:NH1	2.05	0.89
1:S:219:ARG:NH1	2:Z:64:GLU:OE2	2.06	0.88
1:G:72:ASP:OD1	1:G:75:ARG:NH1	2.06	0.87
1:Q:87:TYR:O	2:X:57:ARG:NH1	2.09	0.86
1:G:92:ARG:NH1	1:G:132:GLU:OE2	2.09	0.85
1:B:163:ILE:HD11	1:B:188:LEU:HA	1.57	0.85
1:O:182:ARG:NH2	1:O:234:LEU:HA	1.92	0.83
2:H:38:ASP:HB3	2:H:41:THR:HB	1.61	0.83
1:R:214:ASP:OD2	1:R:223:ARG:NH2	2.13	0.82
1:F:16:ARG:NH2	1:F:111:PHE:O	2.13	0.82
1:S:87:TYR:O	2:Z:57:ARG:NH2	2.13	0.82
1:D:87:TYR:O	2:K:57:ARG:NH2	2.13	0.81
1:B:97:ARG:HH21	1:C:51:GLN:HE22	1.28	0.81
1:A:134:LYS:NZ	1:A:137:GLU:OE2	2.13	0.81
2:J:75:THR:HG23	2:J:78:GLY:H	1.45	0.80
1:B:163:ILE:CD1	1:B:188:LEU:HA	2.10	0.80
1:R:152:HIS:NE2	1:R:173:GLU:OE2	2.13	0.80
1:B:214:ASP:OD2	1:B:223:ARG:NH2	2.15	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:181:LEU:HD13	1:F:233:LEU:HD23	1.65	0.79
1:C:17:SER:O	1:C:21:ARG:HG3	1.83	0.79
1:E:87:TYR:O	2:L:57:ARG:NH2	2.16	0.78
1:D:217:ARG:NH1	1:D:223:ARG:HB3	1.99	0.78
1:R:58:ASP:CG	1:R:91:ARG:NH1	2.38	0.77
1:F:205:VAL:HG11	1:F:230:LEU:HG	1.65	0.77
1:D:178:THR:HG23	1:D:233:LEU:O	1.84	0.77
1:Q:137:GLU:OE1	1:Q:139:TYR:OH	2.02	0.76
2:X:38:ASP:HB3	2:X:41:THR:HB	1.66	0.76
1:U:159:THR:HG22	1:U:162:PRO:HD2	1.68	0.76
1:R:92:ARG:HB3	2:Z:75:THR:HG21	1.66	0.76
1:G:48:ARG:N	1:G:48:ARG:HD2	2.01	0.75
1:O:182:ARG:HH22	1:O:234:LEU:CA	2.01	0.74
2:X:132:GLU:OE1	2:X:134:GLU:N	2.19	0.74
1:D:18:GLU:O	1:D:22:LYS:HG3	1.89	0.73
1:B:31:VAL:HG12	1:B:155:VAL:HG22	1.70	0.73
1:Q:205:VAL:HG23	1:Q:230:LEU:HD23	1.70	0.73
1:F:33:LEU:CD1	1:F:153:PHE:HB3	2.17	0.72
1:C:189:ARG:NH2	1:C:190:ALA:O	2.23	0.72
1:F:33:LEU:HD11	1:F:153:PHE:HB3	1.71	0.72
1:R:92:ARG:NH2	1:R:92:ARG:HG3	2.04	0.71
1:P:87:TYR:O	2:W:57:ARG:NH2	2.24	0.70
2:L:156:GLN:OE1	2:L:165:ARG:NH2	2.23	0.70
1:P:97:ARG:NH1	1:Q:49:SER:O	2.24	0.70
2:J:48:THR:HG22	3:J:301:7HJ:C22	2.21	0.70
1:O:140:ARG:NH1	1:O:155:VAL:O	2.24	0.70
1:G:87:TYR:O	2:N:57:ARG:NH2	2.25	0.70
1:F:233:LEU:N	1:F:233:LEU:HD13	2.04	0.69
2:N:209:ARG:NH1	2:N:212:GLU:OE1	2.26	0.69
2:M:208:SER:O	2:M:212:GLU:HG3	1.92	0.69
1:B:163:ILE:O	1:B:167:LEU:HD12	1.93	0.69
1:C:189:ARG:NH2	1:C:190:ALA:C	2.47	0.68
1:C:30:VAL:HG13	1:C:43:ALA:HB2	1.75	0.68
1:R:58:ASP:OD2	1:R:91:ARG:NH1	2.27	0.68
1:B:16:ARG:NH1	1:B:111:PHE:O	2.28	0.67
1:B:219:ARG:NH1	2:I:64:GLU:OE1	2.26	0.67
1:G:16:ARG:NH2	1:G:114:GLN:O	2.25	0.67
1:F:189:ARG:CG	1:F:203:LEU:HD21	2.21	0.67
1:F:135:ARG:NH1	1:F:173:GLU:OE1	2.27	0.67
1:F:182:ARG:HA	1:F:185:VAL:HG12	1.77	0.67
1:U:149:ASP:N	1:U:149:ASP:OD1	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:ARG:HD2	1:C:48:ARG:N	2.11	0.66
1:F:189:ARG:HE	1:F:203:LEU:CD1	2.05	0.66
1:P:178:THR:HG22	1:P:233:LEU:HD21	1.77	0.66
1:B:161:GLU:N	1:B:161:GLU:OE1	2.22	0.66
1:U:178:THR:O	1:U:182:ARG:HG2	1.96	0.65
1:D:134:LYS:NZ	1:D:137:GLU:OE2	2.29	0.65
1:O:85:ARG:HH21	1:O:98:GLN:CD	2.00	0.65
2:Z:165:ARG:HB2	2:Z:213:LEU:HD22	1.79	0.65
1:F:42:VAL:HG23	1:F:210:VAL:HG22	1.78	0.65
1:O:18:GLU:O	1:O:22:LYS:HG3	1.96	0.65
2:X:64:GLU:HG2	2:X:68:LYS:HE2	1.79	0.64
1:B:230:LEU:O	1:B:234:LEU:HD12	1.97	0.64
1:Q:89:TYR:CE1	2:Y:82:ARG:HD3	2.32	0.64
2:X:208:SER:O	2:X:212:GLU:HG3	1.98	0.64
1:C:10:GLU:HG2	1:D:15:GLU:OE2	1.97	0.64
1:Q:236:ASP:OD1	1:Q:237:GLN:N	2.31	0.64
1:B:16:ARG:NH2	1:B:114:GLN:O	2.31	0.64
1:O:90:ASP:HB3	1:O:93:ASP:OD1	1.97	0.64
1:P:179:ASP:O	1:P:183:ILE:HD12	1.98	0.64
1:F:189:ARG:NE	1:F:203:LEU:HD11	2.06	0.63
1:B:230:LEU:HG	1:B:234:LEU:HD11	1.80	0.63
1:Q:10:GLU:HG3	1:R:15:GLU:HB3	1.80	0.63
1:O:151:PRO:HB3	1:P:48:ARG:NH2	2.14	0.63
1:C:53:ILE:HD12	1:C:209:GLU:HG2	1.81	0.63
1:P:53:ILE:HD12	1:P:209:GLU:HG2	1.81	0.63
2:K:62:GLU:OE1	2:K:82:ARG:NE	2.31	0.62
1:F:40:LEU:HD21	1:F:181:LEU:HA	1.81	0.62
1:U:11:GLN:O	1:U:15:GLU:HG2	2.00	0.62
1:B:142:THR:HG22	1:B:146:SER:HB2	1.80	0.62
1:A:9:MET:HE1	1:B:16:ARG:HA	1.81	0.62
1:O:49:SER:O	1:U:97:ARG:NH1	2.32	0.62
1:T:16:ARG:NH1	1:T:111:PHE:O	2.33	0.61
1:G:48:ARG:HD2	1:G:48:ARG:H	1.64	0.61
2:W:215:ARG:O	2:W:219:GLU:HG3	2.00	0.61
1:C:176:SER:OG	1:C:179:ASP:OD2	2.18	0.61
1:O:179:ASP:O	1:O:183:ILE:HD12	2.00	0.61
1:D:18:GLU:HB3	1:D:22:LYS:HE2	1.83	0.61
2:Z:132:GLU:HG3	2:Z:137:GLN:HB2	1.83	0.61
2:L:132:GLU:HG3	2:L:137:GLN:HB2	1.83	0.61
1:Q:89:TYR:CD1	2:Y:82:ARG:HD3	2.35	0.61
2:Z:88:ARG:HD3	2:Z:126:ALA:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:98:GLN:O	1:G:102:VAL:HG23	2.00	0.60
1:D:164:ALA:O	1:D:168:LYS:HG3	2.01	0.60
1:C:68:PHE:HA	1:C:71:PHE:CE2	2.36	0.60
1:T:53:ILE:HD12	1:T:209:GLU:HG2	1.83	0.60
1:A:53:ILE:HD12	1:A:209:GLU:HG2	1.82	0.60
1:D:28:LYS:HD3	1:D:44:GLU:HG2	1.82	0.60
1:B:155:VAL:HG11	1:B:163:ILE:CG2	2.31	0.60
2:L:48:THR:HG22	3:L:301:7HJ:C25	2.32	0.60
1:O:116:LYS:NZ	1:O:119:GLU:OE1	2.30	0.59
1:O:18:GLU:OE1	1:O:21:ARG:NH1	2.35	0.59
1:A:152:HIS:HD2	1:A:171:TYR:CE2	2.21	0.59
2:L:94:ALA:HB1	2:L:99:LEU:HD23	1.84	0.59
2:W:88:ARG:HD3	2:W:126:ALA:O	2.01	0.59
1:A:152:HIS:HD2	1:A:171:TYR:HE2	1.49	0.59
1:D:18:GLU:OE1	1:D:21:ARG:NH2	2.35	0.59
2:V:48:THR:HG22	3:V:301:7HJ:C22	2.32	0.59
1:F:31:VAL:HG12	1:F:155:VAL:HG22	1.84	0.58
1:R:98:GLN:O	1:R:102:VAL:HG23	2.03	0.58
1:D:53:ILE:O	1:D:224:ARG:NH2	2.36	0.58
1:P:55:GLU:OE1	1:P:220:ARG:NH1	2.36	0.58
1:T:28:LYS:HE3	1:T:46:PRO:HG3	1.84	0.58
1:U:53:ILE:HD12	1:U:209:GLU:HG2	1.85	0.58
1:B:151:PRO:CG	1:C:48:ARG:HH22	2.16	0.58
1:O:189:ARG:HH12	1:O:202:THR:N	2.01	0.58
1:B:164:ALA:O	1:B:168:LYS:HG3	2.04	0.58
1:B:204:GLY:O	1:B:208:LEU:HD12	2.04	0.58
1:D:217:ARG:HD2	1:D:223:ARG:HH11	1.69	0.58
2:Y:20:SER:HB2	2:Y:31:VAL:HG21	1.85	0.58
1:B:89:TYR:CD1	2:J:82:ARG:HD3	2.39	0.57
2:M:48:THR:HG22	3:M:301:7HJ:C22	2.34	0.57
1:S:53:ILE:HD12	1:S:209:GLU:HG2	1.85	0.57
1:G:33:LEU:HD11	1:G:180:ALA:HB1	1.86	0.57
1:R:22:LYS:O	1:R:26:ARG:HG3	2.04	0.57
2:H:37:THR:OG1	2:H:41:THR:HG22	2.05	0.57
1:R:53:ILE:HD12	1:R:209:GLU:HG2	1.85	0.57
2:K:132:GLU:HG3	2:K:137:GLN:HB2	1.84	0.57
2:X:88:ARG:HD3	2:X:126:ALA:O	2.05	0.57
2:H:7:LYS:NZ	2:H:118:GLY:O	2.24	0.57
1:F:72:ASP:O	1:F:76:ARG:HG3	2.05	0.57
1:O:89:TYR:CE1	2:W:82:ARG:HD3	2.40	0.57
1:P:235:VAL:HG23	1:P:236:ASP:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:11:GLN:HE21	1:D:14:ARG:HH22	1.53	0.56
1:B:93:ASP:OD2	2:J:75:THR:HG22	2.05	0.56
2:N:161:ASP:OD2	2:N:209:ARG:NH2	2.37	0.56
1:O:140:ARG:NH1	1:O:155:VAL:H	2.03	0.56
1:U:182:ARG:NH2	1:U:234:LEU:O	2.38	0.56
1:B:97:ARG:NH2	1:C:51:GLN:HE22	2.01	0.56
2:L:88:ARG:HD3	2:L:126:ALA:O	2.05	0.56
1:C:89:TYR:CE1	2:K:82:ARG:HD2	2.40	0.56
2:N:161:ASP:CG	2:N:209:ARG:HH21	2.09	0.56
2:K:2:THR:HG21	2:K:174:ALA:HB1	1.87	0.56
1:S:98:GLN:O	1:S:102:VAL:HG23	2.06	0.56
1:B:151:PRO:HB3	1:C:48:ARG:HH22	1.70	0.56
1:P:230:LEU:O	1:P:234:LEU:HD13	2.06	0.56
1:B:25:ALA:O	1:B:158:GLY:HA2	2.06	0.56
1:C:22:LYS:O	1:C:26:ARG:HG3	2.06	0.56
1:F:89:TYR:CD1	2:N:82:ARG:HD3	2.41	0.56
1:Q:207:SER:OG	1:Q:207:SER:O	2.24	0.56
1:P:178:THR:HG22	1:P:233:LEU:CD2	2.36	0.56
1:B:232:ALA:O	1:B:235:VAL:HB	2.05	0.55
1:R:121:GLU:OE2	1:R:140:ARG:NH1	2.39	0.55
1:T:182:ARG:NH2	1:T:234:LEU:C	2.60	0.55
1:D:225:ILE:HD13	1:D:233:LEU:HD11	1.89	0.55
1:T:182:ARG:CZ	1:T:233:LEU:O	2.54	0.55
1:F:181:LEU:CD1	1:F:233:LEU:HD23	2.33	0.55
2:M:30:ASP:N	2:M:30:ASP:OD1	2.39	0.55
1:S:229:ALA:O	1:S:233:LEU:HD12	2.06	0.55
1:R:89:TYR:CD1	2:Z:82:ARG:HD3	2.42	0.55
1:B:92:ARG:HG3	1:B:92:ARG:O	2.07	0.55
1:B:53:ILE:HD12	1:B:209:GLU:HG2	1.87	0.55
2:K:2:THR:HG23	2:K:181:THR:OG1	2.05	0.55
1:U:56:LEU:HD13	1:U:99:LEU:HD13	1.87	0.55
1:C:214:ASP:OD2	1:C:223:ARG:NH2	2.39	0.55
2:L:62:GLU:OE2	2:L:82:ARG:HD3	2.07	0.55
2:N:64:GLU:HG2	2:N:68:LYS:HE2	1.89	0.55
1:O:182:ARG:HH12	1:O:234:LEU:C	2.10	0.55
2:K:88:ARG:HD3	2:K:126:ALA:O	2.06	0.54
1:G:56:LEU:HG	1:G:62:PHE:HB2	1.89	0.54
1:G:75:ARG:NH2	2:N:69:LEU:O	2.40	0.54
2:I:156:GLN:NE2	2:I:165:ARG:HH22	2.06	0.54
1:R:89:TYR:CE1	2:Z:82:ARG:HD3	2.42	0.54
1:B:149:ASP:OD2	1:C:48:ARG:HD3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:GLU:HB3	1:D:118:TYR:CD2	2.43	0.54
1:U:110:ILE:HA	1:U:114:GLN:HG3	1.91	0.53
2:Z:18:ARG:NH2	2:Z:30:ASP:O	2.32	0.53
1:F:35:TYR:CZ	1:F:177:LEU:HD13	2.43	0.53
2:N:12:VAL:HG12	2:N:197:ILE:HB	1.90	0.53
1:P:121:GLU:OE2	1:P:140:ARG:NH1	2.41	0.53
1:B:108:GLY:O	1:B:112:THR:HG23	2.08	0.53
1:Q:219:ARG:NH2	2:X:64:GLU:OE2	2.41	0.53
1:R:189:ARG:HH12	1:R:203:LEU:N	2.07	0.53
1:S:92:ARG:NH2	1:S:129:HIS:CE1	2.77	0.53
1:O:140:ARG:HH12	1:O:155:VAL:H	1.56	0.53
1:O:89:TYR:CD1	2:W:82:ARG:HD3	2.43	0.53
2:W:116:SER:O	2:W:119:ARG:NH1	2.38	0.53
2:Y:88:ARG:HD3	2:Y:126:ALA:O	2.09	0.53
2:Y:137:GLN:HG3	2:Y:138:ALA:N	2.24	0.53
2:M:78:GLY:O	2:M:82:ARG:HG2	2.09	0.53
1:P:85:ARG:NH1	1:P:98:GLN:OE1	2.42	0.53
1:B:10:GLU:HG3	1:B:10:GLU:O	2.08	0.53
1:Q:182:ARG:NH2	1:Q:236:ASP:O	2.41	0.53
1:C:56:LEU:HG	1:C:62:PHE:HB2	1.91	0.52
1:E:149:ASP:OD2	1:F:48:ARG:HG2	2.09	0.52
1:G:89:TYR:CE1	2:H:82:ARG:HD3	2.45	0.52
1:T:67:LYS:HE3	1:T:69:ASN:OD1	2.09	0.52
2:K:2:THR:HG22	2:K:142:GLY:H	1.74	0.52
1:T:45:ASN:ND2	1:T:209:GLU:OE2	2.39	0.52
1:O:98:GLN:O	1:O:102:VAL:HG23	2.09	0.52
2:W:48:THR:HG22	3:W:301:7HJ:C22	2.39	0.52
1:A:9:MET:CE	1:B:16:ARG:HA	2.40	0.52
1:G:93:ASP:OD1	2:H:75:THR:HG23	2.09	0.52
1:G:30:VAL:HG13	1:G:43:ALA:HB2	1.92	0.52
1:R:121:GLU:CD	1:R:140:ARG:HH11	2.13	0.52
1:C:189:ARG:HH21	1:C:190:ALA:C	2.13	0.51
1:F:121:GLU:HG2	1:F:156:MET:HG2	1.92	0.51
2:M:51:VAL:HG21	2:M:98:LEU:HB3	1.91	0.51
1:A:151:PRO:HG2	1:A:152:HIS:ND1	2.25	0.51
1:B:151:PRO:CB	1:C:48:ARG:HH22	2.24	0.51
2:W:194:ALA:HB3	2:W:205:VAL:HB	1.93	0.51
1:A:42:VAL:HG22	1:A:210:VAL:HG22	1.92	0.51
2:M:132:GLU:OE1	2:M:137:GLN:NE2	2.43	0.51
1:D:11:GLN:HE21	1:D:14:ARG:NH2	2.07	0.51
1:G:181:LEU:HD22	1:G:233:LEU:HD23	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:38:ASP:OD1	2:N:41:THR:HG23	2.11	0.51
1:D:41:PHE:HB3	1:D:53:ILE:HD13	1.92	0.51
1:G:112:THR:HG22	1:G:113:GLU:HG2	1.93	0.51
1:U:134:LYS:HB2	4:U:313:HOH:O	2.10	0.51
1:B:155:VAL:HG21	1:B:163:ILE:HG23	1.92	0.51
1:R:56:LEU:HG	1:R:62:PHE:HB2	1.93	0.51
1:S:121:GLU:OE1	4:S:301:HOH:O	2.19	0.51
1:A:150:GLU:OE2	1:A:151:PRO:HD2	2.10	0.50
1:A:10:GLU:O	1:A:14:ARG:HG3	2.11	0.50
1:E:11:GLN:NE2	1:E:15:GLU:OE2	2.44	0.50
2:N:88:ARG:HD3	2:N:126:ALA:O	2.12	0.50
1:O:219:ARG:NH2	2:V:64:GLU:OE2	2.45	0.50
1:T:182:ARG:HD3	1:T:182:ARG:N	2.26	0.50
2:Y:8:TYR:CE1	2:Y:196:ILE:HD11	2.47	0.50
1:B:167:LEU:O	1:B:171:TYR:HB2	2.11	0.50
1:F:165:ASN:OD1	1:F:166:ALA:N	2.44	0.50
1:R:92:ARG:NH2	1:R:92:ARG:CG	2.73	0.50
1:S:92:ARG:NH2	1:S:129:HIS:ND1	2.59	0.50
1:T:182:ARG:HH22	1:T:233:LEU:C	2.02	0.50
1:D:239:SER:OG	1:D:240:PRO:HD3	2.11	0.50
1:D:98:GLN:O	1:D:102:VAL:HG23	2.12	0.50
1:F:152:HIS:HB3	1:F:171:TYR:CE2	2.47	0.50
1:G:53:ILE:HD12	1:G:209:GLU:HG2	1.92	0.50
2:N:31:VAL:HG11	3:N:301:7HJ:C15	2.41	0.50
1:D:161:GLU:HB3	1:D:162:PRO:HD3	1.94	0.50
2:K:18:ARG:O	2:K:31:VAL:HG22	2.12	0.50
2:M:18:ARG:NH1	2:M:30:ASP:O	2.44	0.50
1:P:32:ALA:HA	1:P:40:LEU:O	2.11	0.50
2:K:177:ASP:OD1	2:V:29:ARG:NH2	2.44	0.50
1:B:163:ILE:HD11	1:B:188:LEU:HD23	1.92	0.50
1:F:33:LEU:HD13	1:F:153:PHE:HB3	1.92	0.50
1:F:152:HIS:HD1	1:F:171:TYR:HE2	1.58	0.50
1:E:89:TYR:CD1	2:M:82:ARG:HD3	2.46	0.50
1:A:137:GLU:HG2	1:B:48:ARG:NH2	2.26	0.50
1:U:72:ASP:OD1	1:U:75:ARG:NH1	2.44	0.50
1:P:9:MET:HE1	1:Q:116:LYS:HG3	1.94	0.50
1:A:68:PHE:HA	1:A:71:PHE:CE2	2.47	0.49
1:B:155:VAL:HG11	1:B:163:ILE:HG21	1.92	0.49
1:B:30:VAL:HG13	1:B:43:ALA:HB2	1.93	0.49
2:Z:20:SER:HB2	2:Z:31:VAL:HG21	1.93	0.49
1:A:179:ASP:OD1	1:A:182:ARG:NH2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:GLU:O	1:D:22:LYS:CG	2.58	0.49
1:G:33:LEU:HD21	1:G:184:ALA:HB2	1.93	0.49
2:J:156:GLN:OE1	2:J:165:ARG:NH1	2.34	0.49
1:O:31:VAL:HG12	1:O:155:VAL:HG22	1.95	0.49
2:I:122:SER:O	2:I:129:TRP:HA	2.13	0.49
2:X:41:THR:HG23	2:X:104:LEU:HD11	1.95	0.49
1:B:92:ARG:HD2	1:B:129:HIS:CE1	2.48	0.49
1:F:30:VAL:HG13	1:F:43:ALA:HB2	1.95	0.49
1:F:31:VAL:CG2	1:F:42:VAL:HG13	2.43	0.49
1:G:89:TYR:CD1	2:H:82:ARG:HD3	2.48	0.49
1:Q:21:ARG:HD2	1:Q:143:TYR:HE2	1.77	0.49
1:S:140:ARG:NH1	1:S:155:VAL:O	2.44	0.49
1:B:10:GLU:OE1	1:C:22:LYS:NZ	2.46	0.49
1:D:11:GLN:HG2	1:D:14:ARG:HH22	1.78	0.49
2:J:51:VAL:HG21	2:J:98:LEU:HB3	1.95	0.49
1:E:81:PHE:CZ	1:E:102:VAL:HG21	2.48	0.49
1:A:10:GLU:HG3	1:B:19:LEU:HD12	1.95	0.48
1:B:142:THR:CG2	1:B:146:SER:HB2	2.43	0.48
1:R:30:VAL:HG13	1:R:43:ALA:HB2	1.94	0.48
2:H:132:GLU:CD	2:H:137:GLN:HE21	2.16	0.48
2:J:113:ASP:N	4:J:402:HOH:O	2.34	0.48
2:L:82:ARG:NH2	2:L:85:ILE:HD13	2.28	0.48
1:P:93:ASP:OD1	2:X:75:THR:HG23	2.13	0.48
2:X:32:ARG:CD	2:X:193:THR:HG21	2.43	0.48
1:C:48:ARG:HD2	1:C:48:ARG:H	1.76	0.48
1:F:9:MET:HE3	1:F:13:MET:HG2	1.95	0.48
1:F:42:VAL:HG23	1:F:210:VAL:CG2	2.44	0.48
2:Y:161:ASP:CG	2:Y:209:ARG:HH21	2.16	0.48
1:A:68:PHE:HA	1:A:71:PHE:CZ	2.48	0.48
1:D:81:PHE:CZ	1:D:102:VAL:HG21	2.49	0.48
1:O:33:LEU:HD11	1:O:180:ALA:HB1	1.95	0.48
1:O:85:ARG:NH2	1:O:98:GLN:CD	2.66	0.48
1:Q:152:HIS:HB3	1:Q:171:TYR:CE2	2.48	0.48
1:T:56:LEU:HG	1:T:62:PHE:HB2	1.96	0.48
2:V:32:ARG:NE	2:V:34:VAL:O	2.45	0.48
1:B:151:PRO:HG3	1:C:48:ARG:HH22	1.78	0.48
1:F:33:LEU:HD12	1:F:33:LEU:HA	1.47	0.48
1:A:33:LEU:HD11	1:A:180:ALA:HB1	1.96	0.48
2:W:20:SER:HB2	2:W:31:VAL:HG21	1.95	0.48
1:B:178:THR:CG2	1:B:233:LEU:HD12	2.44	0.47
1:F:227:GLY:O	1:F:231:GLN:N	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:53:ILE:HD12	1:Q:209:GLU:HG2	1.96	0.47
1:B:24:ILE:HG22	1:B:157:GLY:HA2	1.96	0.47
1:P:231:GLN:O	1:P:234:LEU:N	2.48	0.47
1:U:182:ARG:NH2	1:U:235:VAL:HA	2.29	0.47
1:C:48:ARG:CD	1:C:48:ARG:N	2.76	0.47
2:W:115:GLN:NE2	4:W:402:HOH:O	2.46	0.47
1:G:81:PHE:CZ	1:G:102:VAL:HG21	2.49	0.47
1:Q:90:ASP:HB3	1:Q:93:ASP:OD2	2.13	0.47
2:Z:208:SER:O	2:Z:212:GLU:HG3	2.14	0.47
2:M:156:GLN:OE1	2:M:165:ARG:NH2	2.43	0.47
1:Q:177:LEU:HG	1:Q:233:LEU:HD21	1.96	0.47
1:T:179:ASP:O	1:T:183:ILE:HD12	2.14	0.47
2:X:32:ARG:HD3	2:X:193:THR:HG21	1.95	0.47
2:Y:38:ASP:HB3	2:Y:41:THR:OG1	2.14	0.47
1:G:219:ARG:NH2	2:N:64:GLU:OE1	2.48	0.47
1:O:162:PRO:HB2	1:O:190:ALA:O	2.14	0.47
1:Q:121:GLU:OE2	1:Q:140:ARG:NH1	2.48	0.47
1:A:123:CYS:HA	1:A:139:TYR:O	2.14	0.47
2:N:22:GLN:NE2	3:N:301:7HJ:O35	2.42	0.47
1:R:163:ILE:HG23	1:R:187:ALA:HB1	1.97	0.47
1:A:89:TYR:CD2	2:I:74:LEU:HD21	2.49	0.47
1:G:72:ASP:O	1:G:76:ARG:HG3	2.15	0.47
2:I:3:ILE:HB	2:I:139:VAL:HG12	1.96	0.47
2:K:48:THR:HG21	2:K:98:LEU:HA	1.96	0.47
1:T:18:GLU:OE2	1:T:21:ARG:NH1	2.26	0.47
1:R:11:GLN:O	1:R:15:GLU:HG3	2.14	0.47
1:A:186:ALA:O	1:A:189:ARG:HG2	2.14	0.47
2:H:132:GLU:HG3	2:H:137:GLN:HB2	1.97	0.47
2:H:3:ILE:O	2:H:138:ALA:HA	2.14	0.47
1:B:167:LEU:O	1:B:171:TYR:N	2.47	0.47
1:O:18:GLU:CD	1:O:21:ARG:HE	2.17	0.47
1:D:68:PHE:HA	1:D:71:PHE:CZ	2.50	0.46
1:Q:227:GLY:O	1:Q:231:GLN:HG2	2.15	0.46
1:R:163:ILE:HG12	1:R:187:ALA:O	2.15	0.46
2:N:51:VAL:HG21	2:N:98:LEU:HB3	1.97	0.46
1:B:105:GLN:O	1:B:109:THR:HG23	2.15	0.46
1:F:89:TYR:CE1	2:N:82:ARG:HD3	2.50	0.46
2:I:137:GLN:HG3	2:I:138:ALA:N	2.30	0.46
1:P:36:ALA:HA	1:P:174:ASN:HD22	1.80	0.46
1:B:74:LEU:HD13	1:B:122:LEU:HD11	1.97	0.46
1:F:189:ARG:HG2	1:F:203:LEU:CD2	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:22:GLN:HG2	3:J:301:7HJ:O46	2.16	0.46
1:B:173:GLU:HG3	1:B:174:ASN:N	2.30	0.46
1:G:121:GLU:OE1	1:G:140:ARG:HD3	2.15	0.46
1:O:212:VAL:HG23	1:O:223:ARG:HG2	1.98	0.46
1:P:150:GLU:HG3	1:P:154:VAL:HG22	1.98	0.46
1:Q:167:LEU:HG	1:Q:187:ALA:CB	2.46	0.46
1:U:159:THR:HG22	1:U:162:PRO:CD	2.44	0.46
1:E:56:LEU:HG	1:E:62:PHE:HB2	1.98	0.46
1:P:152:HIS:HB3	1:P:171:TYR:CE2	2.50	0.46
1:A:56:LEU:HG	1:A:62:PHE:HB2	1.97	0.46
1:F:110:ILE:HA	1:F:114:GLN:HG3	1.98	0.46
2:J:78:GLY:O	2:J:82:ARG:HG2	2.15	0.46
1:S:33:LEU:HD11	1:S:180:ALA:HB1	1.98	0.46
1:A:152:HIS:CD2	1:A:171:TYR:CE2	3.04	0.46
1:C:109:THR:HG22	1:C:113:GLU:HG3	1.97	0.46
2:K:112:SER:O	2:K:114:PRO:HD3	2.16	0.46
1:O:56:LEU:HG	1:O:62:PHE:HB2	1.98	0.46
1:S:236:ASP:OD1	1:S:236:ASP:N	2.49	0.46
1:F:70:GLU:HB3	1:F:118:TYR:CD2	2.51	0.45
2:L:51:VAL:HG21	2:L:98:LEU:HB3	1.98	0.45
2:Z:31:VAL:HG11	3:Z:301:7HJ:C15	2.45	0.45
1:D:56:LEU:HG	1:D:62:PHE:HB2	1.98	0.45
2:H:209:ARG:NH2	2:H:212:GLU:OE1	2.50	0.45
1:P:56:LEU:HG	1:P:62:PHE:HB2	1.97	0.45
1:S:178:THR:O	1:S:182:ARG:HG3	2.16	0.45
1:P:89:TYR:CD1	2:X:82:ARG:HD3	2.52	0.45
2:J:88:ARG:HD3	2:J:126:ALA:O	2.15	0.45
1:B:97:ARG:HH21	1:C:51:GLN:NE2	2.05	0.45
1:F:42:VAL:CG2	1:F:210:VAL:HG22	2.46	0.45
1:O:167:LEU:O	1:O:171:TYR:N	2.46	0.45
2:V:188:ARG:NH2	2:W:134:GLU:OE2	2.46	0.45
2:W:20:SER:HB3	2:W:28:GLY:HA3	1.99	0.45
1:F:142:THR:HG22	1:F:146:SER:HB2	1.99	0.45
1:G:48:ARG:N	1:G:48:ARG:CD	2.72	0.45
1:P:110:ILE:HA	1:P:114:GLN:HG3	1.98	0.45
2:V:48:THR:HG21	2:V:97:GLY:O	2.17	0.45
1:C:21:ARG:HG3	1:C:21:ARG:H	1.57	0.45
2:N:207:GLU:H	2:N:207:GLU:CD	2.18	0.45
1:O:149:ASP:OD2	1:P:48:ARG:NH1	2.49	0.45
1:S:9:MET:CE	1:T:19:LEU:HD13	2.46	0.45
1:D:236:ASP:OD1	1:D:237:GLN:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:70:GLU:HB3	1:G:118:TYR:CD2	2.51	0.45
1:O:182:ARG:NH1	1:O:234:LEU:O	2.41	0.45
1:R:161:GLU:HB2	1:R:162:PRO:HD3	1.99	0.45
1:S:152:HIS:HB3	1:S:171:TYR:CE2	2.51	0.45
1:S:92:ARG:HH12	1:S:132:GLU:CD	2.10	0.45
1:U:28:LYS:H	1:U:28:LYS:HG2	1.61	0.45
2:W:156:GLN:OE1	2:W:165:ARG:NH1	2.44	0.45
1:E:140:ARG:NH1	1:E:155:VAL:O	2.50	0.45
1:S:58:ASP:OD1	1:S:91:ARG:NH2	2.36	0.45
2:V:107:TYR:CE1	2:V:117:ALA:HB3	2.52	0.45
2:Z:137:GLN:HG3	2:Z:138:ALA:N	2.32	0.45
2:W:8:TYR:CE2	2:W:196:ILE:HD11	2.52	0.44
2:X:37:THR:OG1	2:X:41:THR:HG22	2.17	0.44
1:C:179:ASP:O	1:C:183:ILE:HG22	2.18	0.44
1:R:137:GLU:OE2	1:S:48:ARG:NH2	2.50	0.44
1:T:182:ARG:NH1	1:T:233:LEU:O	2.50	0.44
1:C:155:VAL:HG11	1:C:163:ILE:HB	1.98	0.44
2:V:72:VAL:CG2	2:V:73:PRO:HD2	2.48	0.44
2:N:22:GLN:HG2	3:N:301:7HJ:O46	2.18	0.44
1:P:9:MET:CE	1:Q:19:LEU:HD13	2.48	0.44
1:U:48:ARG:HG2	1:U:48:ARG:O	2.16	0.44
2:W:33:LYS:O	2:W:44:GLY:HA2	2.17	0.44
1:D:68:PHE:HA	1:D:71:PHE:CE2	2.51	0.44
1:T:231:GLN:O	1:T:234:LEU:N	2.49	0.44
2:Y:30:ASP:N	2:Y:30:ASP:OD1	2.47	0.44
1:B:56:LEU:HG	1:B:62:PHE:HB2	2.00	0.44
1:D:116:LYS:NZ	1:D:119:GLU:OE1	2.31	0.44
1:P:30:VAL:HG13	1:P:43:ALA:HB2	1.99	0.44
1:B:42:VAL:HG13	1:B:210:VAL:HG22	2.00	0.44
1:C:9:MET:HB3	1:D:15:GLU:OE1	2.17	0.44
1:D:162:PRO:HB2	1:D:191:GLY:HA2	2.00	0.44
1:D:89:TYR:CE1	2:L:82:ARG:HD2	2.53	0.44
1:F:152:HIS:CE1	1:F:173:GLU:HB2	2.53	0.44
1:F:68:PHE:HA	1:F:71:PHE:CE2	2.52	0.44
1:O:151:PRO:HB3	1:P:48:ARG:HH21	1.80	0.44
1:T:182:ARG:NH2	1:T:234:LEU:CA	2.80	0.44
1:A:203:LEU:HD23	1:A:203:LEU:HA	1.74	0.44
1:G:168:LYS:HA	1:G:168:LYS:HD2	1.83	0.44
1:D:33:LEU:HD11	1:D:180:ALA:HB1	2.00	0.43
2:L:38:ASP:OD1	2:L:41:THR:N	2.51	0.43
1:B:163:ILE:CG2	1:B:164:ALA:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:VAL:HG22	1:C:210:VAL:HG22	2.00	0.43
1:E:18:GLU:OE1	1:E:21:ARG:NH2	2.43	0.43
1:A:15:GLU:HB3	1:G:9:MET:HB3	1.99	0.43
2:H:18:ARG:HD3	2:H:193:THR:HG23	1.99	0.43
1:P:33:LEU:HD11	1:P:180:ALA:HB1	1.99	0.43
1:P:214:ASP:HB3	1:P:217:ARG:HG3	1.99	0.43
1:U:181:LEU:O	1:U:185:VAL:HG23	2.18	0.43
1:E:112:THR:HG21	1:F:116:LYS:HE3	1.99	0.43
1:O:53:ILE:HD12	1:O:209:GLU:HG2	2.01	0.43
1:B:89:TYR:CE1	2:J:82:ARG:HD3	2.54	0.43
1:C:116:LYS:NZ	1:C:119:GLU:OE2	2.41	0.43
1:Q:16:ARG:NH2	1:Q:114:GLN:O	2.32	0.43
2:Y:32:ARG:HD3	2:Y:35:TYR:CE1	2.53	0.43
1:F:33:LEU:HD13	1:F:153:PHE:CB	2.48	0.43
1:F:51:GLN:OE1	1:F:54:SER:HB2	2.18	0.43
1:F:99:LEU:O	1:F:102:VAL:HG12	2.18	0.43
1:P:89:TYR:CE1	2:X:82:ARG:HD3	2.53	0.43
1:Q:14:ARG:HA	1:Q:14:ARG:HD3	1.71	0.43
1:U:188:LEU:HA	1:U:188:LEU:HD23	1.89	0.43
2:Z:112:SER:O	2:Z:114:PRO:HD3	2.18	0.43
2:J:137:GLN:HG3	2:J:138:ALA:N	2.34	0.43
2:L:64:GLU:HG2	2:L:68:LYS:HE2	2.00	0.43
1:U:161:GLU:O	1:U:165:ASN:OD1	2.36	0.43
2:V:72:VAL:HG22	2:V:73:PRO:HD2	2.00	0.43
1:B:58:ASP:OD1	1:B:91:ARG:NH1	2.52	0.43
1:C:9:MET:HG3	1:C:10:GLU:N	2.32	0.43
1:E:89:TYR:CE1	2:M:82:ARG:HD3	2.54	0.43
1:P:18:GLU:O	1:P:22:LYS:HG3	2.18	0.43
1:U:55:GLU:CD	1:U:220:ARG:HH21	2.21	0.43
1:U:55:GLU:HB2	1:U:222:PHE:CG	2.53	0.43
1:U:67:LYS:HE2	1:U:69:ASN:OD1	2.19	0.43
2:V:78:GLY:O	2:V:82:ARG:HG2	2.19	0.43
1:A:110:ILE:HA	1:A:114:GLN:HG3	2.01	0.43
1:A:163:ILE:HG23	1:A:187:ALA:O	2.19	0.43
1:A:22:LYS:O	1:A:26:ARG:HG3	2.19	0.43
2:L:150:MET:O	2:L:154:TYR:HB2	2.19	0.43
1:Q:217:ARG:NH1	1:Q:223:ARG:HH11	2.16	0.43
2:I:215:ARG:O	2:I:219:GLU:HG3	2.18	0.43
1:O:112:THR:HG22	1:O:113:GLU:CG	2.49	0.43
1:Q:93:ASP:OD1	2:Y:75:THR:HG23	2.19	0.43
1:F:54:SER:CB	1:F:75:ARG:HD2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:205:VAL:HG11	1:P:231:GLN:HG2	2.01	0.43
1:G:151:PRO:HG2	1:G:152:HIS:ND1	2.33	0.42
2:H:48:THR:HG22	3:H:301:7HJ:C25	2.49	0.42
1:S:72:ASP:OD1	1:S:75:ARG:NH1	2.52	0.42
2:Y:18:ARG:HD3	2:Y:193:THR:HG23	2.01	0.42
1:A:9:MET:O	1:A:12:ALA:N	2.52	0.42
1:C:168:LYS:HA	1:C:168:LYS:HD3	1.61	0.42
2:H:51:VAL:HG21	2:H:98:LEU:HB3	2.01	0.42
2:Y:165:ARG:O	2:Y:165:ARG:HG3	2.19	0.42
1:C:150:GLU:HA	1:C:151:PRO:HD3	1.82	0.42
1:C:72:ASP:O	1:C:76:ARG:HG3	2.19	0.42
1:E:72:ASP:O	1:E:76:ARG:HG3	2.19	0.42
2:I:64:GLU:HG2	2:I:68:LYS:HE2	2.01	0.42
1:P:62:PHE:CZ	1:P:75:ARG:HB2	2.54	0.42
1:Q:70:GLU:HB3	1:Q:118:TYR:CD2	2.54	0.42
1:T:54:SER:CB	1:T:75:ARG:HD2	2.48	0.42
1:F:129:HIS:O	1:F:132:GLU:HB2	2.19	0.42
1:F:31:VAL:HG12	1:F:155:VAL:HG13	2.01	0.42
1:F:152:HIS:ND1	1:F:171:TYR:HE2	2.18	0.42
1:T:9:MET:HG3	1:U:19:LEU:HD13	2.02	0.42
2:Z:51:VAL:HG21	2:Z:98:LEU:HB3	2.01	0.42
1:T:182:ARG:HA	1:T:182:ARG:HD2	1.69	0.42
1:T:182:ARG:NH2	1:T:234:LEU:HA	2.35	0.42
1:U:150:GLU:HA	1:U:151:PRO:HD3	1.91	0.42
2:W:12:VAL:HG12	2:W:197:ILE:HB	2.02	0.42
1:S:137:GLU:HG2	1:T:48:ARG:HH12	1.85	0.42
2:H:112:SER:O	2:H:114:PRO:HD3	2.20	0.42
1:B:155:VAL:HG12	1:B:160:THR:HG22	2.01	0.42
1:G:55:GLU:HB2	1:G:222:PHE:CG	2.55	0.42
2:J:12:VAL:HG12	2:J:197:ILE:HB	2.01	0.42
1:O:112:THR:HG22	1:O:113:GLU:HG3	2.02	0.42
1:T:167:LEU:HD23	1:T:183:ILE:HG22	2.02	0.42
1:U:60:VAL:HG22	1:U:126:GLU:HG3	2.02	0.42
1:U:92:ARG:HB2	2:V:75:THR:HG21	2.02	0.42
1:C:109:THR:CG2	1:C:113:GLU:HG3	2.49	0.42
2:K:45:ILE:HB	2:K:52:ALA:HB1	2.02	0.42
1:Q:234:LEU:HA	1:Q:234:LEU:HD23	1.89	0.42
2:V:123:PHE:HA	2:V:128:GLY:O	2.20	0.42
1:B:163:ILE:CD1	1:B:188:LEU:HD23	2.50	0.42
1:B:229:ALA:O	1:B:233:LEU:HD22	2.20	0.42
1:D:230:LEU:O	1:D:233:LEU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:33:LYS:O	2:H:44:GLY:HA2	2.20	0.42
2:H:72:VAL:HG22	2:H:73:PRO:HD2	2.02	0.42
1:T:13:MET:O	1:T:17:SER:OG	2.34	0.42
2:H:121:VAL:HG22	2:H:131:ILE:HG12	2.03	0.41
2:K:107:TYR:CE1	2:K:117:ALA:HB3	2.55	0.41
1:U:56:LEU:HG	1:U:62:PHE:HB2	2.02	0.41
1:D:217:ARG:NH1	1:D:222:PHE:O	2.50	0.41
1:G:12:ALA:O	1:G:16:ARG:HG3	2.20	0.41
2:I:57:ARG:NH1	2:J:81:ASN:HD21	2.17	0.41
2:J:20:SER:HB2	2:J:31:VAL:HG21	2.02	0.41
2:M:137:GLN:HG3	2:M:138:ALA:N	2.35	0.41
1:T:161:GLU:OE1	1:T:161:GLU:N	2.40	0.41
1:C:10:GLU:HG3	1:C:11:GLN:N	2.36	0.41
2:H:88:ARG:HD2	2:H:88:ARG:HA	1.83	0.41
2:N:3:ILE:HG21	2:N:44:GLY:HA3	2.00	0.41
1:G:152:HIS:HD2	1:G:171:TYR:HE2	1.68	0.41
2:I:18:ARG:HD3	2:I:193:THR:HG23	2.03	0.41
2:N:69:LEU:HA	2:N:69:LEU:HD23	1.74	0.41
1:O:189:ARG:HG2	1:O:203:LEU:HD12	2.01	0.41
1:F:140:ARG:HH11	1:F:140:ARG:HD2	1.75	0.41
1:F:152:HIS:HE1	1:F:173:GLU:HB2	1.86	0.41
1:F:233:LEU:N	1:F:233:LEU:CD1	2.73	0.41
2:H:173:ASP:OD2	2:Z:152:LYS:NZ	2.40	0.41
2:L:82:ARG:HH21	2:L:85:ILE:HD13	1.86	0.41
1:O:189:ARG:NH1	1:O:202:THR:N	2.68	0.41
1:P:51:GLN:HB3	1:P:209:GLU:OE2	2.20	0.41
1:R:74:LEU:HD23	1:R:74:LEU:HA	1.80	0.41
1:T:99:LEU:O	1:T:102:VAL:HG12	2.20	0.41
1:U:155:VAL:HG12	1:U:160:THR:HG22	2.03	0.41
2:X:20:SER:HB2	2:X:31:VAL:HG21	2.01	0.41
1:B:152:HIS:CG	1:B:171:TYR:HH	2.38	0.41
1:F:180:ALA:HA	1:F:183:ILE:HG22	2.01	0.41
1:G:116:LYS:NZ	1:G:119:GLU:OE1	2.40	0.41
1:O:189:ARG:HH22	1:O:202:THR:HG23	1.86	0.41
1:P:98:GLN:O	1:P:102:VAL:HG23	2.20	0.41
1:T:132:GLU:HG2	1:T:133:THR:N	2.35	0.41
2:I:151:LYS:NZ	2:Y:176:ASP:OD2	2.37	0.41
2:H:41:THR:HG23	2:H:104:LEU:HD11	2.03	0.41
2:I:156:GLN:HE21	2:I:165:ARG:HH22	1.67	0.41
1:P:167:LEU:HA	1:P:167:LEU:HD23	1.86	0.41
1:P:95:THR:O	1:P:99:LEU:HD23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:81:ASN:O	2:X:85:ILE:HG12	2.21	0.41
1:C:181:LEU:O	1:C:185:VAL:HG13	2.20	0.41
2:L:30:ASP:OD2	2:M:133:GLU:HB2	2.21	0.41
2:M:3:ILE:O	2:M:138:ALA:HA	2.20	0.41
1:T:57:TYR:O	1:T:58:ASP:C	2.59	0.41
2:V:113:ASP:OD2	2:V:115:GLN:HB2	2.20	0.41
2:W:101:LEU:HA	2:W:102:PRO:HD3	1.94	0.41
1:B:155:VAL:CG1	1:B:163:ILE:HG21	2.50	0.41
1:C:55:GLU:HB2	1:C:222:PHE:CG	2.56	0.41
1:D:11:GLN:NE2	1:D:14:ARG:NH2	2.68	0.41
1:R:209:GLU:OE1	1:R:224:ARG:NH1	2.47	0.41
1:U:213:LEU:HA	1:U:213:LEU:HD23	1.84	0.41
1:U:68:PHE:HA	1:U:71:PHE:CE2	2.56	0.41
2:W:153:LEU:HD23	2:W:153:LEU:HA	1.84	0.41
2:Z:31:VAL:HG12	2:Z:32:ARG:N	2.36	0.41
1:D:207:SER:O	1:D:207:SER:OG	2.37	0.41
1:G:123:CYS:HA	1:G:139:TYR:O	2.21	0.41
1:P:54:SER:CB	1:P:75:ARG:HD2	2.50	0.41
1:U:85:ARG:HB3	4:U:305:HOH:O	2.21	0.41
1:B:70:GLU:HB3	1:B:118:TYR:CD2	2.56	0.40
1:C:177:LEU:HD12	1:C:177:LEU:HA	1.75	0.40
1:C:54:SER:CB	1:C:75:ARG:HD2	2.51	0.40
1:F:9:MET:HE2	1:G:19:LEU:HD13	2.03	0.40
2:J:176:ASP:OD2	2:W:188:ARG:NH1	2.48	0.40
2:J:194:ALA:HB3	2:J:210:ILE:HD11	2.03	0.40
1:O:182:ARG:HH22	1:O:234:LEU:C	2.24	0.40
1:R:58:ASP:CG	1:R:91:ARG:HH12	2.05	0.40
1:U:81:PHE:CZ	1:U:102:VAL:HG21	2.55	0.40
1:U:14:ARG:NH2	1:U:18:GLU:HG3	2.36	0.40
2:W:51:VAL:HG21	2:W:98:LEU:HB3	2.03	0.40
1:A:10:GLU:CG	1:B:19:LEU:HD12	2.51	0.40
1:C:89:TYR:CE1	2:K:82:ARG:CD	3.04	0.40
2:H:137:GLN:HG3	2:H:138:ALA:N	2.36	0.40
2:I:123:PHE:HA	2:I:128:GLY:O	2.21	0.40
2:M:18:ARG:HD2	2:M:31:VAL:O	2.21	0.40
1:O:150:GLU:HA	1:O:151:PRO:HD3	1.90	0.40
1:O:92:ARG:HE	1:O:92:ARG:HB3	1.71	0.40
1:P:152:HIS:CD2	1:P:171:TYR:HE2	2.39	0.40
1:P:81:PHE:CZ	1:P:102:VAL:HG21	2.56	0.40
1:R:214:ASP:HB3	1:R:217:ARG:HG3	2.02	0.40
2:V:188:ARG:HD3	2:V:188:ARG:HH21	1.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ARG:HH22	1:A:132:GLU:CD	2.25	0.40
1:C:171:TYR:HA	1:C:183:ILE:CD1	2.51	0.40
1:C:183:ILE:HG21	1:C:183:ILE:HD13	1.76	0.40
2:H:122:SER:O	2:H:129:TRP:HA	2.22	0.40
2:J:112:SER:HB3	4:J:402:HOH:O	2.21	0.40
1:O:189:ARG:CG	1:O:203:LEU:HD12	2.51	0.40
1:S:57:TYR:O	1:S:58:ASP:C	2.60	0.40
1:T:231:GLN:HA	1:T:234:LEU:HB2	2.04	0.40
1:U:161:GLU:HB2	1:U:162:PRO:HD3	2.03	0.40
1:Q:142:THR:OG1	1:Q:146:SER:HB2	2.21	0.40
1:D:123:CYS:HB2	1:D:156:MET:SD	2.62	0.40
1:D:188:LEU:HD23	1:D:188:LEU:HA	1.83	0.40
1:F:151:PRO:HB2	1:F:152:HIS:CD2	2.57	0.40
2:K:91:LEU:O	2:K:95:MET:HG2	2.22	0.40
2:Z:38:ASP:HB3	2:Z:41:THR:OG1	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:LYS:CE	2:Z:219:GLU:OE1[2_555]	1.89	0.31
1:D:22:LYS:NZ	2:Z:219:GLU:OE1[2_555]	2.19	0.01

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%)	209 (98%)	4 (2%)	1 (0%)	29	61
1	B	211/240 (88%)	204 (97%)	6 (3%)	1 (0%)	29	61
1	C	212/240 (88%)	206 (97%)	5 (2%)	1 (0%)	29	61
1	D	219/240 (91%)	210 (96%)	8 (4%)	1 (0%)	29	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	214/240 (89%)	208 (97%)	6 (3%)	0	100	100
1	F	211/240 (88%)	204 (97%)	7 (3%)	0	100	100
1	G	212/240 (88%)	208 (98%)	4 (2%)	0	100	100
1	O	214/240 (89%)	206 (96%)	6 (3%)	2 (1%)	17	46
1	P	215/240 (90%)	210 (98%)	5 (2%)	0	100	100
1	Q	213/240 (89%)	210 (99%)	2 (1%)	1 (0%)	29	61
1	R	211/240 (88%)	203 (96%)	6 (3%)	2 (1%)	17	46
1	S	214/240 (89%)	208 (97%)	6 (3%)	0	100	100
1	T	213/240 (89%)	207 (97%)	5 (2%)	1 (0%)	29	61
1	U	212/240 (88%)	204 (96%)	6 (3%)	2 (1%)	17	46
2	H	220/240 (92%)	216 (98%)	4 (2%)	0	100	100
2	I	220/240 (92%)	216 (98%)	4 (2%)	0	100	100
2	J	220/240 (92%)	217 (99%)	3 (1%)	0	100	100
2	K	221/240 (92%)	218 (99%)	3 (1%)	0	100	100
2	L	221/240 (92%)	217 (98%)	4 (2%)	0	100	100
2	M	220/240 (92%)	217 (99%)	3 (1%)	0	100	100
2	N	221/240 (92%)	218 (99%)	3 (1%)	0	100	100
2	V	221/240 (92%)	218 (99%)	3 (1%)	0	100	100
2	W	221/240 (92%)	218 (99%)	3 (1%)	0	100	100
2	X	220/240 (92%)	217 (99%)	3 (1%)	0	100	100
2	Y	221/240 (92%)	218 (99%)	3 (1%)	0	100	100
2	Z	220/240 (92%)	217 (99%)	3 (1%)	0	100	100
2	a	221/240 (92%)	218 (99%)	3 (1%)	0	100	100
2	b	221/240 (92%)	217 (98%)	4 (2%)	0	100	100
All	All	6073/6720 (90%)	5939 (98%)	122 (2%)	12 (0%)	47	78

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	174	ASN
1	T	174	ASN
1	U	174	ASN
1	R	174	ASN
1	A	174	ASN

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Mol	Chain	Res	Type
1	B	174	ASN
1	C	151	PRO
1	O	190	ALA
1	R	190	ALA
1	Q	151	PRO
1	O	151	PRO
1	U	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%)	167 (100%)	0	100	100
1	B	165/184 (90%)	162 (98%)	3 (2%)	59	86
1	C	165/184 (90%)	160 (97%)	5 (3%)	41	75
1	D	172/184 (94%)	172 (100%)	0	100	100
1	E	167/184 (91%)	166 (99%)	1 (1%)	86	96
1	F	164/184 (89%)	162 (99%)	2 (1%)	71	92
1	G	165/184 (90%)	164 (99%)	1 (1%)	86	96
1	O	167/184 (91%)	162 (97%)	5 (3%)	41	75
1	P	168/184 (91%)	167 (99%)	1 (1%)	86	96
1	Q	167/184 (91%)	167 (100%)	0	100	100
1	R	164/184 (89%)	162 (99%)	2 (1%)	71	92
1	S	167/184 (91%)	165 (99%)	2 (1%)	71	92
1	T	166/184 (90%)	166 (100%)	0	100	100
1	U	165/184 (90%)	164 (99%)	1 (1%)	86	96
2	H	165/178 (93%)	165 (100%)	0	100	100
2	I	165/178 (93%)	165 (100%)	0	100	100
2	J	165/178 (93%)	165 (100%)	0	100	100
2	K	165/178 (93%)	165 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	L	165/178 (93%)	165 (100%)	0	100 100
2	M	165/178 (93%)	165 (100%)	0	100 100
2	N	165/178 (93%)	164 (99%)	1 (1%)	86 96
2	V	165/178 (93%)	165 (100%)	0	100 100
2	W	165/178 (93%)	162 (98%)	3 (2%)	59 86
2	X	165/178 (93%)	165 (100%)	0	100 100
2	Y	165/178 (93%)	163 (99%)	2 (1%)	71 92
2	Z	165/178 (93%)	165 (100%)	0	100 100
2	a	165/178 (93%)	165 (100%)	0	100 100
2	b	165/178 (93%)	162 (98%)	3 (2%)	59 86
All	All	4639/5068 (92%)	4607 (99%)	32 (1%)	84 95

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

Mol	Chain	Res	Type
1	B	101	ASN
1	B	135	ARG
1	B	231	GLN
1	C	48	ARG
1	C	101	ASN
1	C	163	ILE
1	C	168	LYS
1	C	189	ARG
1	E	178	THR
1	F	176	SER
1	F	233	LEU
1	G	101	ASN
2	N	57	ARG
1	O	48	ARG
1	O	101	ASN
1	O	133	THR
1	O	135	ARG
1	O	182	ARG
1	P	101	ASN
1	R	91	ARG
1	R	97	ARG
1	S	92	ARG
1	S	233	LEU

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Mol	Chain	Res	Type
1	U	142	THR
2	W	38	ASP
2	W	161	ASP
2	W	209	ARG
2	Y	38	ASP
2	Y	208	SER
2	b	13	VAL
2	b	38	ASP
2	b	48	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	51	GLN
1	C	165	ASN
1	D	11	GLN
1	E	101	ASN
1	F	231	GLN
1	G	73	ASN
2	I	156	GLN
2	L	96	GLN
2	N	137	GLN
1	P	73	ASN
1	P	165	ASN
1	P	174	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

14 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	7HJ	b	301	-	49,49,49	1.78	7 (14%)	64,65,65	1.44	6 (9%)
3	7HJ	a	301	-	49,49,49	1.70	3 (6%)	64,65,65	1.53	11 (17%)
3	7HJ	X	301	-	49,49,49	1.88	5 (10%)	64,65,65	1.40	7 (10%)
3	7HJ	Z	301	-	49,49,49	1.71	8 (16%)	64,65,65	1.37	5 (7%)
3	7HJ	Y	301	-	49,49,49	1.68	4 (8%)	64,65,65	1.28	6 (9%)
3	7HJ	V	301	-	49,49,49	1.60	3 (6%)	64,65,65	1.62	8 (12%)
3	7HJ	W	301	-	49,49,49	1.56	6 (12%)	64,65,65	1.53	9 (14%)
3	7HJ	L	301	-	49,49,49	1.69	4 (8%)	64,65,65	1.42	6 (9%)
3	7HJ	N	301	-	49,49,49	1.54	6 (12%)	64,65,65	1.45	8 (12%)
3	7HJ	M	301	-	49,49,49	1.90	7 (14%)	64,65,65	1.31	9 (14%)
3	7HJ	H	301	-	49,49,49	1.72	7 (14%)	64,65,65	1.42	8 (12%)
3	7HJ	J	301	-	49,49,49	1.85	9 (18%)	64,65,65	1.34	7 (10%)
3	7HJ	I	301	-	49,49,49	1.78	3 (6%)	64,65,65	1.32	7 (10%)
3	7HJ	K	301	-	49,49,49	1.44	5 (10%)	64,65,65	1.35	6 (9%)

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	7HJ	b	301	-	-	4/42/42/42	0/4/4/4
3	7HJ	a	301	-	-	6/42/42/42	0/4/4/4
3	7HJ	X	301	-	-	4/42/42/42	0/4/4/4
3	7HJ	Z	301	-	-	5/42/42/42	0/4/4/4
3	7HJ	Y	301	-	-	6/42/42/42	0/4/4/4
3	7HJ	V	301	-	-	8/42/42/42	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	7HJ	W	301	-	-	7/42/42/42	0/4/4/4
3	7HJ	L	301	-	-	5/42/42/42	0/4/4/4
3	7HJ	N	301	-	-	8/42/42/42	0/4/4/4
3	7HJ	M	301	-	-	6/42/42/42	0/4/4/4
3	7HJ	H	301	-	-	4/42/42/42	0/4/4/4
3	7HJ	J	301	-	-	7/42/42/42	0/4/4/4
3	7HJ	I	301	-	-	6/42/42/42	0/4/4/4
3	7HJ	K	301	-	-	6/42/42/42	0/4/4/4

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	301	7HJ	C38-C39	9.04	1.56	1.33
3	J	301	7HJ	C38-C39	8.85	1.56	1.33
3	X	301	7HJ	C38-C39	8.60	1.55	1.33
3	M	301	7HJ	C38-C39	8.33	1.54	1.33
3	V	301	7HJ	C38-C39	8.01	1.53	1.33
3	a	301	7HJ	C38-C39	7.77	1.53	1.33
3	L	301	7HJ	C38-C39	7.63	1.52	1.33
3	b	301	7HJ	C38-C39	7.48	1.52	1.33
3	W	301	7HJ	C38-C39	7.42	1.52	1.33
3	H	301	7HJ	C38-C39	7.42	1.52	1.33
3	Y	301	7HJ	C38-C39	7.23	1.51	1.33
3	Z	301	7HJ	C38-C39	6.98	1.51	1.33
3	K	301	7HJ	C38-C39	6.62	1.50	1.33
3	N	301	7HJ	C38-C39	6.47	1.49	1.33
3	Y	301	7HJ	C29-N30	5.89	1.47	1.35
3	X	301	7HJ	C29-N30	5.89	1.47	1.35
3	M	301	7HJ	C29-N30	5.86	1.47	1.35
3	L	301	7HJ	C29-N30	5.84	1.47	1.35
3	I	301	7HJ	C29-N30	5.46	1.46	1.35
3	b	301	7HJ	C29-N30	5.34	1.46	1.35
3	H	301	7HJ	C29-N30	5.11	1.45	1.35
3	a	301	7HJ	C29-N30	4.90	1.45	1.35
3	N	301	7HJ	C27-C02	4.65	1.65	1.52
3	J	301	7HJ	C29-N30	4.22	1.43	1.35
3	Z	301	7HJ	C29-N30	4.03	1.43	1.35
3	V	301	7HJ	C29-N30	3.87	1.43	1.35
3	K	301	7HJ	C29-N30	3.78	1.42	1.35
3	X	301	7HJ	C02-N03	3.73	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	W	301	7HJ	C29-N30	3.71	1.42	1.35
3	b	301	7HJ	C07-C08	-3.69	1.41	1.52
3	W	301	7HJ	C05-N06	3.45	1.41	1.33
3	Z	301	7HJ	C07-N06	-3.40	1.39	1.46
3	Z	301	7HJ	C37-N36	3.36	1.42	1.34
3	Y	301	7HJ	C37-N36	3.27	1.42	1.34
3	M	301	7HJ	C19-C20	-3.15	1.43	1.51
3	H	301	7HJ	C37-N36	3.14	1.42	1.34
3	L	301	7HJ	C05-N06	3.01	1.40	1.33
3	N	301	7HJ	C05-N06	3.01	1.40	1.33
3	M	301	7HJ	C05-N06	3.00	1.40	1.33
3	X	301	7HJ	C05-N06	2.85	1.39	1.33
3	L	301	7HJ	C37-N36	2.82	1.41	1.34
3	J	301	7HJ	C07-N06	-2.79	1.40	1.46
3	Y	301	7HJ	C07-N06	-2.76	1.40	1.46
3	Z	301	7HJ	C28-C29	2.74	1.56	1.51
3	J	301	7HJ	C19-C20	-2.72	1.44	1.51
3	H	301	7HJ	C13-C12	-2.67	1.38	1.43
3	N	301	7HJ	C29-N30	2.66	1.40	1.35
3	b	301	7HJ	C37-N36	2.63	1.40	1.34
3	M	301	7HJ	C04-C05	-2.53	1.46	1.52
3	Z	301	7HJ	C02-N03	2.52	1.39	1.34
3	H	301	7HJ	C05-N06	2.51	1.39	1.33
3	J	301	7HJ	C38-C37	2.51	1.53	1.48
3	J	301	7HJ	C07-C08	-2.49	1.45	1.52
3	a	301	7HJ	C27-C02	2.44	1.59	1.52
3	M	301	7HJ	C37-N36	2.42	1.40	1.34
3	H	301	7HJ	C04-C05	-2.41	1.46	1.52
3	N	301	7HJ	C13-C12	-2.41	1.38	1.43
3	J	301	7HJ	C37-N36	2.38	1.40	1.34
3	K	301	7HJ	C05-N06	2.36	1.38	1.33
3	Z	301	7HJ	C05-N06	2.34	1.38	1.33
3	Z	301	7HJ	C28-C27	2.33	1.58	1.53
3	W	301	7HJ	C04-C05	-2.28	1.46	1.52
3	M	301	7HJ	C38-C37	2.26	1.53	1.48
3	V	301	7HJ	C04-C05	-2.26	1.46	1.52
3	K	301	7HJ	C37-N36	2.25	1.39	1.34
3	X	301	7HJ	C37-N36	2.24	1.39	1.34
3	J	301	7HJ	C27-C02	2.21	1.58	1.52
3	N	301	7HJ	C04-N03	-2.19	1.41	1.45
3	b	301	7HJ	C02-N03	2.18	1.38	1.34
3	W	301	7HJ	O18-C05	-2.14	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	W	301	7HJ	C02-N03	2.13	1.38	1.34
3	I	301	7HJ	C38-C37	2.12	1.52	1.48
3	H	301	7HJ	C04-N03	-2.12	1.41	1.45
3	K	301	7HJ	C02-N03	2.12	1.38	1.34
3	J	301	7HJ	C02-N03	2.04	1.38	1.34
3	b	301	7HJ	C04-C05	-2.03	1.47	1.52
3	b	301	7HJ	C13-C12	-2.01	1.39	1.43

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	301	7HJ	C40-C39-C38	-6.17	112.78	126.91
3	X	301	7HJ	C40-C39-C38	-5.83	113.56	126.91
3	b	301	7HJ	C40-C39-C38	-5.74	113.78	126.91
3	Z	301	7HJ	C40-C39-C38	-5.72	113.82	126.91
3	W	301	7HJ	C07-N06-C05	5.51	130.27	122.34
3	N	301	7HJ	C40-C39-C38	-5.47	114.39	126.91
3	W	301	7HJ	C40-C39-C38	-5.31	114.76	126.91
3	H	301	7HJ	C40-C39-C38	-5.18	115.06	126.91
3	M	301	7HJ	C40-C39-C38	-4.97	115.54	126.91
3	b	301	7HJ	C39-C38-C37	-4.94	111.90	121.56
3	W	301	7HJ	C39-C38-C37	-4.89	112.00	121.56
3	V	301	7HJ	O46-C37-N36	-4.84	115.95	122.35
3	V	301	7HJ	C40-C39-C38	-4.81	115.90	126.91
3	K	301	7HJ	C39-C38-C37	-4.80	112.18	121.56
3	a	301	7HJ	O46-C37-N36	-4.64	116.22	122.35
3	V	301	7HJ	C27-C28-C29	4.62	121.39	112.25
3	I	301	7HJ	C40-C39-C38	-4.62	116.33	126.91
3	V	301	7HJ	C07-N06-C05	4.53	128.86	122.34
3	a	301	7HJ	C38-C37-N36	4.47	123.16	114.56
3	Y	301	7HJ	C39-C38-C37	-4.47	112.82	121.56
3	K	301	7HJ	C40-C39-C38	-4.44	116.74	126.91
3	J	301	7HJ	C39-C38-C37	-4.36	113.04	121.56
3	N	301	7HJ	C27-C28-C29	4.33	120.81	112.25
3	J	301	7HJ	O46-C37-N36	-4.26	116.72	122.35
3	Z	301	7HJ	C27-C28-C29	4.24	120.64	112.25
3	Y	301	7HJ	C40-C39-C38	-4.17	117.36	126.91
3	V	301	7HJ	C38-C37-N36	4.01	122.26	114.56
3	V	301	7HJ	C39-C38-C37	-4.00	113.75	121.56
3	a	301	7HJ	C39-C38-C37	-3.91	113.92	121.56
3	N	301	7HJ	C39-C38-C37	-3.88	113.98	121.56
3	L	301	7HJ	C07-N06-C05	3.84	127.86	122.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	a	301	7HJ	C40-C39-C38	-3.78	118.26	126.91
3	H	301	7HJ	C27-C28-C29	3.78	119.72	112.25
3	Z	301	7HJ	C39-C38-C37	-3.76	114.21	121.56
3	K	301	7HJ	C07-N06-C05	3.68	127.64	122.34
3	I	301	7HJ	C39-C38-C37	-3.62	114.49	121.56
3	J	301	7HJ	C38-C37-N36	3.62	121.51	114.56
3	M	301	7HJ	C07-N06-C05	3.59	127.50	122.34
3	b	301	7HJ	C27-C28-C29	3.58	119.33	112.25
3	J	301	7HJ	C27-C28-C29	3.54	119.25	112.25
3	I	301	7HJ	O46-C37-N36	-3.51	117.71	122.35
3	X	301	7HJ	C27-C28-C29	3.40	118.97	112.25
3	W	301	7HJ	C27-C28-C29	3.37	118.91	112.25
3	K	301	7HJ	C38-C37-N36	3.34	120.98	114.56
3	a	301	7HJ	O35-C29-C28	-3.34	116.18	122.20
3	L	301	7HJ	C27-C28-C29	3.29	118.76	112.25
3	I	301	7HJ	C27-C28-C29	3.28	118.74	112.25
3	L	301	7HJ	C39-C38-C37	-3.27	115.17	121.56
3	N	301	7HJ	O46-C37-N36	-3.21	118.10	122.35
3	J	301	7HJ	C40-C39-C38	-3.15	119.70	126.91
3	H	301	7HJ	C28-C27-C02	-3.14	103.03	110.42
3	X	301	7HJ	O46-C37-N36	-3.13	118.22	122.35
3	Z	301	7HJ	C07-N06-C05	3.12	126.82	122.34
3	H	301	7HJ	C07-N06-C05	3.11	126.81	122.34
3	Y	301	7HJ	C38-C37-N36	3.00	120.33	114.56
3	H	301	7HJ	C39-C38-C37	-2.96	115.78	121.56
3	N	301	7HJ	O01-C02-N03	-2.94	117.49	122.93
3	Y	301	7HJ	C27-C28-C29	2.88	117.94	112.25
3	X	301	7HJ	C07-N06-C05	2.85	126.44	122.34
3	K	301	7HJ	O46-C37-N36	-2.81	118.63	122.35
3	H	301	7HJ	C27-C02-N03	2.80	122.84	116.70
3	I	301	7HJ	C38-C37-N36	2.74	119.83	114.56
3	M	301	7HJ	C27-C28-C29	2.70	117.58	112.25
3	H	301	7HJ	C38-C37-N36	2.65	119.65	114.56
3	N	301	7HJ	C38-C37-N36	2.64	119.64	114.56
3	b	301	7HJ	C38-C37-N36	2.62	119.60	114.56
3	a	301	7HJ	C28-C29-N30	2.61	123.57	118.52
3	a	301	7HJ	C07-N06-C05	2.60	126.08	122.34
3	I	301	7HJ	C28-C27-C02	-2.59	104.31	110.42
3	N	301	7HJ	C28-C29-N30	-2.55	113.58	118.52
3	b	301	7HJ	C04-N03-C02	2.53	127.09	121.67
3	Y	301	7HJ	O46-C37-N36	-2.53	119.01	122.35
3	X	301	7HJ	C38-C37-N36	2.52	119.40	114.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	301	7HJ	C38-C37-N36	2.47	119.31	114.56
3	X	301	7HJ	C27-C02-N03	2.45	122.08	116.70
3	M	301	7HJ	O46-C37-N36	-2.44	119.12	122.35
3	V	301	7HJ	C08-C13-C12	2.42	121.99	118.98
3	L	301	7HJ	C08-C13-C12	2.31	121.85	118.98
3	N	301	7HJ	C07-N06-C05	2.27	125.60	122.34
3	b	301	7HJ	C28-C27-C02	-2.23	105.17	110.42
3	a	301	7HJ	C27-C02-N03	2.23	121.58	116.70
3	Z	301	7HJ	O35-C29-N30	-2.22	117.73	122.05
3	H	301	7HJ	O46-C37-N36	-2.18	119.47	122.35
3	K	301	7HJ	C27-C02-N03	2.17	121.47	116.70
3	W	301	7HJ	C38-C37-N36	2.17	118.73	114.56
3	M	301	7HJ	C39-C38-C37	-2.15	117.36	121.56
3	M	301	7HJ	C42-C41-C40	2.15	123.25	120.65
3	J	301	7HJ	C28-C27-C02	-2.13	105.41	110.42
3	Y	301	7HJ	C28-C27-C02	-2.12	105.43	110.42
3	a	301	7HJ	C15-C14-C13	2.11	123.82	120.89
3	J	301	7HJ	C27-C02-N03	2.10	121.31	116.70
3	a	301	7HJ	C42-C41-C40	2.10	123.19	120.65
3	a	301	7HJ	C04-N03-C02	2.09	126.15	121.67
3	I	301	7HJ	C27-C02-N03	2.08	121.27	116.70
3	M	301	7HJ	C27-C02-N03	2.08	121.27	116.70
3	M	301	7HJ	C08-C13-C12	2.07	121.55	118.98
3	W	301	7HJ	C28-C27-C02	-2.07	105.55	110.42
3	V	301	7HJ	C28-C27-C02	-2.07	105.55	110.42
3	L	301	7HJ	C27-C02-N03	2.06	121.23	116.70
3	X	301	7HJ	C39-C38-C37	-2.04	117.58	121.56
3	W	301	7HJ	C15-C14-C13	2.03	123.71	120.89
3	W	301	7HJ	C04-N03-C02	2.02	126.00	121.67
3	W	301	7HJ	O46-C37-N36	-2.00	119.71	122.35

There are no chirality outliers.

All (82) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Y	301	7HJ	C34-C33-N30-C29
3	W	301	7HJ	C32-C31-N30-C29
3	W	301	7HJ	C32-C31-N30-C33
3	a	301	7HJ	O46-C37-C38-C39
3	Y	301	7HJ	O46-C37-C38-C39
3	H	301	7HJ	O46-C37-C38-C39
3	a	301	7HJ	N36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
3	b	301	7HJ	C38-C39-C40-C45
3	a	301	7HJ	C38-C39-C40-C41
3	X	301	7HJ	C38-C39-C40-C45
3	W	301	7HJ	C38-C39-C40-C45
3	J	301	7HJ	C38-C39-C40-C45
3	K	301	7HJ	C38-C39-C40-C45
3	H	301	7HJ	C38-C39-C40-C45
3	Z	301	7HJ	C38-C39-C40-C41
3	W	301	7HJ	C38-C39-C40-C41
3	H	301	7HJ	C38-C39-C40-C41
3	b	301	7HJ	C38-C39-C40-C41
3	a	301	7HJ	C38-C39-C40-C45
3	X	301	7HJ	C38-C39-C40-C41
3	J	301	7HJ	C38-C39-C40-C41
3	K	301	7HJ	C38-C39-C40-C41
3	b	301	7HJ	O46-C37-C38-C39
3	X	301	7HJ	O46-C37-C38-C39
3	V	301	7HJ	O46-C37-C38-C39
3	K	301	7HJ	O46-C37-C38-C39
3	L	301	7HJ	C38-C39-C40-C45
3	N	301	7HJ	C34-C33-N30-C29
3	Z	301	7HJ	C37-C38-C39-C40
3	J	301	7HJ	C37-C38-C39-C40
3	M	301	7HJ	C38-C39-C40-C45
3	V	301	7HJ	C38-C39-C40-C45
3	Z	301	7HJ	C38-C39-C40-C45
3	Y	301	7HJ	C34-C33-N30-C31
3	L	301	7HJ	C38-C39-C40-C41
3	I	301	7HJ	C38-C39-C40-C45
3	J	301	7HJ	O46-C37-C38-C39
3	M	301	7HJ	C32-C31-N30-C29
3	V	301	7HJ	C38-C39-C40-C41
3	M	301	7HJ	C38-C39-C40-C41
3	b	301	7HJ	N36-C37-C38-C39
3	X	301	7HJ	N36-C37-C38-C39
3	Y	301	7HJ	N36-C37-C38-C39
3	H	301	7HJ	N36-C37-C38-C39
3	K	301	7HJ	N36-C37-C38-C39
3	I	301	7HJ	C32-C31-N30-C29
3	W	301	7HJ	O46-C37-C38-C39
3	I	301	7HJ	C38-C39-C40-C41
3	V	301	7HJ	N36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
3	W	301	7HJ	N36-C37-C38-C39
3	J	301	7HJ	N36-C37-C38-C39
3	I	301	7HJ	N36-C37-C38-C39
3	Y	301	7HJ	C38-C39-C40-C45
3	a	301	7HJ	C32-C31-N30-C29
3	N	301	7HJ	C32-C31-N30-C29
3	N	301	7HJ	C34-C33-N30-C31
3	Y	301	7HJ	C38-C39-C40-C41
3	N	301	7HJ	C38-C39-C40-C41
3	N	301	7HJ	N36-C37-C38-C39
3	M	301	7HJ	N36-C37-C38-C39
3	W	301	7HJ	N36-C27-C28-C29
3	N	301	7HJ	C32-C31-N30-C33
3	I	301	7HJ	O46-C37-C38-C39
3	N	301	7HJ	C38-C39-C40-C45
3	N	301	7HJ	O46-C37-C38-C39
3	M	301	7HJ	O46-C37-C38-C39
3	M	301	7HJ	C32-C31-N30-C33
3	V	301	7HJ	C27-C28-C29-O35
3	J	301	7HJ	C27-C28-C29-O35
3	I	301	7HJ	C32-C31-N30-C33
3	V	301	7HJ	C32-C31-N30-C29
3	K	301	7HJ	C34-C33-N30-C31
3	L	301	7HJ	C34-C33-N30-C31
3	Z	301	7HJ	N36-C37-C38-C39
3	L	301	7HJ	N36-C37-C38-C39
3	Z	301	7HJ	O46-C37-C38-C39
3	L	301	7HJ	O46-C37-C38-C39
3	a	301	7HJ	C32-C31-N30-C33
3	V	301	7HJ	C27-C28-C29-N30
3	J	301	7HJ	C27-C28-C29-N30
3	V	301	7HJ	C32-C31-N30-C33
3	K	301	7HJ	C34-C33-N30-C29

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Z	301	7HJ	1	0
3	V	301	7HJ	1	0
3	W	301	7HJ	1	0
3	L	301	7HJ	1	0

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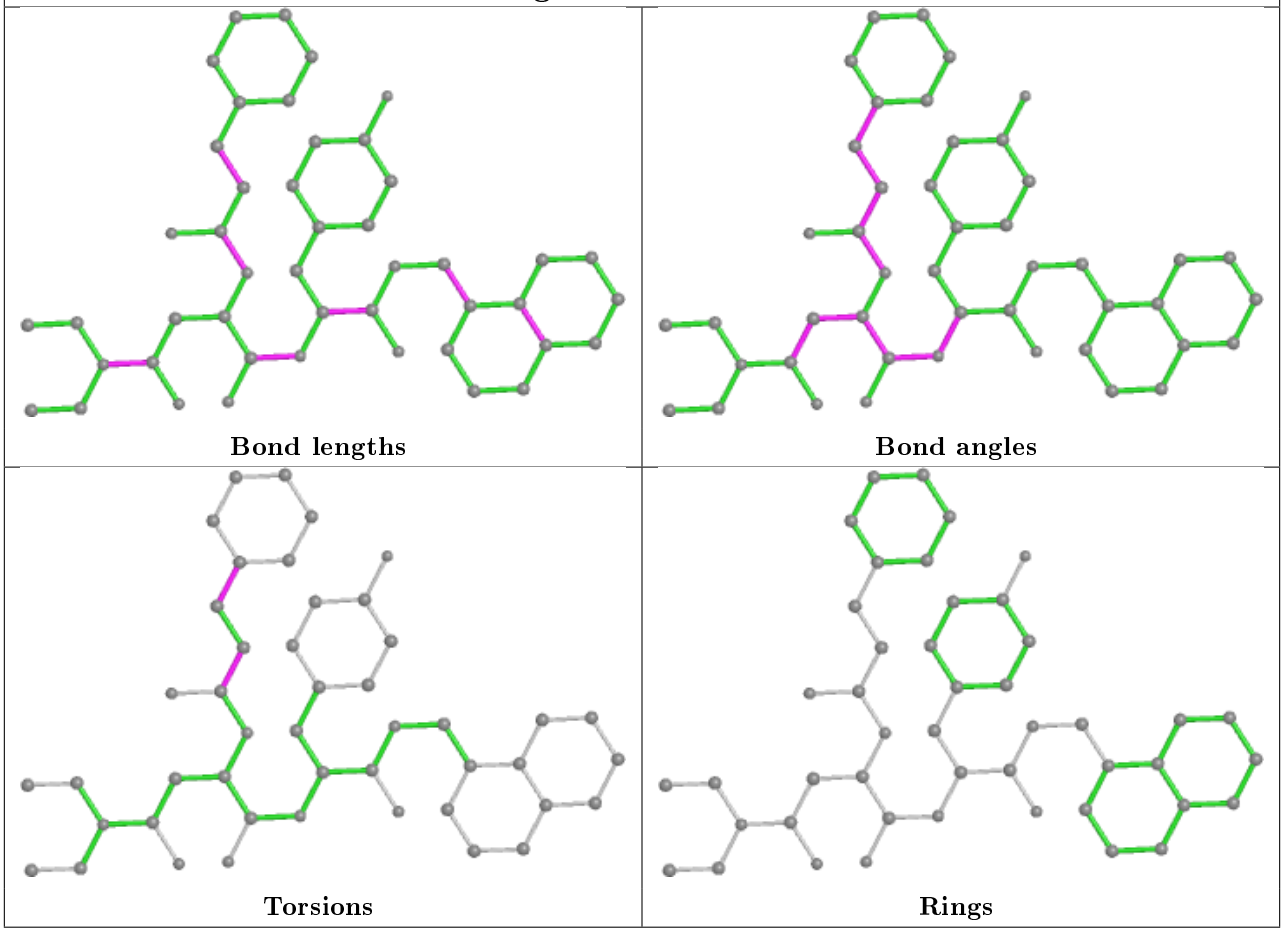
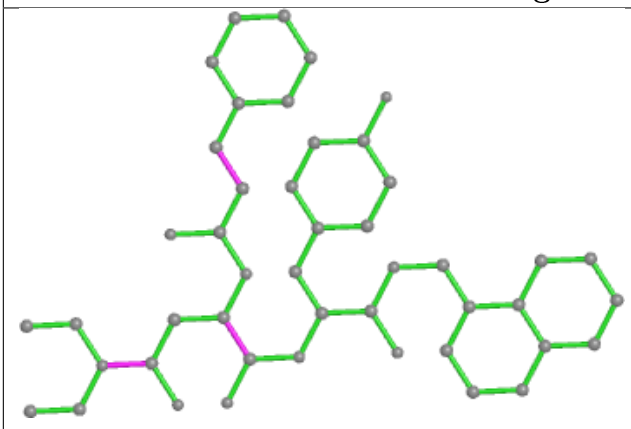
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	N	301	7HJ	3	0
3	M	301	7HJ	1	0
3	H	301	7HJ	1	0
3	J	301	7HJ	2	0

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

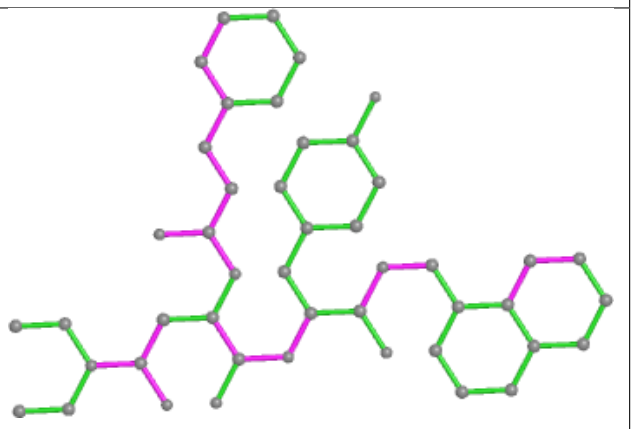
Ligand 7HJ b 301



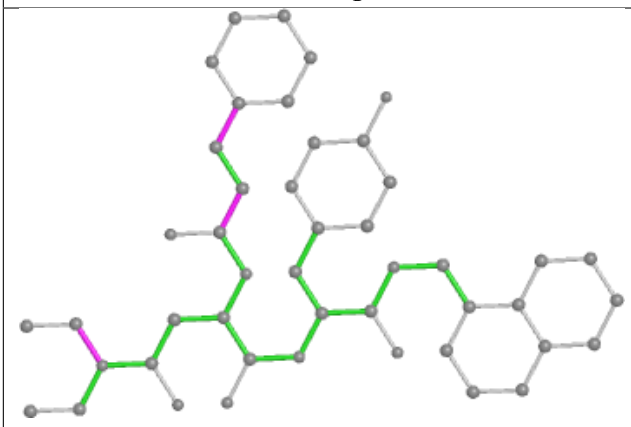
Ligand 7HJ a 301



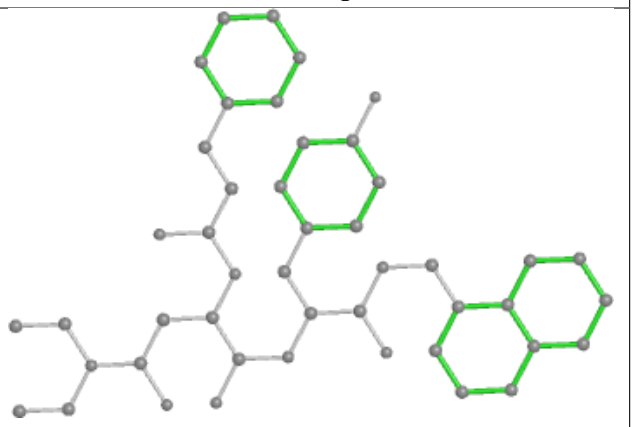
Bond lengths



Bond angles

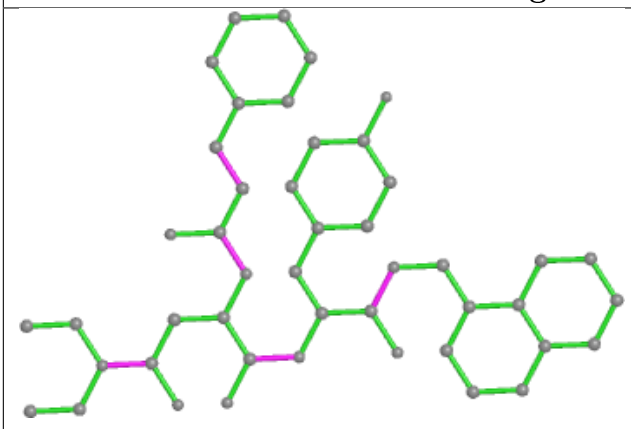


Torsions

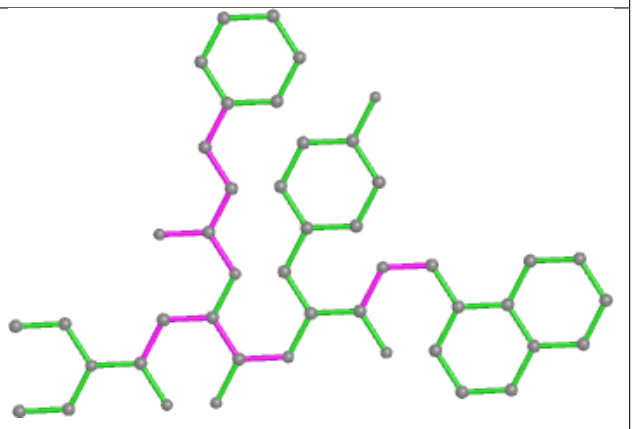


Rings

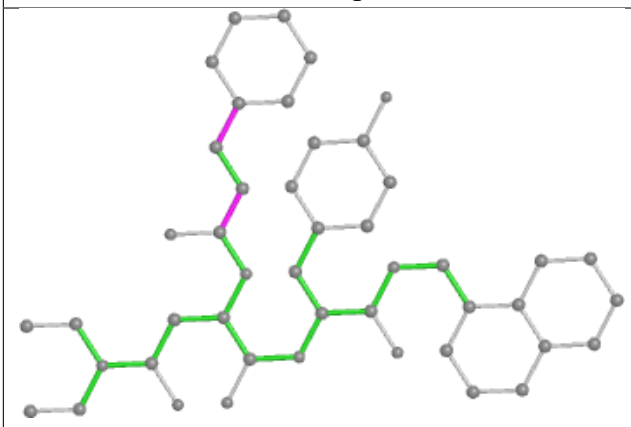
Ligand 7HJ X 301



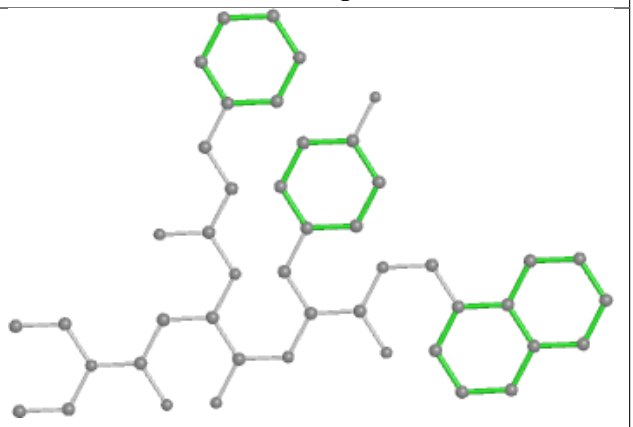
Bond lengths



Bond angles

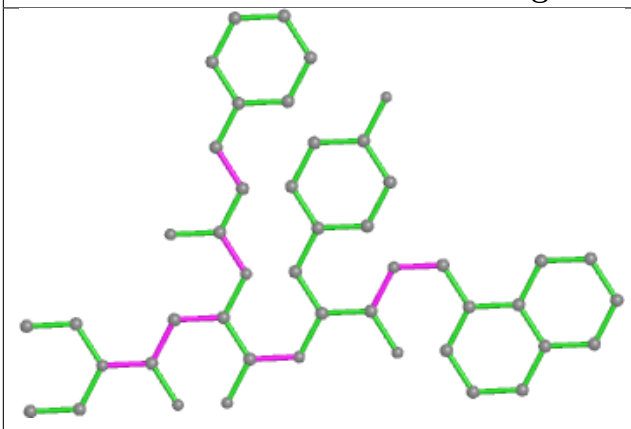


Torsions

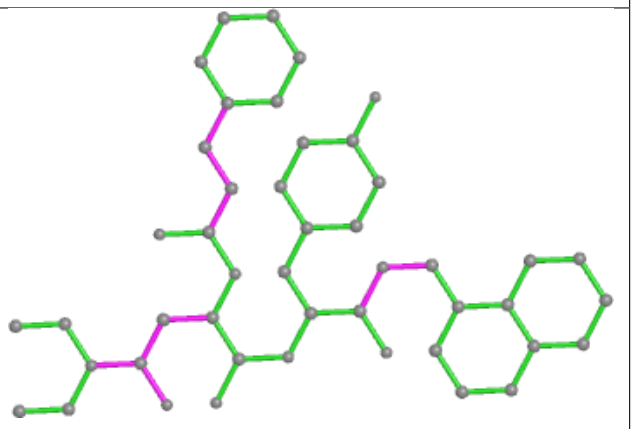


Rings

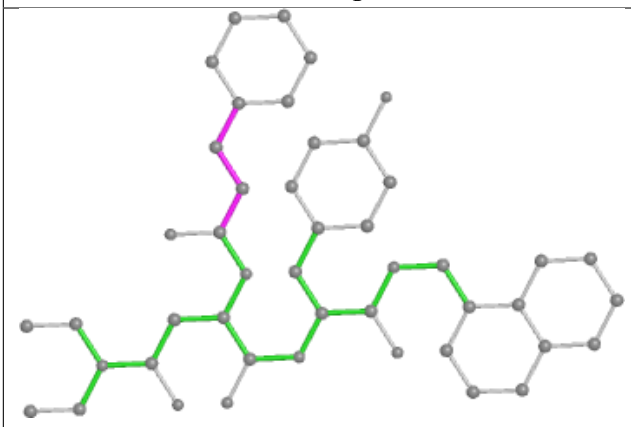
Ligand 7HJ Z 301



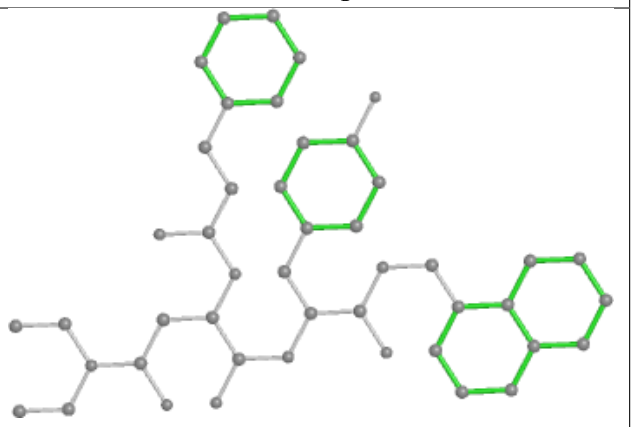
Bond lengths



Bond angles

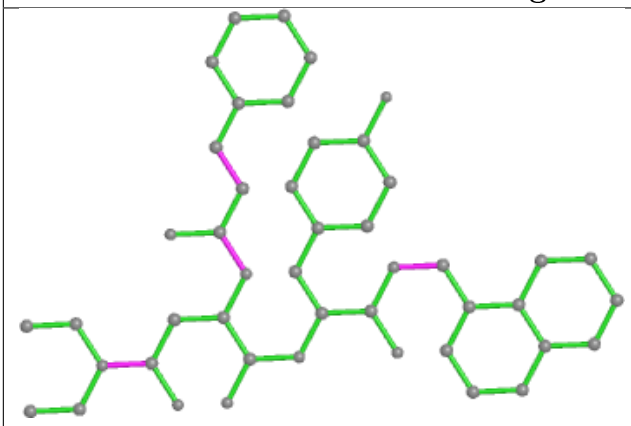


Torsions



Rings

Ligand 7HJ Y 301



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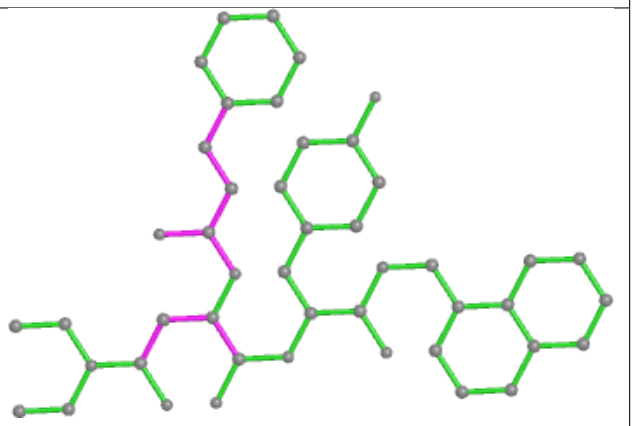

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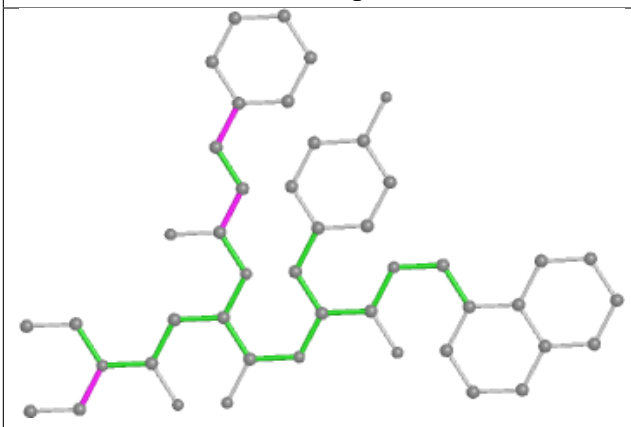

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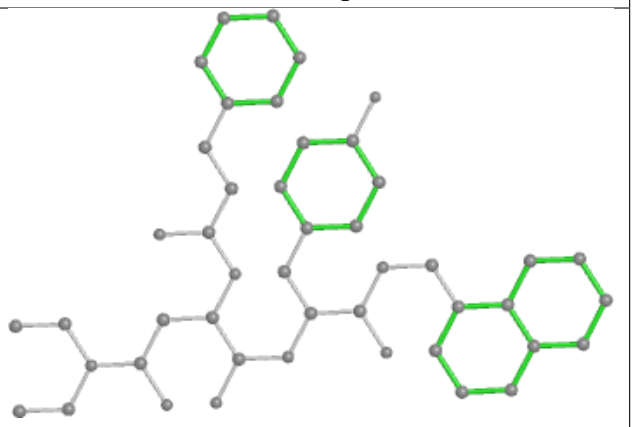
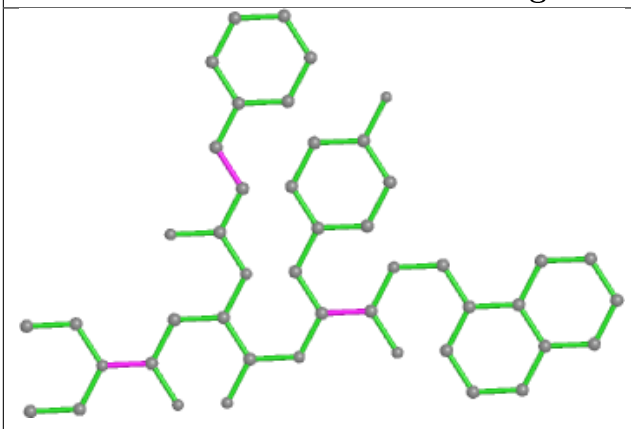


Rings

Ligand 7HJ V 301



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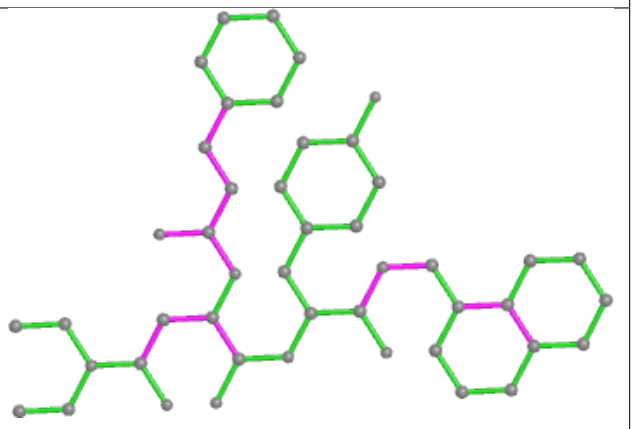

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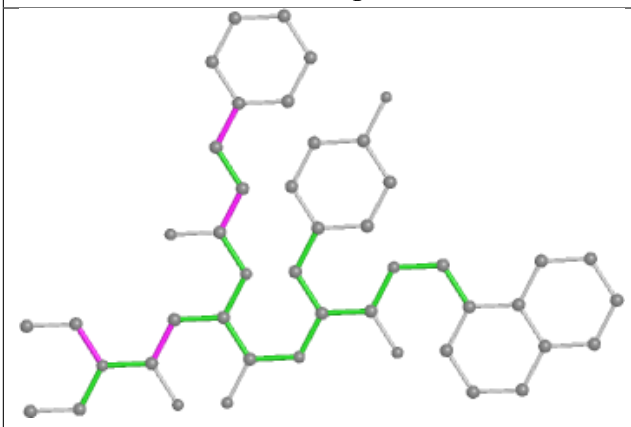
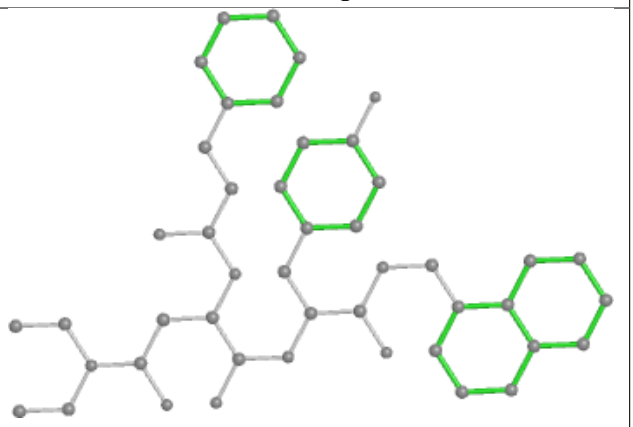
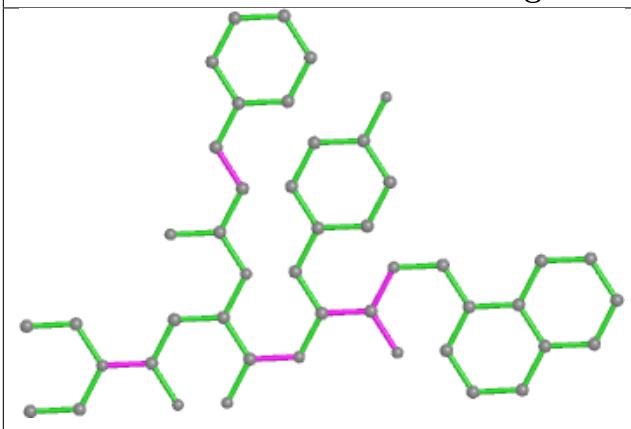


Torsions



Rings

Ligand 7HJ W 301



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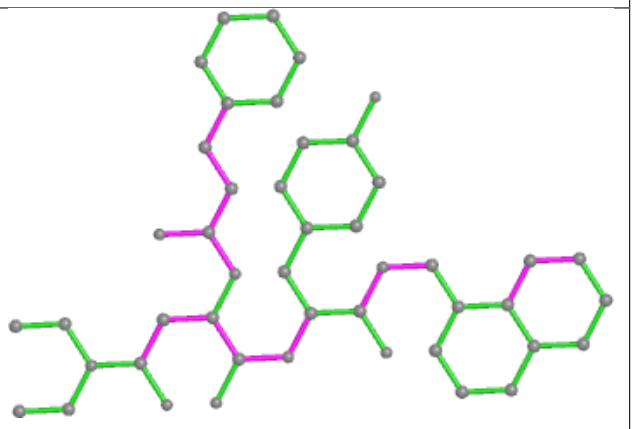
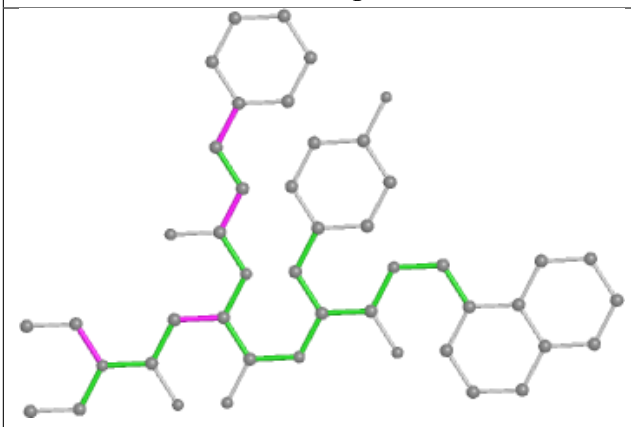


Bond angles



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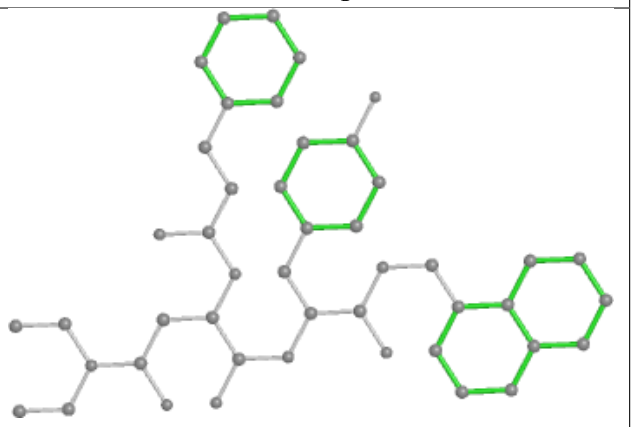
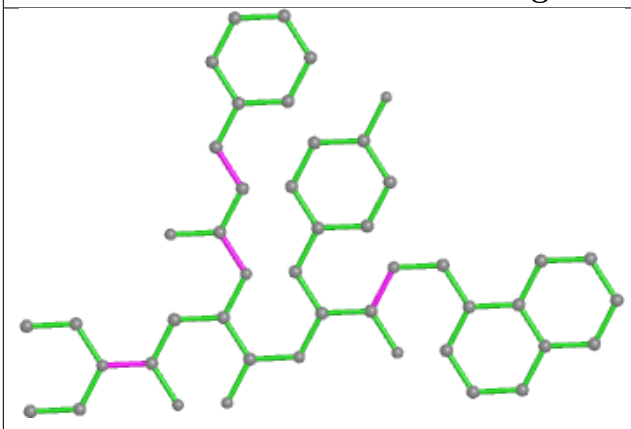


Rings

Ligand 7HJ L 301



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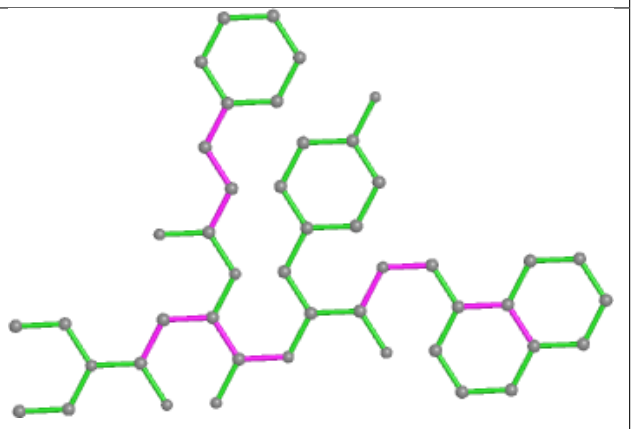

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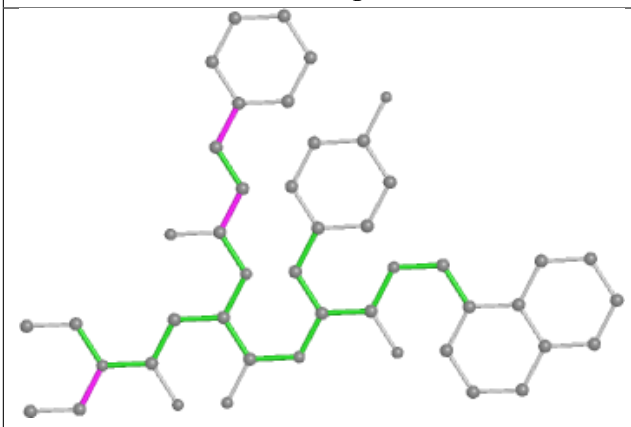

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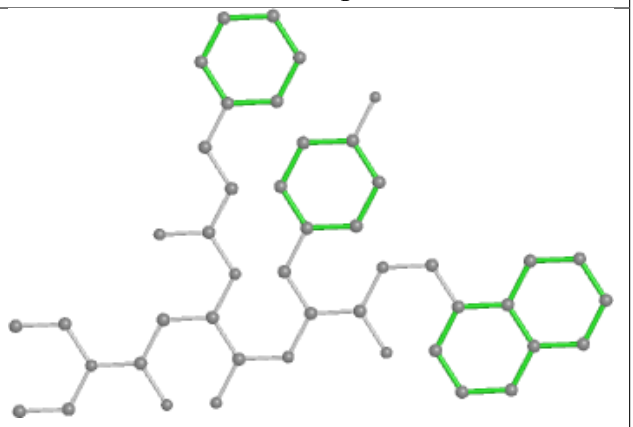
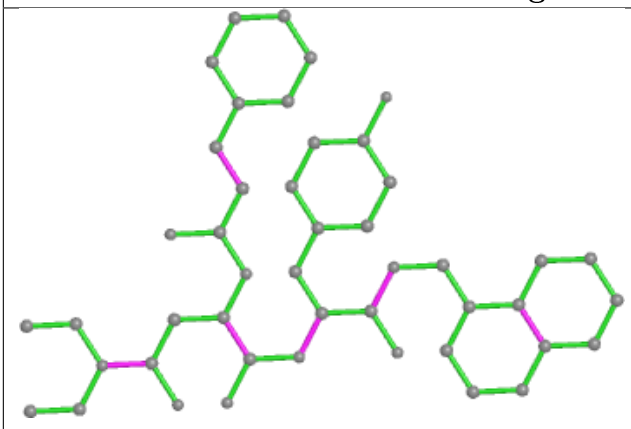


Rings

Ligand 7HJ N 301



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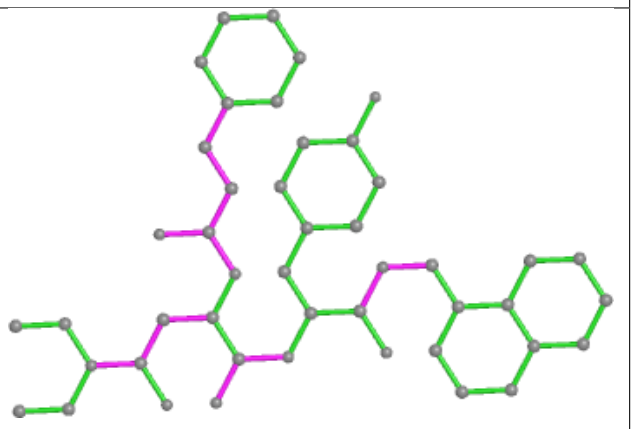
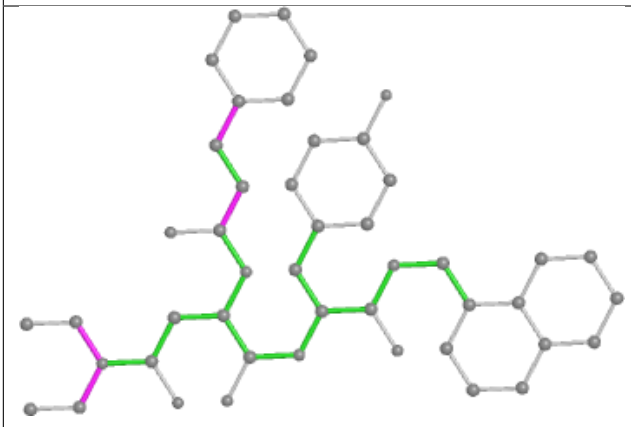


Bond angles



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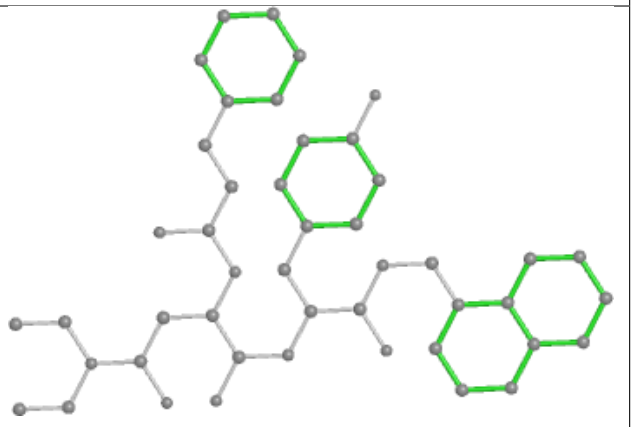
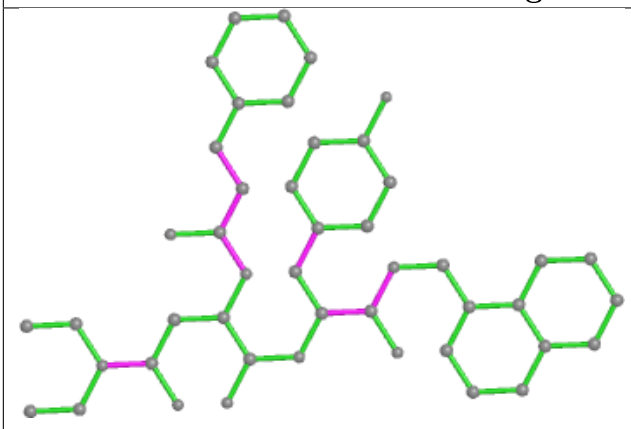


Rings

Ligand 7HJ M 301



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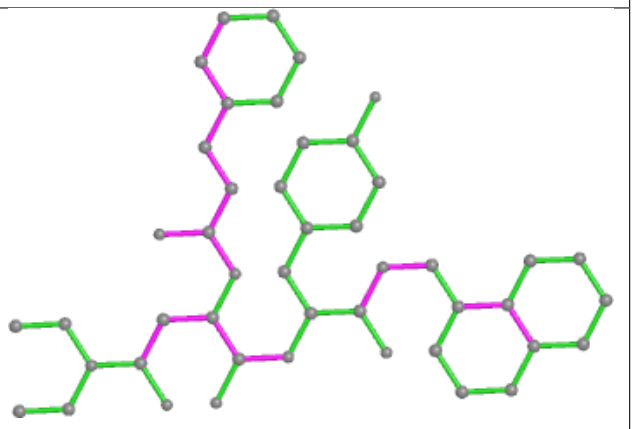

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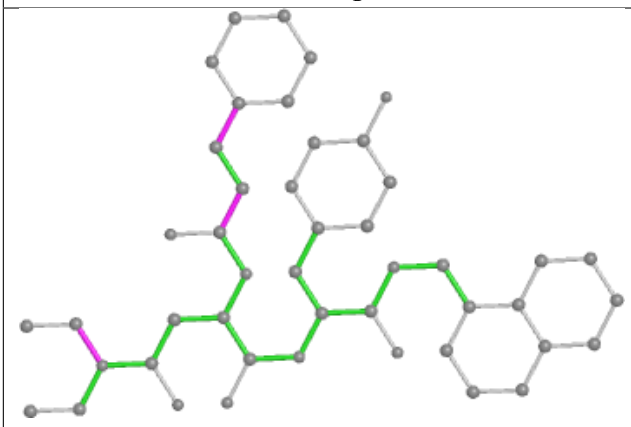

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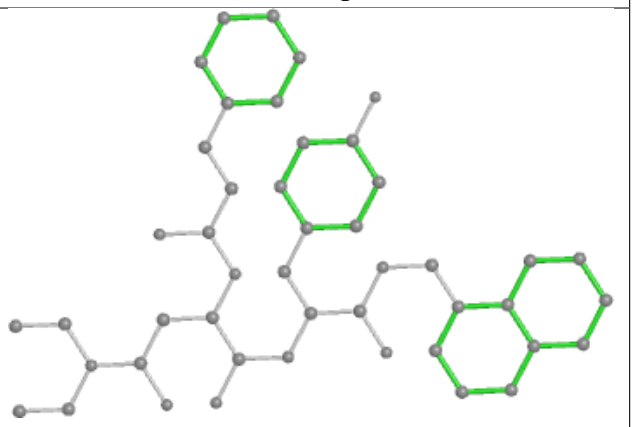
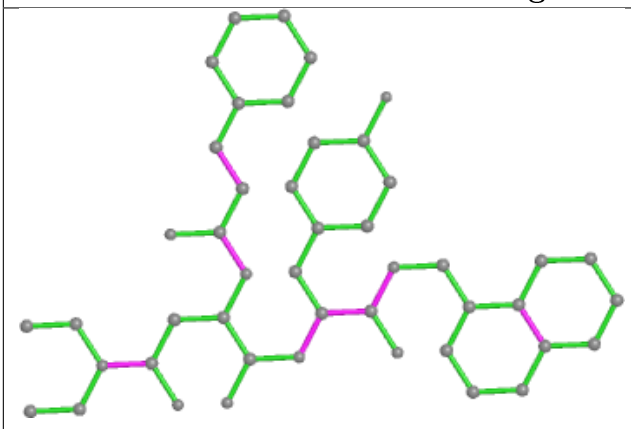


Rings

Ligand 7HJ H 301



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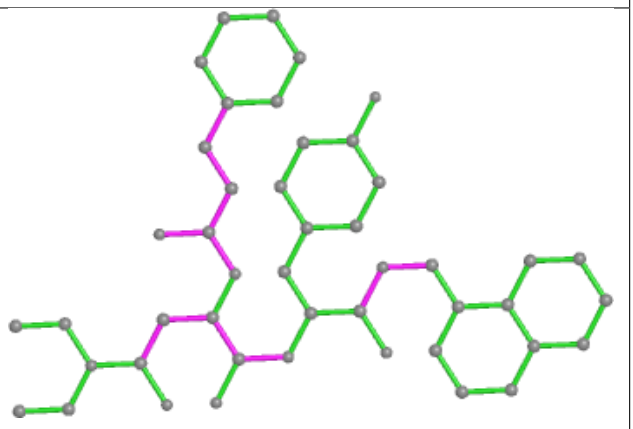
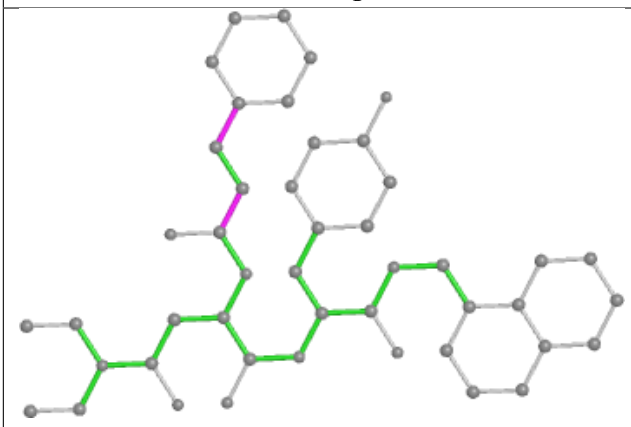


Bond angles



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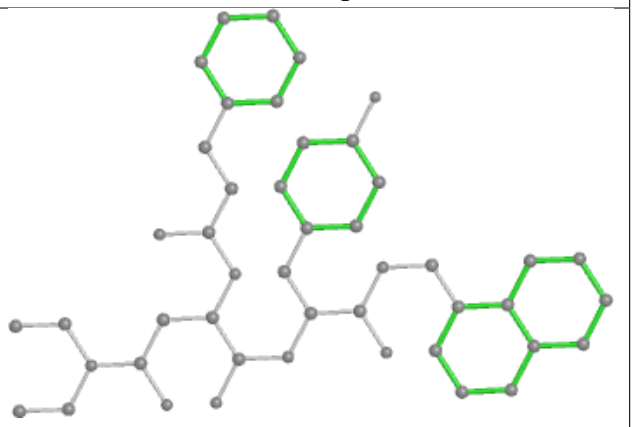
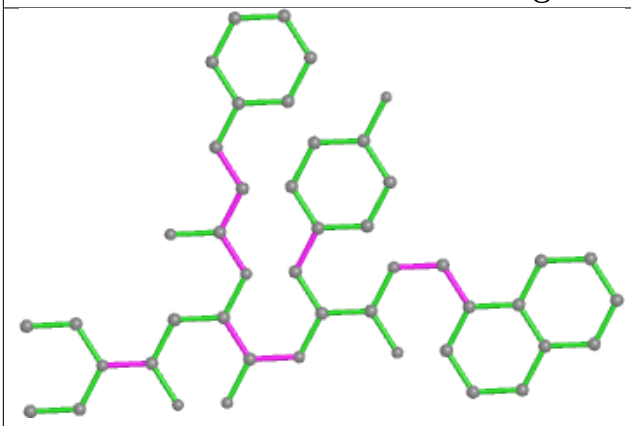


Rings

Ligand 7HJ J 301



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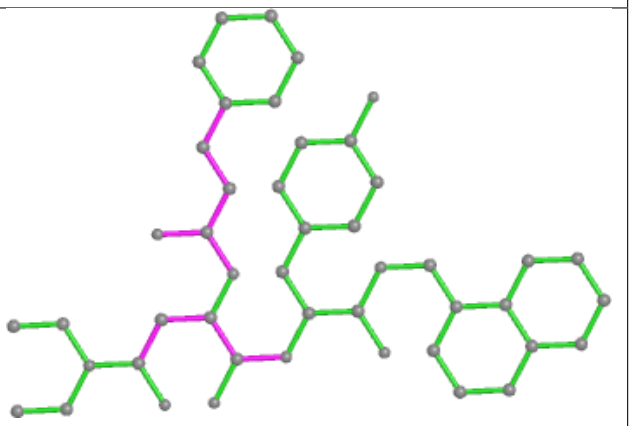
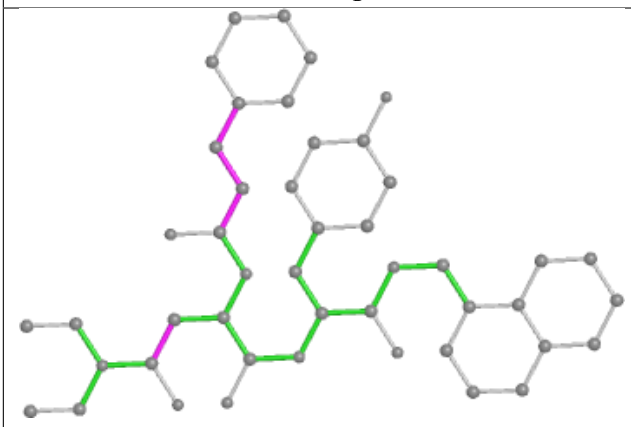


Bond angles



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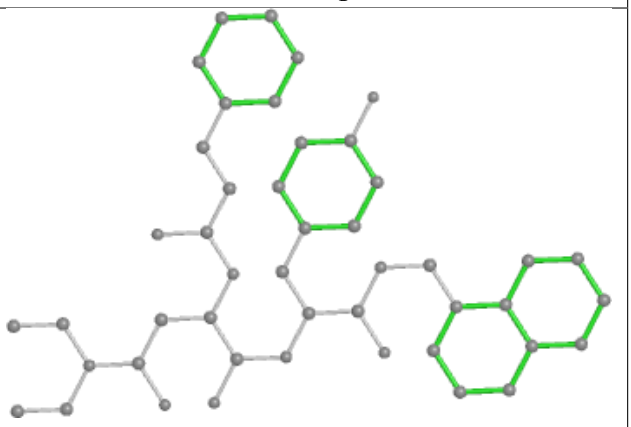
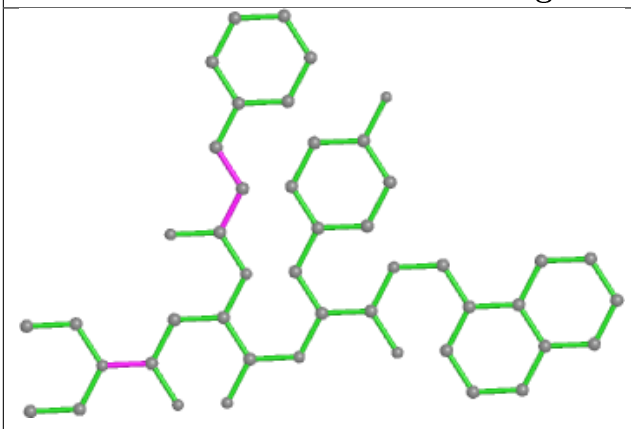
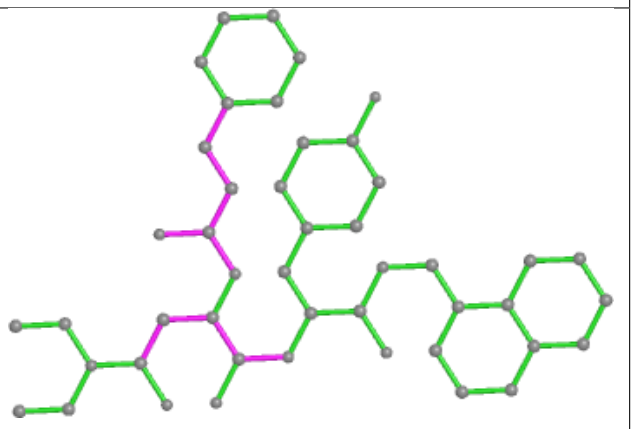


Rings

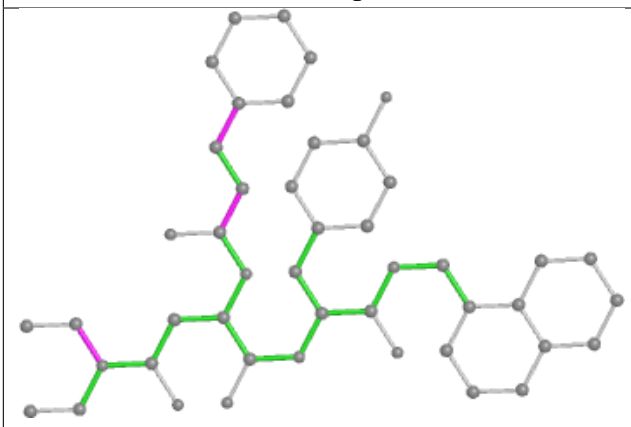
Ligand 7HJ I 301



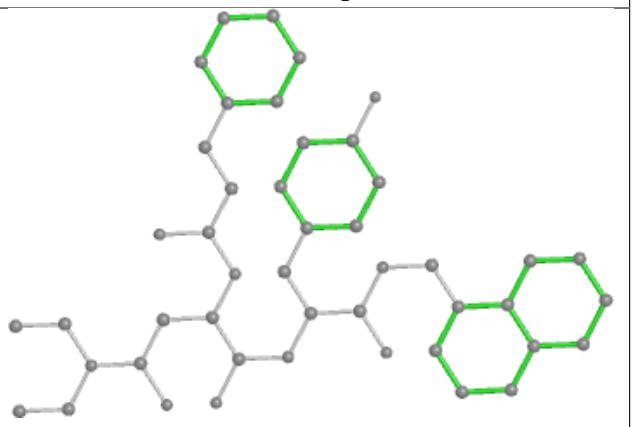
Bond lengths



Bond angles

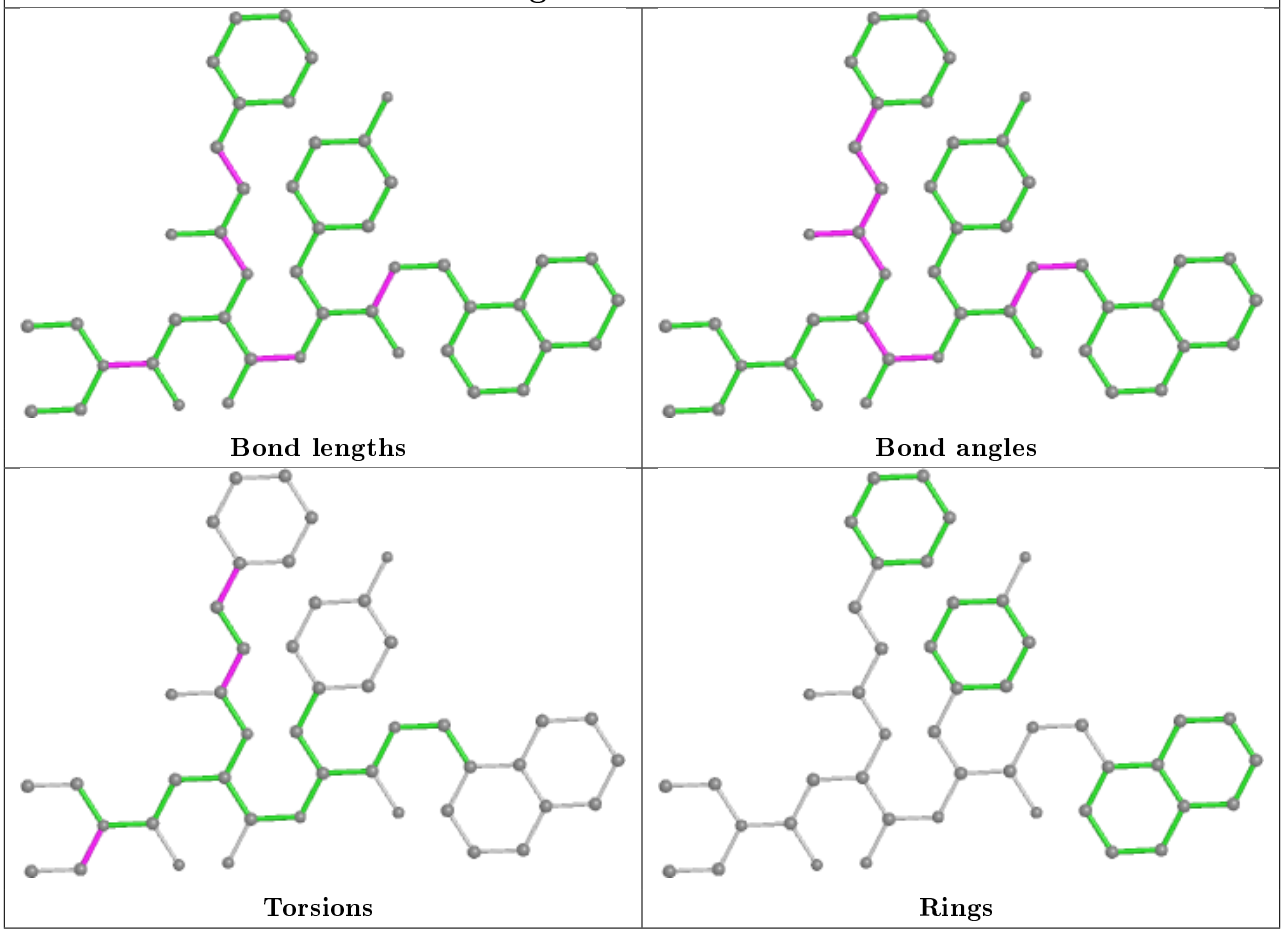


Torsions



Rings

Ligand 7HJ K 301



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.55	1 (0%) 91 88	25, 39, 65, 98	0
1	B	215/240 (89%)	-0.04	9 (4%) 36 26	30, 58, 99, 159	0
1	C	216/240 (90%)	-0.19	4 (1%) 66 59	27, 54, 93, 111	0
1	D	223/240 (92%)	-0.41	1 (0%) 92 91	25, 45, 82, 117	0
1	E	218/240 (90%)	-0.60	0 100 100	24, 38, 68, 103	0
1	F	215/240 (89%)	-0.18	2 (0%) 84 80	27, 57, 117, 144	0
1	G	216/240 (90%)	-0.45	0 100 100	23, 42, 76, 91	0
1	O	218/240 (90%)	-0.43	1 (0%) 91 88	22, 44, 83, 117	0
1	P	219/240 (91%)	-0.49	1 (0%) 91 88	25, 43, 79, 107	0
1	Q	217/240 (90%)	-0.38	1 (0%) 91 88	25, 48, 87, 114	0
1	R	215/240 (89%)	-0.50	0 100 100	24, 41, 72, 88	0
1	S	218/240 (90%)	-0.60	0 100 100	22, 36, 66, 107	0
1	T	217/240 (90%)	-0.48	2 (0%) 84 80	23, 35, 70, 134	0
1	U	216/240 (90%)	-0.44	2 (0%) 84 80	23, 38, 73, 91	0
2	H	222/240 (92%)	-0.48	0 100 100	23, 33, 56, 78	0
2	I	222/240 (92%)	-0.60	0 100 100	23, 33, 52, 72	0
2	J	222/240 (92%)	-0.64	0 100 100	25, 35, 55, 74	0
2	K	223/240 (92%)	-0.69	0 100 100	22, 32, 52, 66	0
2	L	223/240 (92%)	-0.66	0 100 100	20, 30, 50, 74	0
2	M	222/240 (92%)	-0.62	0 100 100	22, 32, 53, 82	0
2	N	223/240 (92%)	-0.60	0 100 100	24, 35, 62, 84	0
2	V	223/240 (92%)	-0.63	0 100 100	21, 29, 48, 69	0
2	W	223/240 (92%)	-0.66	0 100 100	23, 32, 56, 68	0
2	X	222/240 (92%)	-0.65	0 100 100	24, 33, 54, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
2	Y	223/240 (92%)	-0.65	0	100	100	20, 32, 53, 85	0
2	Z	222/240 (92%)	-0.65	0	100	100	22, 34, 55, 70	0
2	a	223/240 (92%)	-0.68	0	100	100	22, 31, 53, 68	0
2	b	223/240 (92%)	-0.60	0	100	100	21, 30, 52, 77	0
All	All	6157/6720 (91%)	-0.52	24 (0%)	92	91	20, 36, 76, 159	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	9	MET	4.0
1	F	205	VAL	3.8
1	F	169	GLU	3.8
1	B	234	LEU	3.7
1	T	9	MET	3.6
1	B	231	GLN	3.1
1	U	203	LEU	2.8
1	D	170	SER	2.7
1	B	203	LEU	2.7
1	T	202	THR	2.7
1	A	9	MET	2.5
1	B	9	MET	2.5
1	C	203	LEU	2.5
1	B	11	GLN	2.3
1	B	171	TYR	2.3
1	Q	133	THR	2.2
1	P	9	MET	2.2
1	B	188	LEU	2.2
1	C	182	ARG	2.2
1	C	9	MET	2.2
1	B	179	ASP	2.1
1	U	9	MET	2.1
1	B	186	ALA	2.1
1	C	169	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

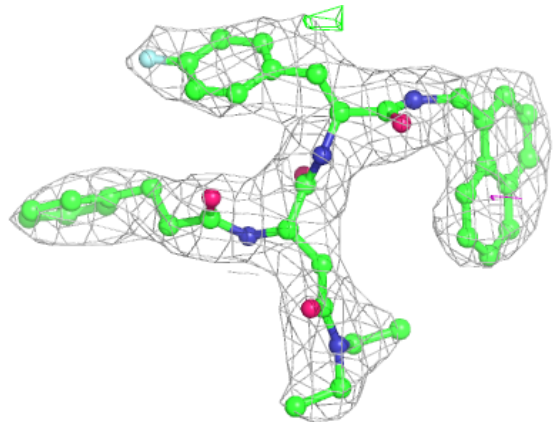
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

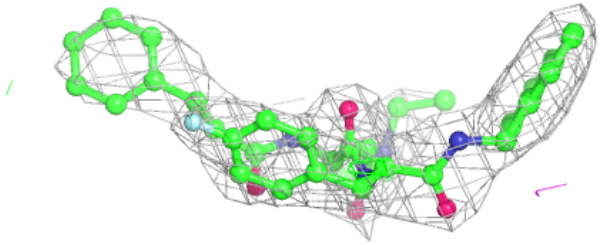
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	7HJ	X	301	46/46	0.95	0.15	29,43,61,64	0
3	7HJ	Z	301	46/46	0.95	0.17	21,34,44,49	0
3	7HJ	Y	301	46/46	0.95	0.15	20,36,49,57	0
3	7HJ	W	301	46/46	0.95	0.16	20,33,49,51	0
3	7HJ	L	301	46/46	0.95	0.17	24,40,54,57	0
3	7HJ	M	301	46/46	0.95	0.17	25,39,55,68	0
3	7HJ	H	301	46/46	0.95	0.17	22,41,53,62	0
3	7HJ	I	301	46/46	0.95	0.15	29,39,50,65	0
3	7HJ	a	301	46/46	0.96	0.15	21,34,44,51	0
3	7HJ	b	301	46/46	0.96	0.15	22,34,42,53	0
3	7HJ	J	301	46/46	0.96	0.17	23,36,45,55	0
3	7HJ	N	301	46/46	0.96	0.15	21,34,45,49	0
3	7HJ	K	301	46/46	0.96	0.15	24,33,47,53	0
3	7HJ	V	301	46/46	0.97	0.14	19,31,46,53	0

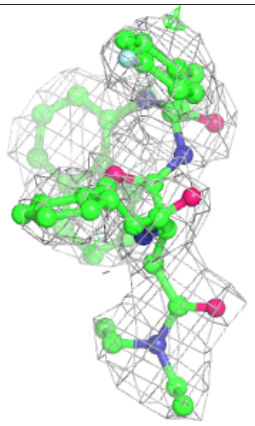
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 7HJ 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)

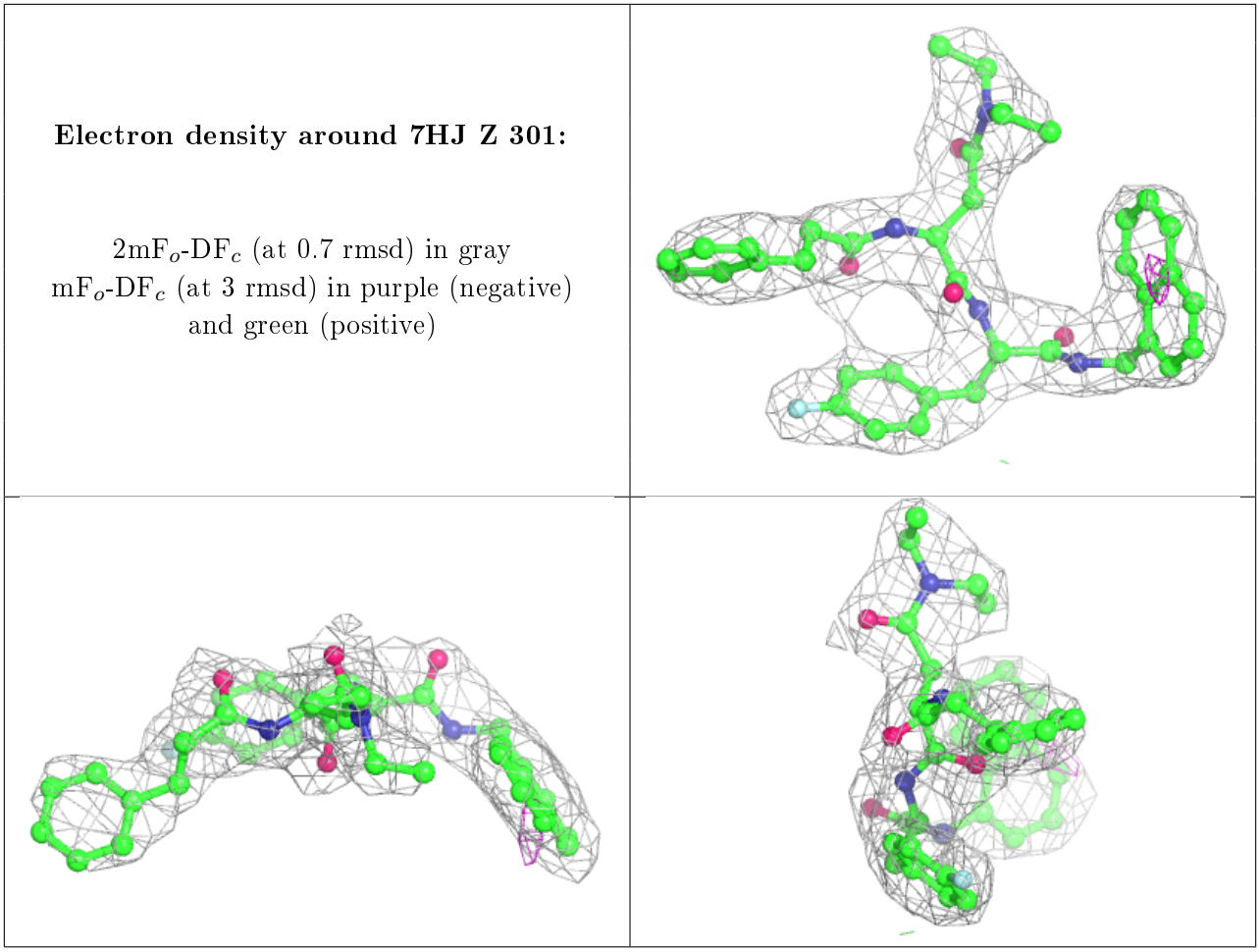






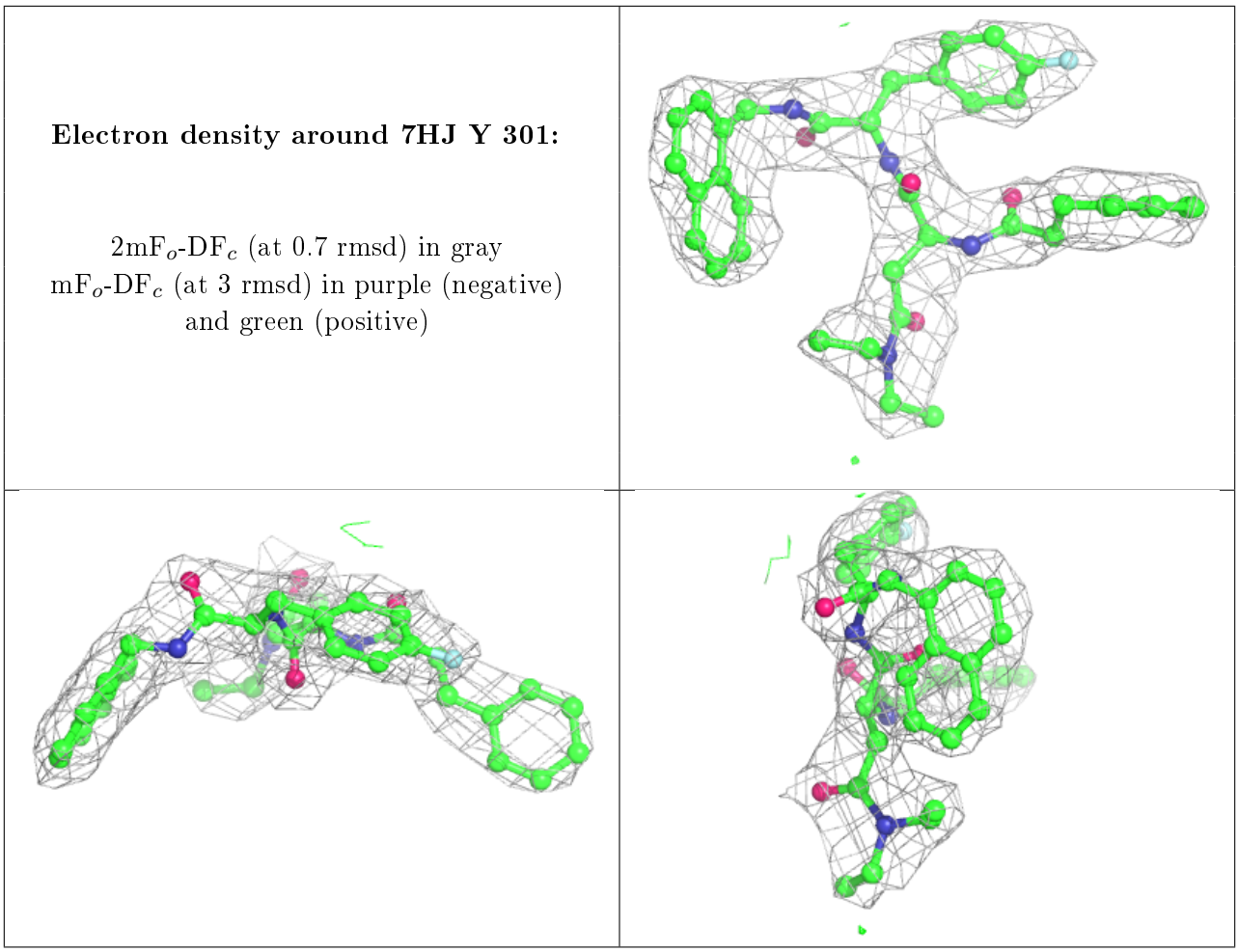
Electron density around 7HJ Z 301:

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



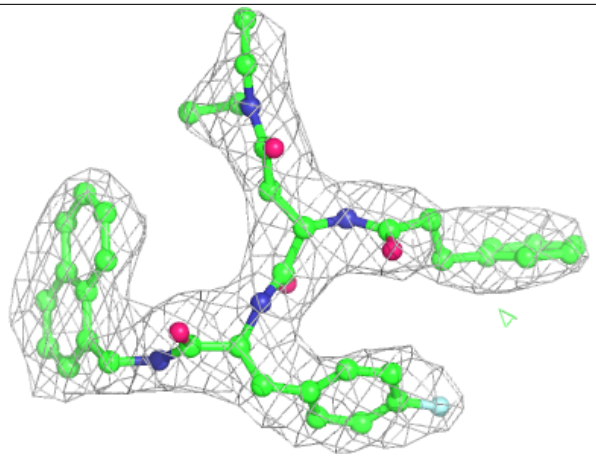
Electron density around 7HJ Y 301:

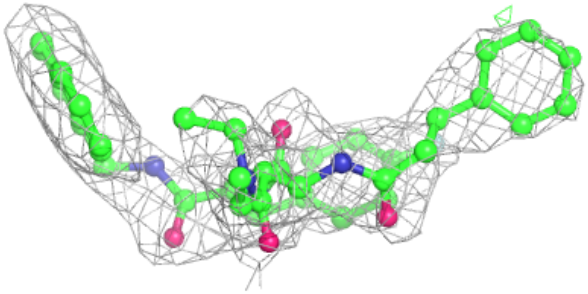
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

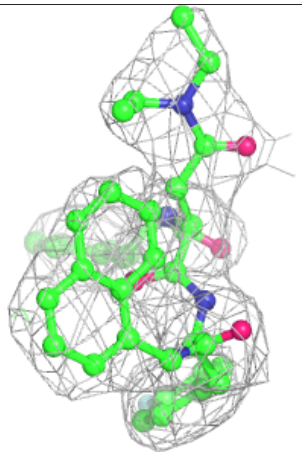


Electron density around 7HJ W 301:

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

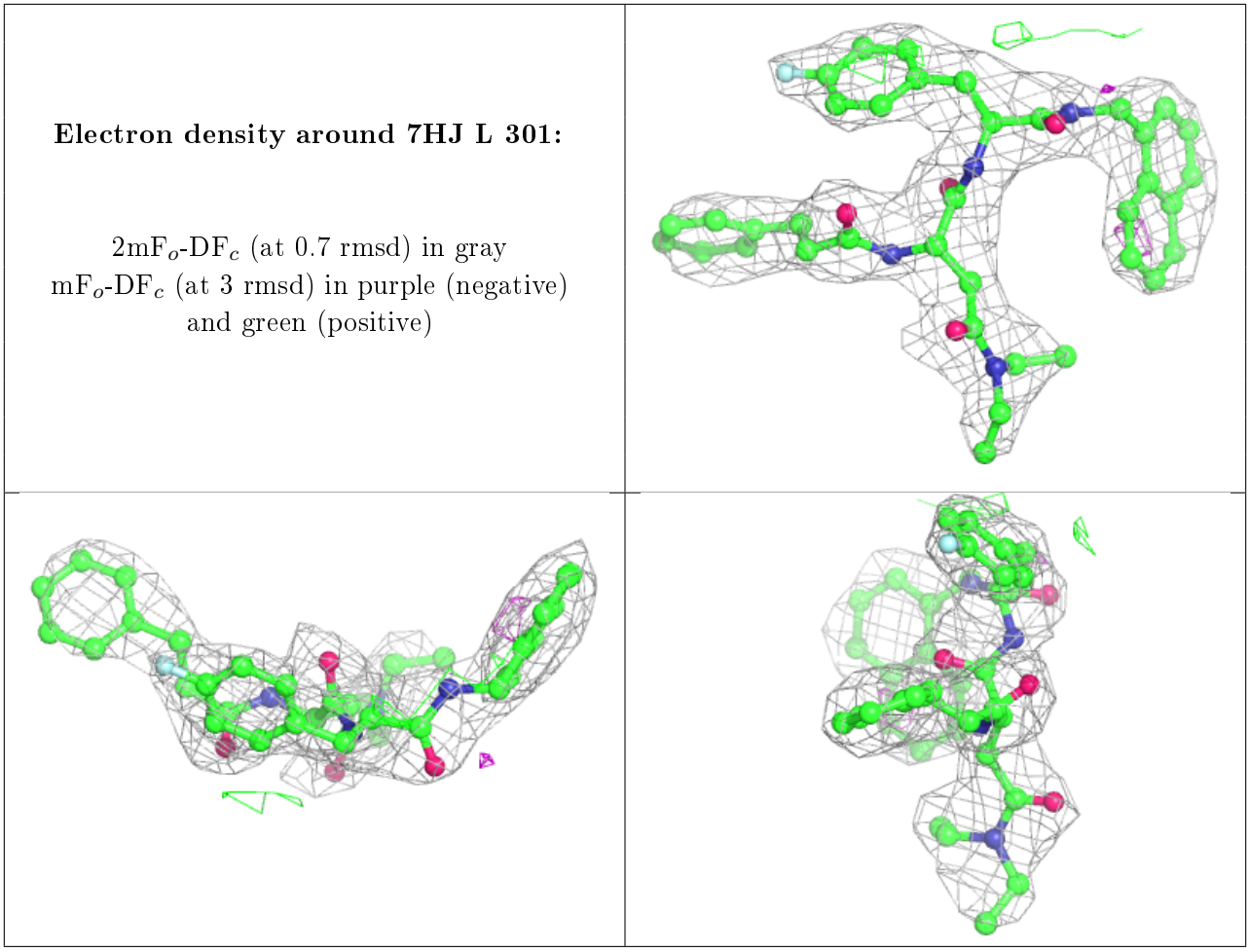






Electron density around 7HJ L 301:

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



Electron density around 7HJ M 301:

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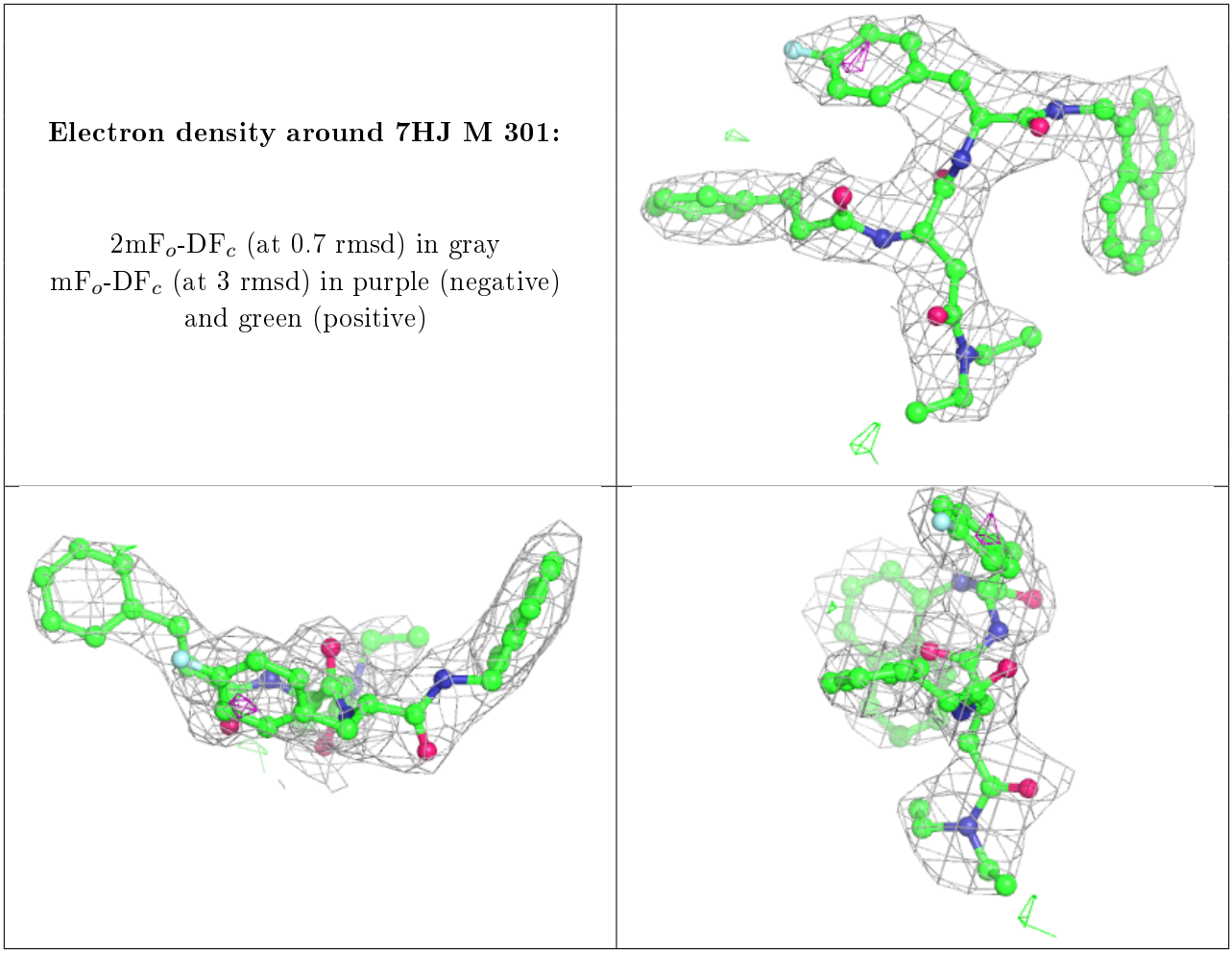
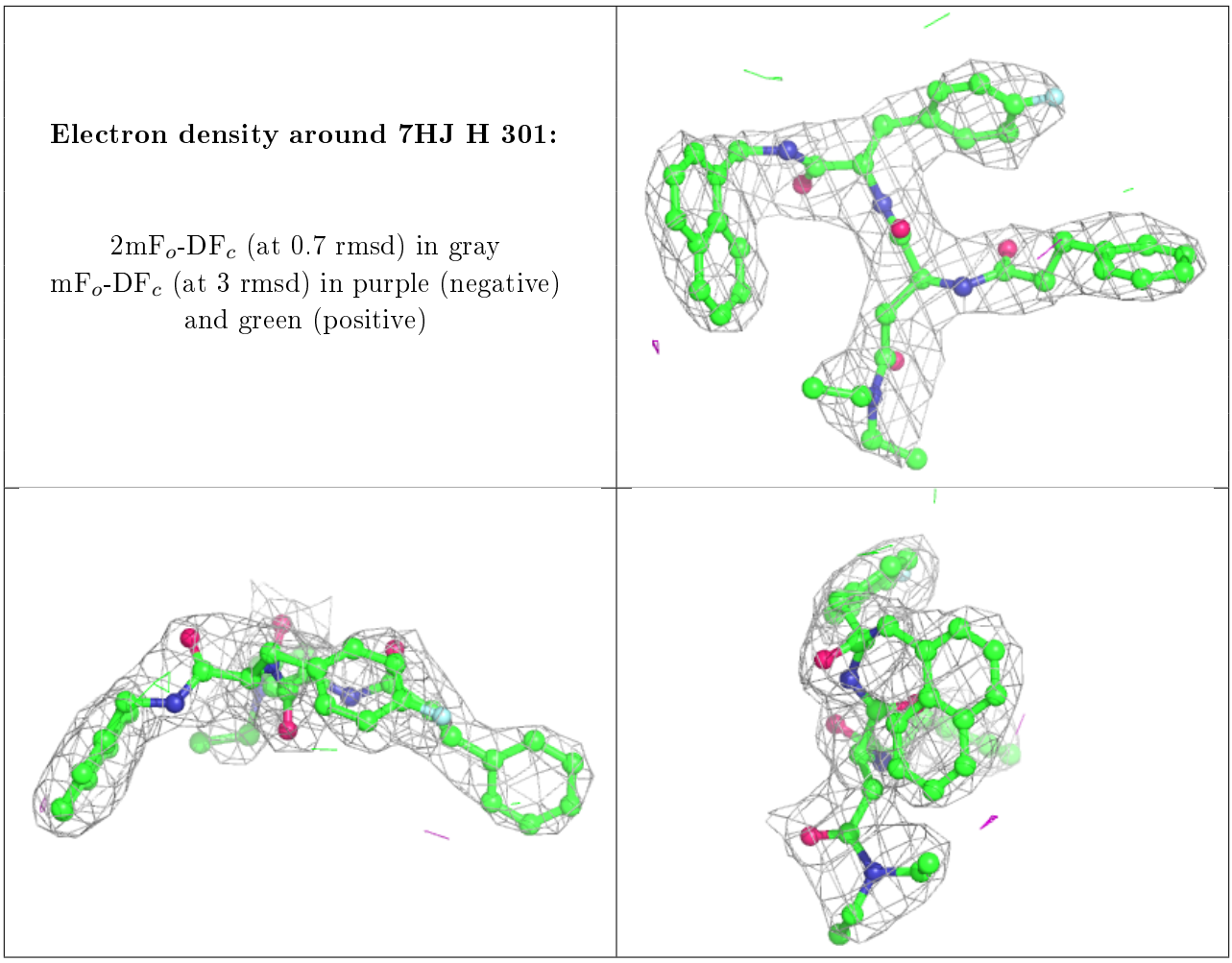
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



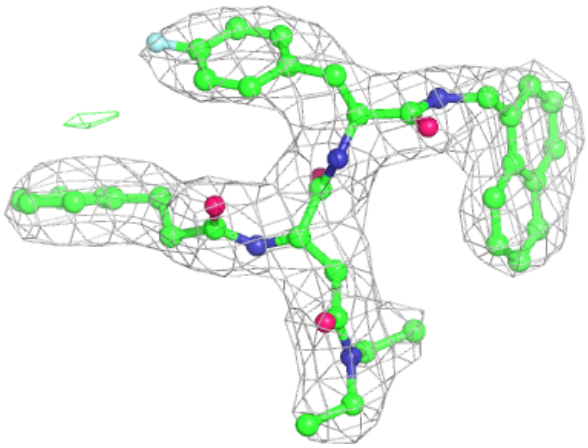
Electron density around 7HJ H 301:

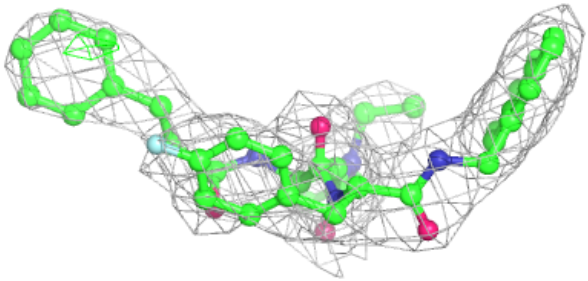
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around 7HJ I 301:

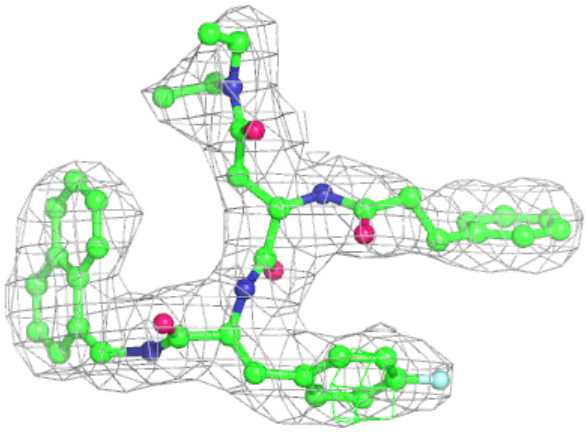
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

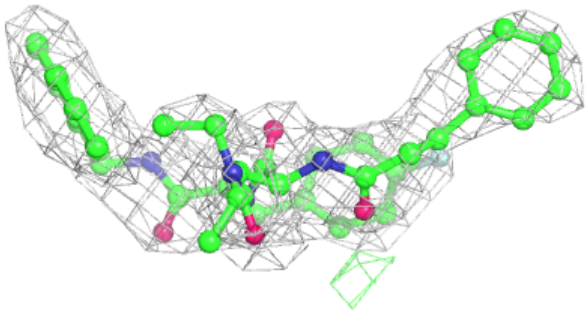


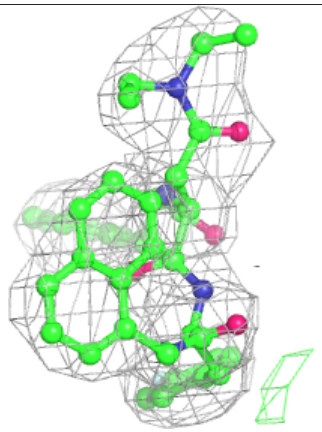


Electron density around 7HJ a 301:

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

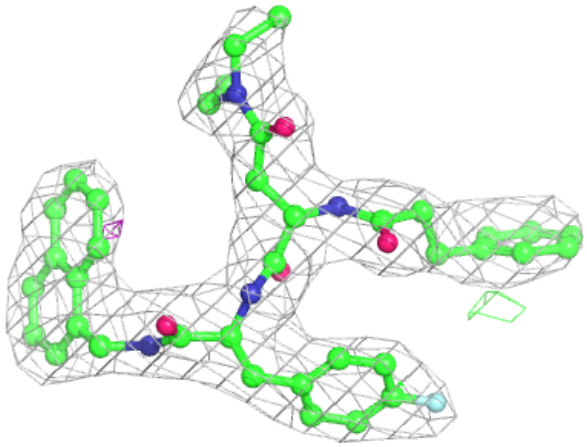


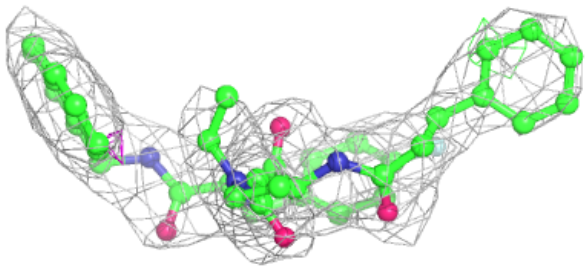


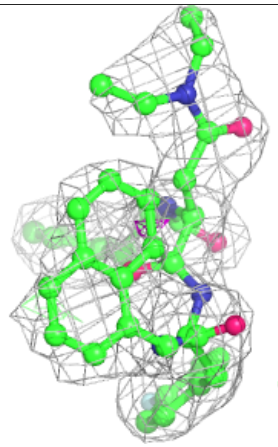


Electron density around 7HJ b 301:

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

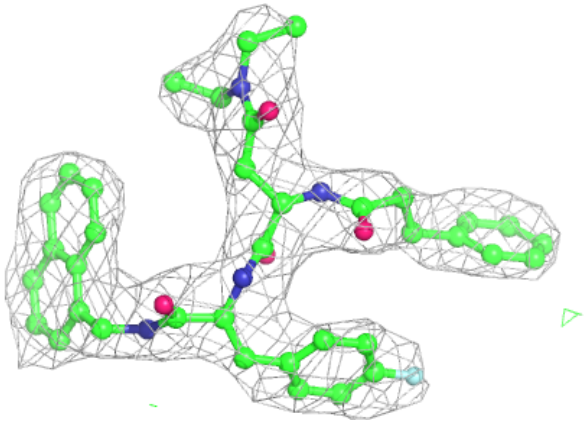


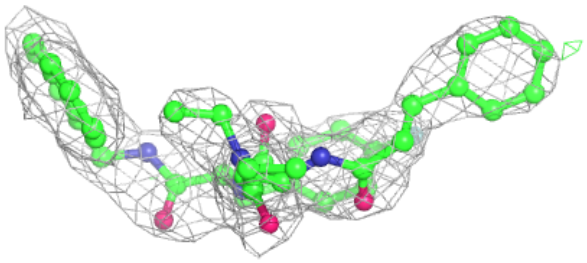


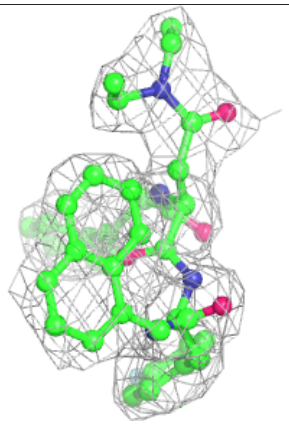


Electron density around 7HJ J 301:

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

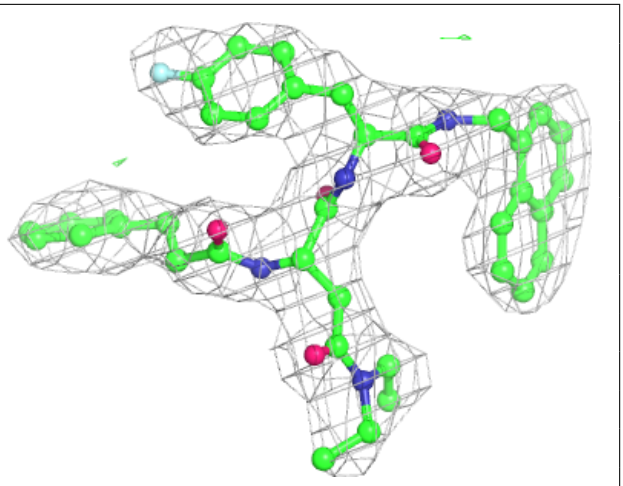


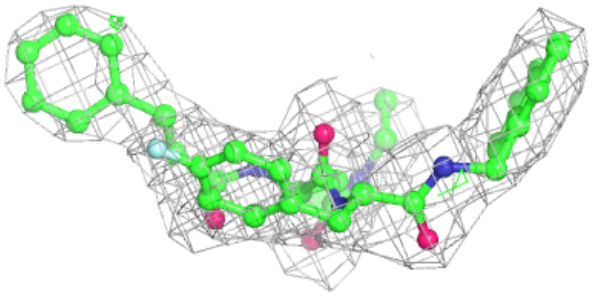


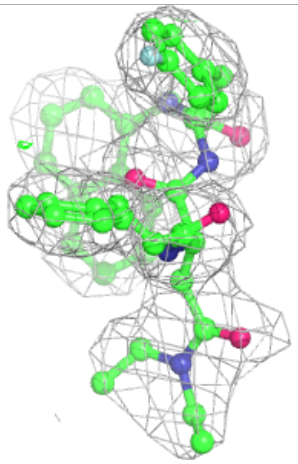


Electron density around 7HJ N 301:

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

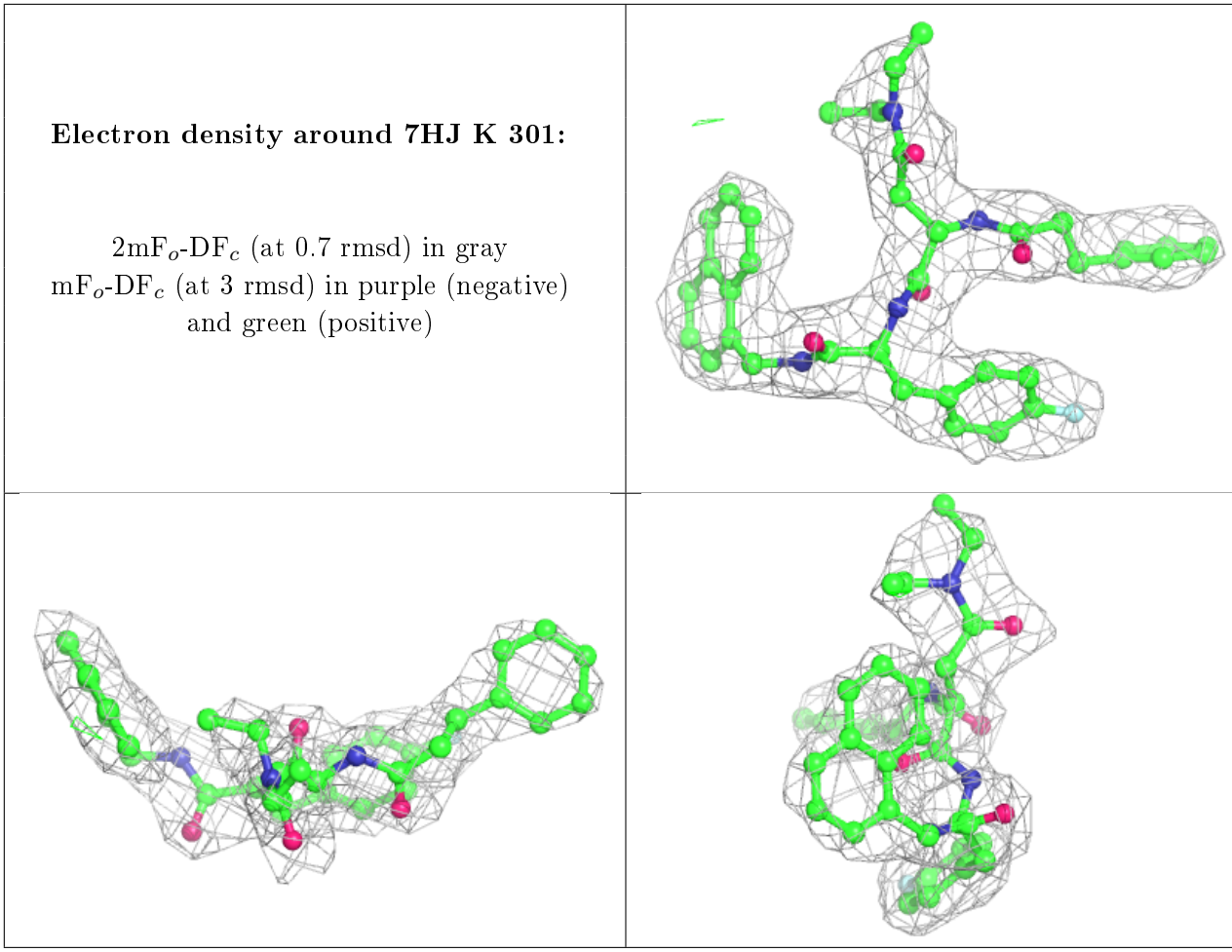






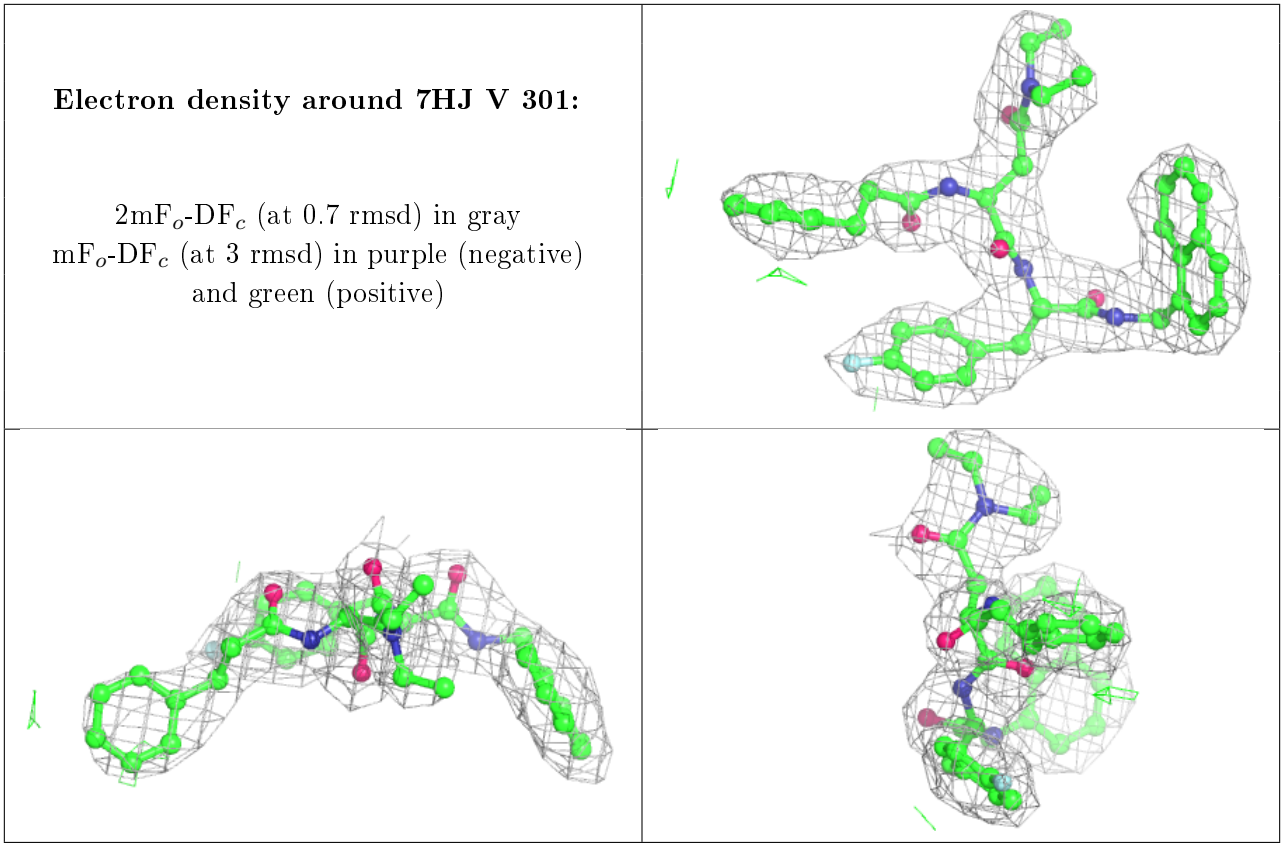
Electron density around 7HJ K 301:

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



Electron density around 7HJ V 301:

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



6.5 Other polymers (i)

There are no such residues in this entry.