



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 12:16 am BST

PDB ID : 3MY0  
Title : Crystal structure of the ACVRL1 (ALK1) kinase domain bound to LDN-193189  
Authors : Chaikuad, A.; Alfano, I.; Cooper, C.; Mahajan, P.; Daga, N.; Sanvitale, C.; Fedorov, O.; Petrie, K.; Savitsky, P.; Gileadi, O.; Sethi, R.; Krojer, T.; Muniz, J.R.C.; Pike, A.C.W.; Vollmar, M.; Carpenter, C.P.; Ugochukwu, E.; Knapp, S.; von Delft, F.; Weigelt, J.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Bullock, A.; Structural Genomics Consortium (SGC)  
Deposited on : 2010-05-08  
Resolution : 2.65 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

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

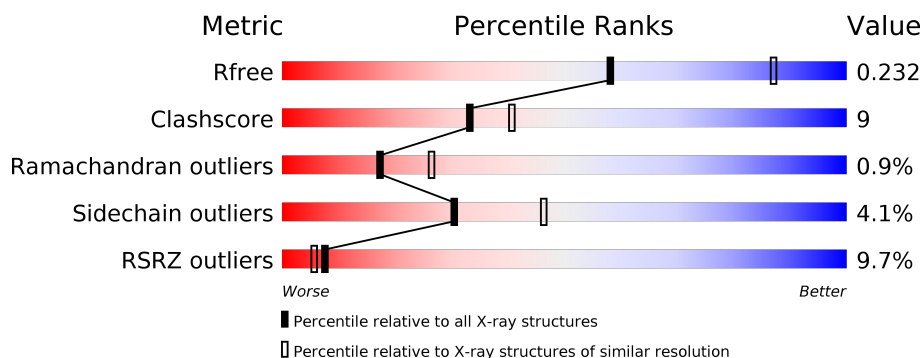
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	305	<div> <div>80%</div> <div>16%</div> <div>••</div> </div>
1	B	305	<div> <div>2%</div> <div>77%</div> <div>18%</div> <div>••</div> </div>
1	C	305	<div> <div>%</div> <div>83%</div> <div>14%</div> <div>••</div> </div>
1	D	305	<div> <div>84%</div> <div>12%</div> <div>••</div> </div>
1	E	305	<div> <div>%</div> <div>77%</div> <div>19%</div> <div>••</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	305	
1	G	305	
1	H	305	
1	I	305	
1	J	305	
1	K	305	
1	L	305	
1	M	305	
1	N	305	
1	O	305	
1	P	305	
1	Q	305	
1	R	305	
1	S	305	
1	T	305	
1	U	305	
1	V	305	
1	W	305	
1	X	305	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LDN	X	600	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 53931 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 Serine/threonine-protein kinase receptor R3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2295	1461	403	418	13			
1	B	295	Total	C	N	O	S	0	0	0
			2303	1470	402	418	13			
1	C	299	Total	C	N	O	S	0	0	0
			2285	1457	401	414	13			
1	D	298	Total	C	N	O	S	0	0	0
			2284	1454	396	421	13			
1	E	294	Total	C	N	O	S	0	0	0
			2251	1446	390	403	12			
1	F	294	Total	C	N	O	S	0	0	0
			2239	1430	396	401	12			
1	G	294	Total	C	N	O	S	0	0	0
			2269	1455	388	413	13			
1	H	294	Total	C	N	O	S	0	0	0
			2233	1428	390	402	13			
1	I	293	Total	C	N	O	S	0	0	0
			2286	1463	399	411	13			
1	J	252	Total	C	N	O	S	0	0	0
			1898	1215	329	342	12			
1	K	261	Total	C	N	O	S	0	0	0
			1937	1241	336	348	12			
1	L	296	Total	C	N	O	S	0	0	0
			2312	1474	406	419	13			
1	M	298	Total	C	N	O	S	0	0	0
			2325	1485	405	422	13			
1	N	300	Total	C	N	O	S	0	0	0
			2295	1464	402	416	13			
1	O	297	Total	C	N	O	S	0	0	0
			2279	1451	398	417	13			
1	P	290	Total	C	N	O	S	0	0	0
			2103	1337	370	385	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	294	Total	C	N	O	S	0	0	0
			2262	1447	399	404	12			
1	R	294	Total	C	N	O	S	0	0	0
			2258	1449	387	409	13			
1	S	294	Total	C	N	O	S	0	0	0
			2236	1430	391	402	13			
1	T	292	Total	C	N	O	S	0	0	0
			2256	1443	391	409	13			
1	U	285	Total	C	N	O	S	0	0	0
			2154	1378	377	386	13			
1	V	282	Total	C	N	O	S	0	0	0
			2122	1358	370	381	13			
1	W	281	Total	C	N	O	S	0	0	0
			2211	1414	386	398	13			
1	X	257	Total	C	N	O	S	0	0	0
			1968	1266	337	354	11			

There are 48 discrepancies between the modelled and reference sequences:

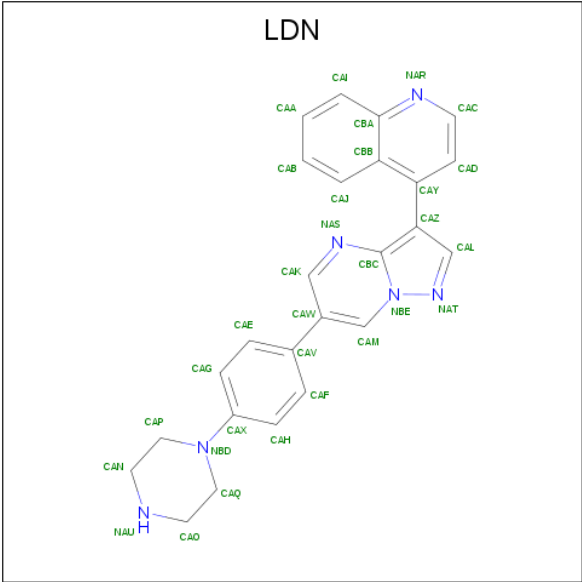
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	EXPRESSION TAG	UNP P37023
A	0	MET	-	EXPRESSION TAG	UNP P37023
B	-1	SER	-	EXPRESSION TAG	UNP P37023
B	0	MET	-	EXPRESSION TAG	UNP P37023
C	-1	SER	-	EXPRESSION TAG	UNP P37023
C	0	MET	-	EXPRESSION TAG	UNP P37023
D	-1	SER	-	EXPRESSION TAG	UNP P37023
D	0	MET	-	EXPRESSION TAG	UNP P37023
E	-1	SER	-	EXPRESSION TAG	UNP P37023
E	0	MET	-	EXPRESSION TAG	UNP P37023
F	-1	SER	-	EXPRESSION TAG	UNP P37023
F	0	MET	-	EXPRESSION TAG	UNP P37023
G	-1	SER	-	EXPRESSION TAG	UNP P37023
G	0	MET	-	EXPRESSION TAG	UNP P37023
H	-1	SER	-	EXPRESSION TAG	UNP P37023
H	0	MET	-	EXPRESSION TAG	UNP P37023
I	-1	SER	-	EXPRESSION TAG	UNP P37023
I	0	MET	-	EXPRESSION TAG	UNP P37023
J	-1	SER	-	EXPRESSION TAG	UNP P37023
J	0	MET	-	EXPRESSION TAG	UNP P37023
K	-1	SER	-	EXPRESSION TAG	UNP P37023
K	0	MET	-	EXPRESSION TAG	UNP P37023
L	-1	SER	-	EXPRESSION TAG	UNP P37023

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Chain	Residue	Modelled	Actual	Comment	Reference
L	0	MET	-	EXPRESSION TAG	UNP P37023
M	-1	SER	-	EXPRESSION TAG	UNP P37023
M	0	MET	-	EXPRESSION TAG	UNP P37023
N	-1	SER	-	EXPRESSION TAG	UNP P37023
N	0	MET	-	EXPRESSION TAG	UNP P37023
O	-1	SER	-	EXPRESSION TAG	UNP P37023
O	0	MET	-	EXPRESSION TAG	UNP P37023
P	-1	SER	-	EXPRESSION TAG	UNP P37023
P	0	MET	-	EXPRESSION TAG	UNP P37023
Q	-1	SER	-	EXPRESSION TAG	UNP P37023
Q	0	MET	-	EXPRESSION TAG	UNP P37023
R	-1	SER	-	EXPRESSION TAG	UNP P37023
R	0	MET	-	EXPRESSION TAG	UNP P37023
S	-1	SER	-	EXPRESSION TAG	UNP P37023
S	0	MET	-	EXPRESSION TAG	UNP P37023
T	-1	SER	-	EXPRESSION TAG	UNP P37023
T	0	MET	-	EXPRESSION TAG	UNP P37023
U	-1	SER	-	EXPRESSION TAG	UNP P37023
U	0	MET	-	EXPRESSION TAG	UNP P37023
V	-1	SER	-	EXPRESSION TAG	UNP P37023
V	0	MET	-	EXPRESSION TAG	UNP P37023
W	-1	SER	-	EXPRESSION TAG	UNP P37023
W	0	MET	-	EXPRESSION TAG	UNP P37023
X	-1	SER	-	EXPRESSION TAG	UNP P37023
X	0	MET	-	EXPRESSION TAG	UNP P37023

- Molecule 2 is 4-[6-(4-piperazin-1-ylphenyl)pyrazolo[1,5-a]pyrimidin-3-yl]quinoline (three-letter code: LDN) (formula: C<sub>25</sub>H<sub>22</sub>N<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			31	25	6		
2	B	1	Total	C	N	0	0
			31	25	6		
2	C	1	Total	C	N	0	0
			31	25	6		
2	D	1	Total	C	N	0	0
			31	25	6		
2	E	1	Total	C	N	0	0
			31	25	6		
2	F	1	Total	C	N	0	0
			31	25	6		
2	G	1	Total	C	N	0	0
			31	25	6		
2	H	1	Total	C	N	0	0
			31	25	6		
2	I	1	Total	C	N	0	0
			31	25	6		
2	J	1	Total	C	N	0	0
			31	25	6		
2	K	1	Total	C	N	0	0
			31	25	6		
2	L	1	Total	C	N	0	0
			31	25	6		
2	M	1	Total	C	N	0	0
			31	25	6		
2	N	1	Total	C	N	0	0
			31	25	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	O	1	Total	C	N	0	0
			31	25	6		
2	P	1	Total	C	N	0	0
			31	25	6		
2	Q	1	Total	C	N	0	0
			31	25	6		
2	R	1	Total	C	N	0	0
			31	25	6		
2	S	1	Total	C	N	0	0
			31	25	6		
2	T	1	Total	C	N	0	0
			31	25	6		
2	U	1	Total	C	N	0	0
			31	25	6		
2	V	1	Total	C	N	0	0
			31	25	6		
2	W	1	Total	C	N	0	0
			31	25	6		
2	X	1	Total	C	N	0	0
			31	25	6		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	O	0	0
			4	4		
3	B	12	Total	O	0	0
			12	12		
3	C	11	Total	O	0	0
			11	11		
3	D	7	Total	O	0	0
			7	7		
3	E	4	Total	O	0	0
			4	4		
3	F	8	Total	O	0	0
			8	8		
3	G	6	Total	O	0	0
			6	6		
3	H	6	Total	O	0	0
			6	6		
3	I	3	Total	O	0	0
			3	3		

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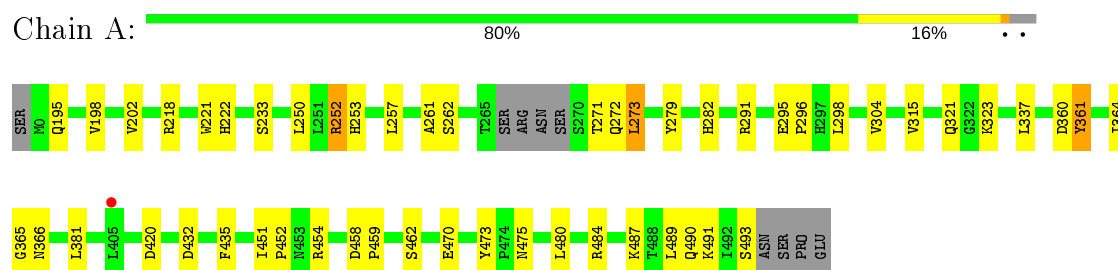
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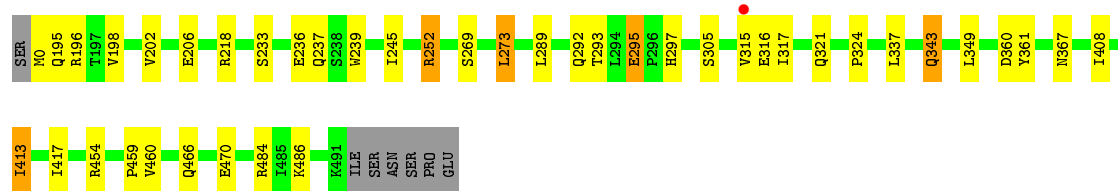
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	2	Total	O	0	0
			2	2		
3	L	6	Total	O	0	0
			6	6		
3	M	1	Total	O	0	0
			1	1		
3	N	6	Total	O	0	0
			6	6		
3	O	2	Total	O	0	0
			2	2		
3	P	4	Total	O	0	0
			4	4		
3	Q	8	Total	O	0	0
			8	8		
3	R	5	Total	O	0	0
			5	5		
3	S	6	Total	O	0	0
			6	6		
3	T	5	Total	O	0	0
			5	5		
3	U	9	Total	O	0	0
			9	9		
3	V	2	Total	O	0	0
			2	2		
3	W	9	Total	O	0	0
			9	9		

### 3 Residue-property plots

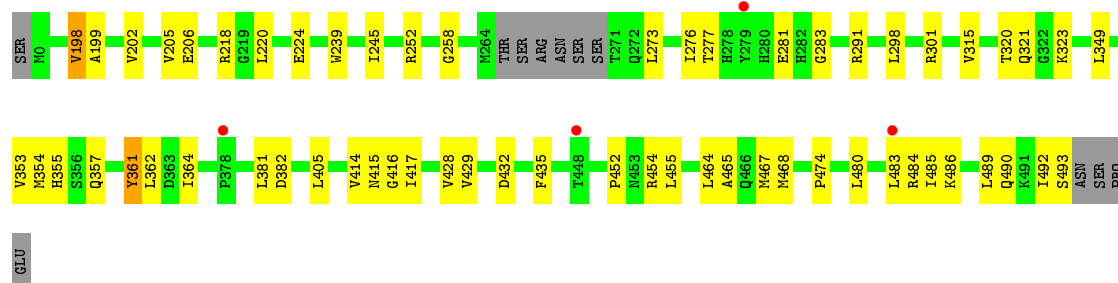
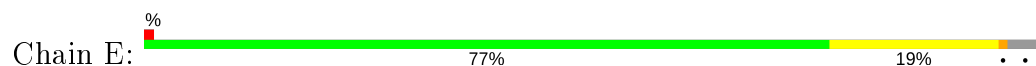
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: Serine/threonine-protein kinase receptor R3

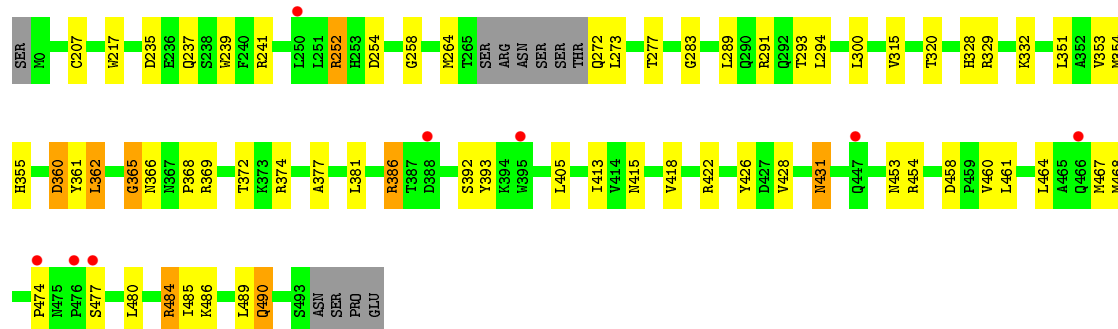




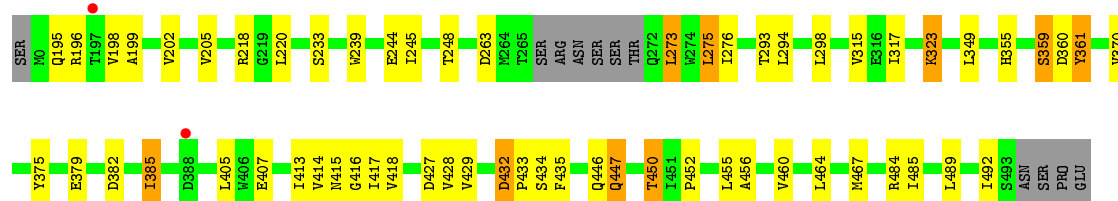
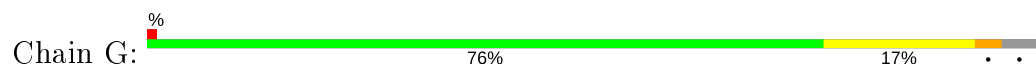
- Molecule 1: Serine/threonine-protein kinase receptor R3



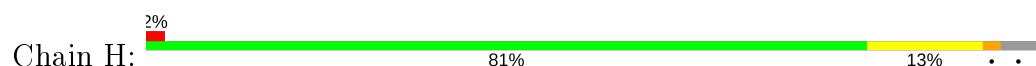
- Molecule 1: Serine/threonine-protein kinase receptor R3

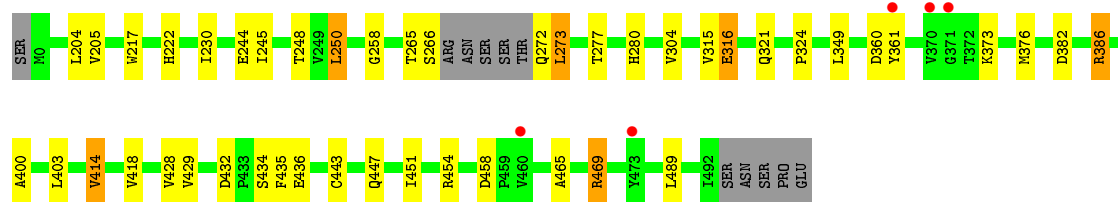


- Molecule 1: Serine/threonine-protein kinase receptor R3



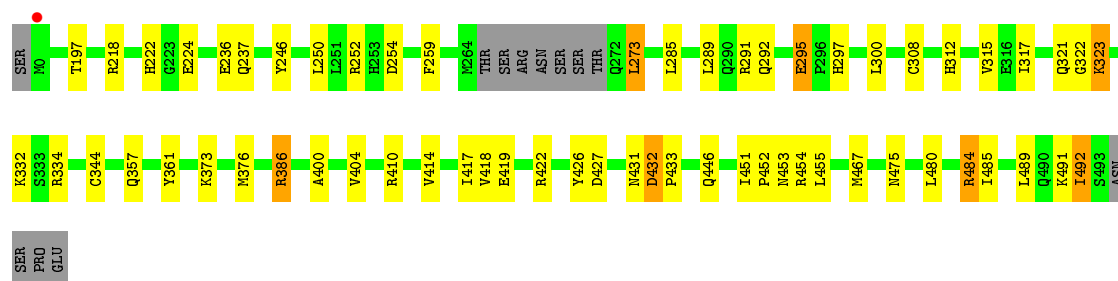
- Molecule 1: Serine/threonine-protein kinase receptor R3





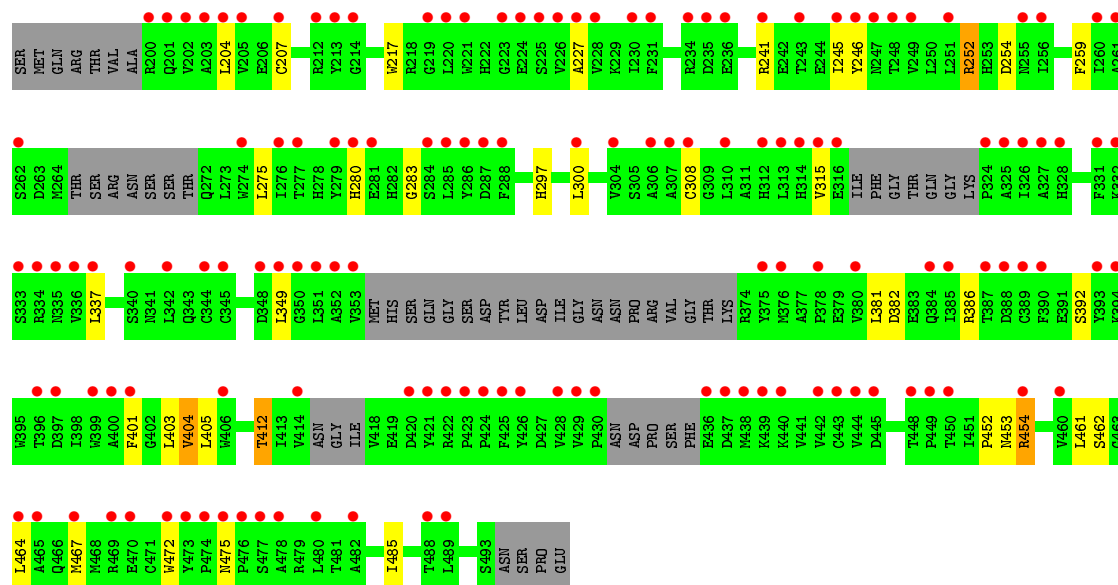
• Molecule 1: Serine/threonine-protein kinase receptor R3

Chain I:



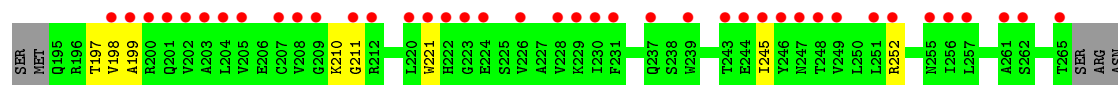
• Molecule 1: Serine/threonine-protein kinase receptor R3

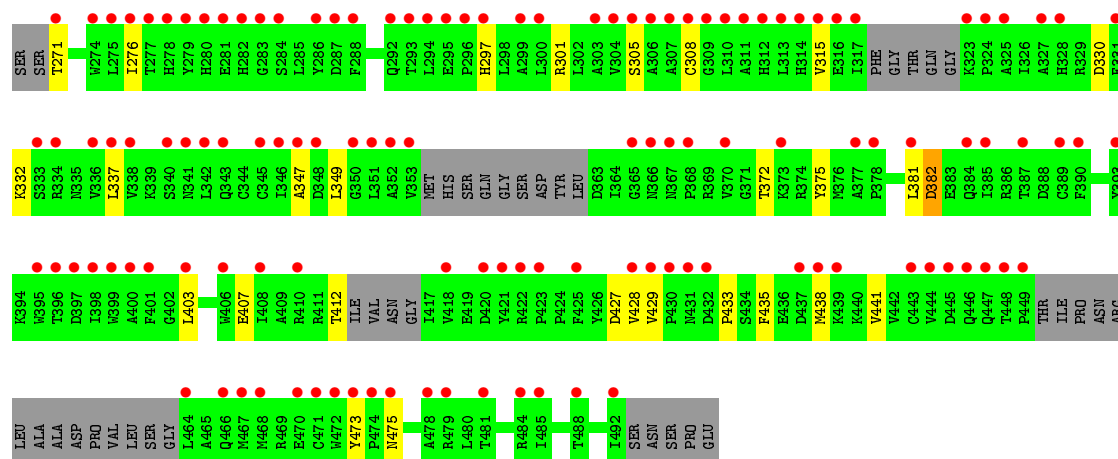
Chain J:



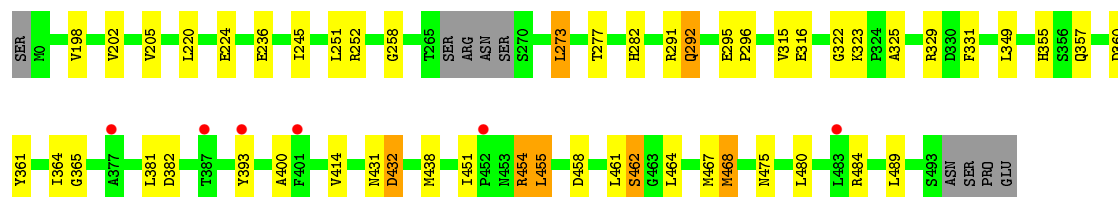
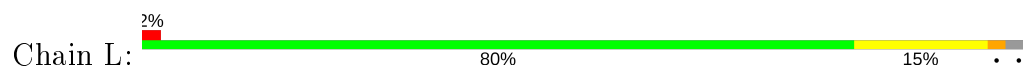
• Molecule 1: Serine/threonine-protein kinase receptor R3

Chain K:

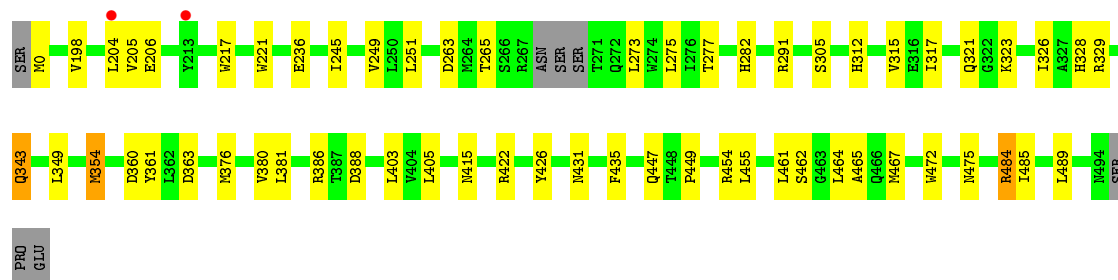
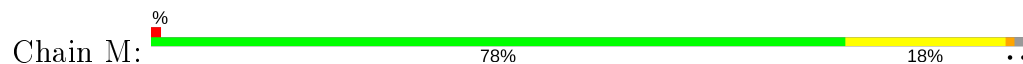




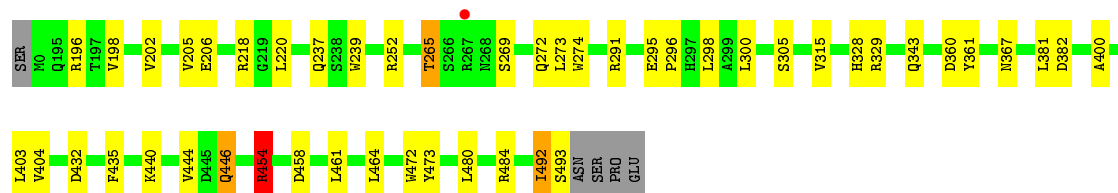
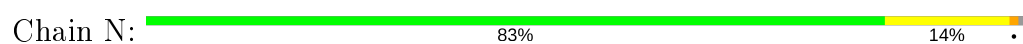
- Molecule 1: Serine/threonine-protein kinase receptor R3



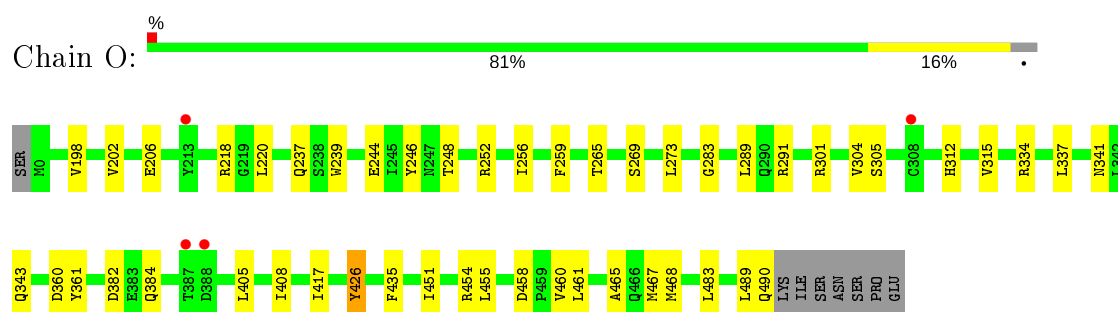
- Molecule 1: Serine/threonine-protein kinase receptor R3



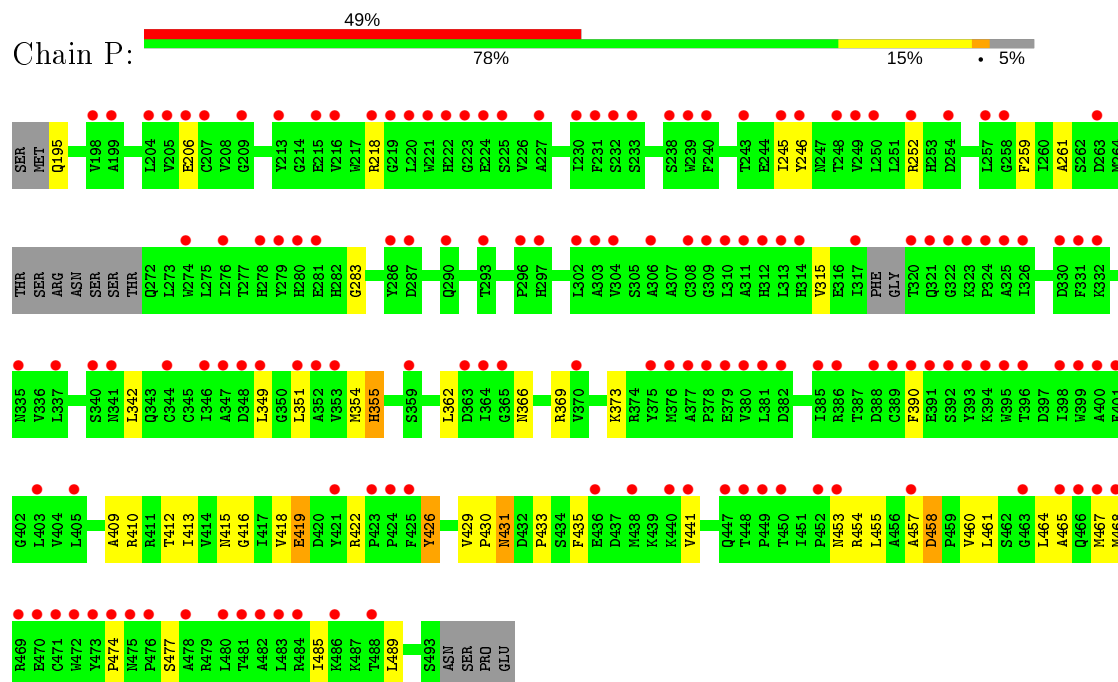
- Molecule 1: Serine/threonine-protein kinase receptor R3



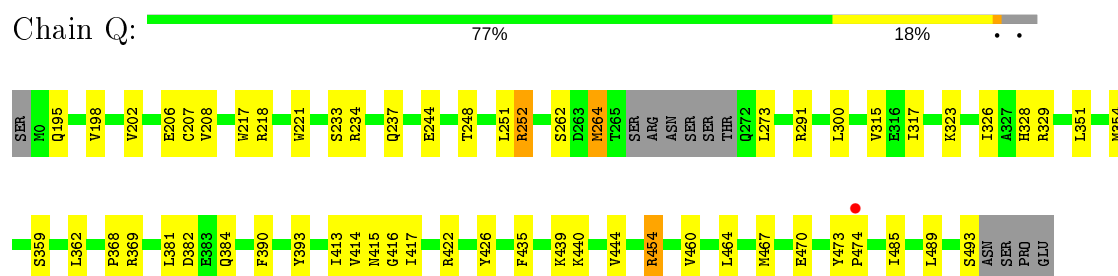
- Molecule 1: Serine/threonine-protein kinase receptor R3



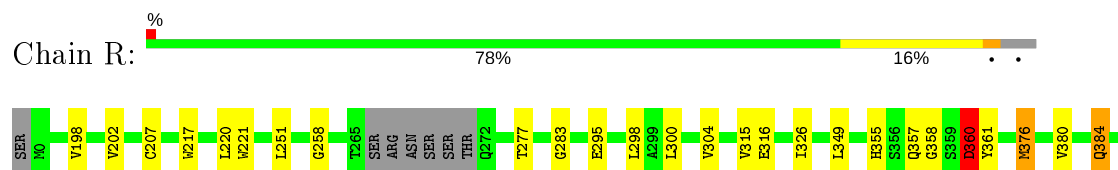
- Molecule 1: Serine/threonine-protein kinase receptor R3

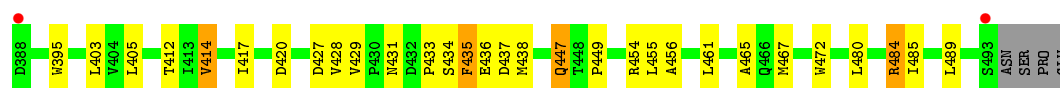


- Molecule 1: Serine/threonine-protein kinase receptor R3

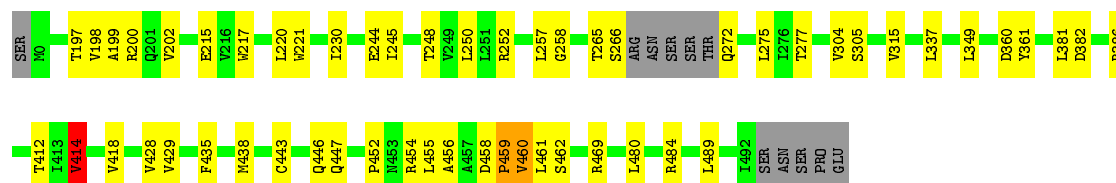


- Molecule 1: Serine/threonine-protein kinase receptor R3

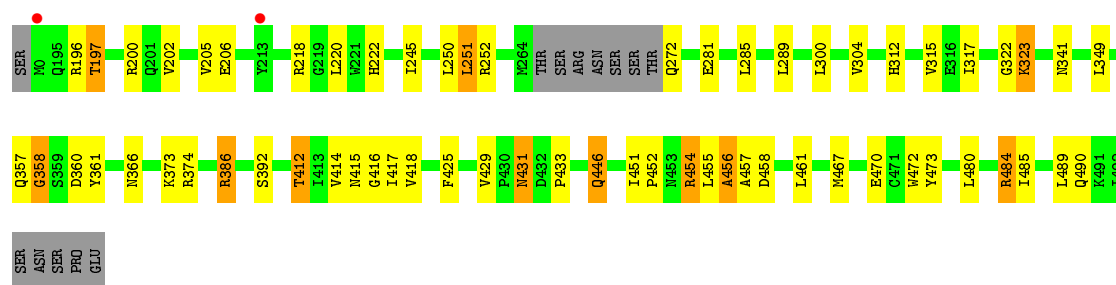
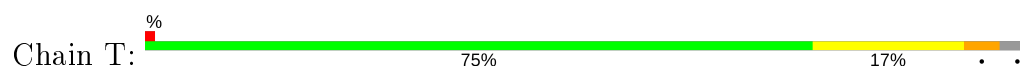




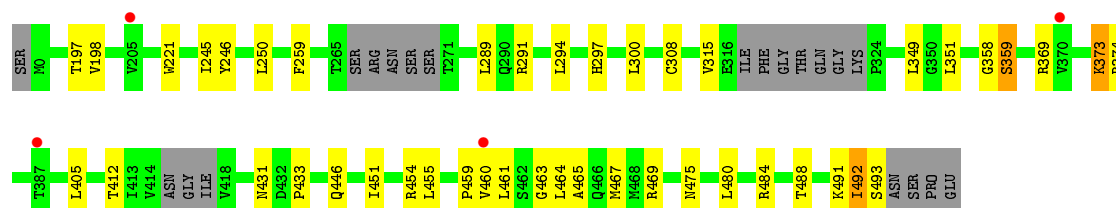
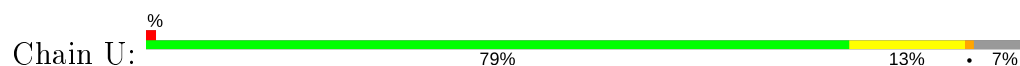
- Molecule 1: Serine/threonine-protein kinase receptor R3



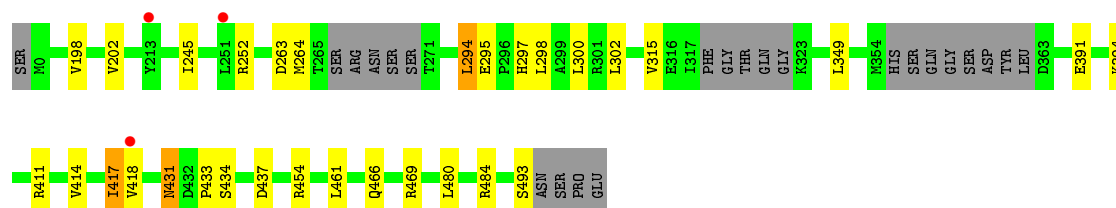
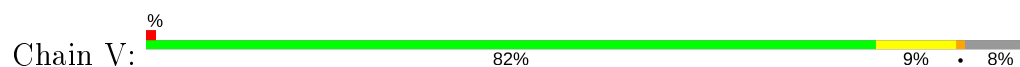
- Molecule 1: Serine/threonine-protein kinase receptor R3



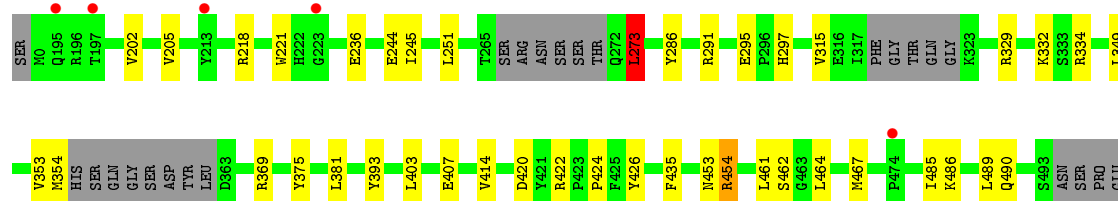
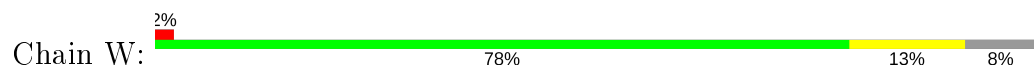
- Molecule 1: Serine/threonine-protein kinase receptor R3



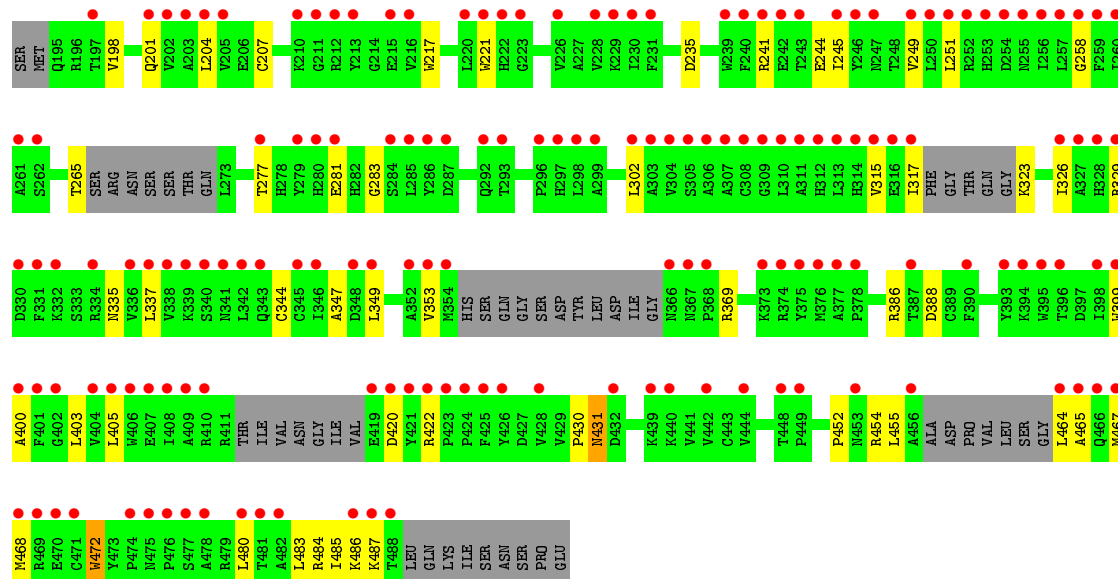
- Molecule 1: Serine/threonine-protein kinase receptor R3



- Molecule 1: Serine/threonine-protein kinase receptor R3



- Molecule 1: Serine/threonine-protein kinase receptor R3





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.77Å 118.77Å 510.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	58.99 – 2.65 58.99 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.7 (58.99-2.65) 99.8 (58.99-2.65)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.96 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.6.0066	Depositor
R, $R_{free}$	0.207 , 0.247 0.208 , 0.232	Depositor DCC
$R_{free}$ test set	11716 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.8	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 7.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.457 for -h,-k,l 0.316 for h,-h-k,-l 0.315 for -k,-h,-l	Xtriage
Reported twinning fraction	0.357 for H, K, L 0.147 for h+k,-k,-l 0.352 for -h,-k,l 0.145 for h,-h-k,-l	Depositor
Outliers	0 of 233740 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	53931	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.52 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.7713e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LDN

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	0.57	2/2352 (0.1%)	0.66	0/3204
1	B	0.57	0/2359	0.70	1/3212 (0.0%)
1	C	0.55	0/2342	0.67	0/3195
1	D	0.58	0/2340	0.67	0/3192
1	E	0.59	0/2308	0.70	1/3150 (0.0%)
1	F	0.52	0/2296	0.64	2/3133 (0.1%)
1	G	0.67	0/2326	0.72	1/3173 (0.0%)
1	H	0.57	0/2289	0.68	0/3124
1	I	0.69	2/2343 (0.1%)	0.73	1/3191 (0.0%)
1	J	0.39	0/1942	0.54	0/2645
1	K	0.39	0/1984	0.55	0/2709
1	L	0.57	0/2369	0.66	0/3226
1	M	0.61	0/2381	0.70	0/3243
1	N	0.63	0/2352	0.69	0/3209
1	O	0.55	0/2335	0.65	0/3185
1	P	0.43	0/2150	0.56	0/2942
1	Q	0.57	0/2319	0.69	0/3160
1	R	0.55	0/2315	0.67	1/3160 (0.0%)
1	S	0.60	0/2292	0.68	1/3128 (0.0%)
1	T	0.53	0/2311	0.64	1/3149 (0.0%)
1	U	0.57	1/2206 (0.0%)	0.62	0/3009
1	V	0.56	0/2174	0.62	0/2969
1	W	0.59	0/2263	0.67	1/3079 (0.0%)
1	X	0.39	0/2014	0.53	0/2743
All	All	0.56	5/54362 (0.0%)	0.66	10/74130 (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	B	0	1
1	C	0	1
1	H	0	1
1	R	0	1
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	282	HIS	CG-CD2	6.62	1.47	1.35
1	U	308	CYS	CB-SG	6.13	1.92	1.82
1	I	308	CYS	CB-SG	-6.00	1.72	1.81
1	I	344	CYS	CB-SG	-5.45	1.73	1.81
1	A	282	HIS	CE1-NE2	5.33	1.45	1.32

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	386	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	S	220	LEU	CA-CB-CG	6.52	130.30	115.30
1	E	301	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	R	220	LEU	CA-CB-CG	6.07	129.26	115.30
1	I	386	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	W	273	LEU	CA-CB-CG	5.60	128.19	115.30
1	F	254	ASP	CB-CG-OD1	5.35	123.11	118.30
1	G	275	LEU	CA-CB-CG	5.28	127.44	115.30
1	F	254	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	T	251	LEU	CA-CB-CG	5.07	126.96	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	320	THR	Peptide
1	C	490	GLN	Peptide
1	H	280	HIS	Sidechain
1	R	360	ASP	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2295	0	2191	29	0
1	B	2303	0	2224	53	1
1	C	2285	0	2171	36	0
1	D	2284	0	2161	34	0
1	E	2251	0	2153	42	1
1	F	2239	0	2112	45	0
1	G	2269	0	2174	47	1
1	H	2233	0	2106	31	1
1	I	2286	0	2215	45	0
1	J	1898	0	1760	29	1
1	K	1937	0	1740	29	1
1	L	2312	0	2228	36	0
1	M	2325	0	2254	41	0
1	N	2295	0	2190	45	0
1	O	2279	0	2161	33	0
1	P	2103	0	1917	41	0
1	Q	2262	0	2164	40	1
1	R	2258	0	2157	52	0
1	S	2236	0	2118	41	1
1	T	2256	0	2171	41	0
1	U	2154	0	2023	32	1
1	V	2122	0	1976	17	0
1	W	2211	0	2148	29	0
1	X	1968	0	1848	62	0
2	A	31	0	22	1	0
2	B	31	0	22	4	0
2	C	31	0	22	1	0
2	D	31	0	22	3	0
2	E	31	0	22	3	0
2	F	31	0	22	3	0
2	G	31	0	22	2	0
2	H	31	0	22	0	0
2	I	31	0	22	1	0
2	J	31	0	22	5	0
2	K	31	0	22	4	0
2	L	31	0	22	3	0
2	M	31	0	22	0	0
2	N	31	0	22	1	0
2	O	31	0	22	5	0
2	P	31	0	22	5	0
2	Q	31	0	22	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	31	0	22	1	1
2	S	31	0	22	0	0
2	T	31	0	22	2	0
2	U	31	0	22	1	0
2	V	31	0	22	3	0
2	W	31	0	22	4	0
2	X	31	0	22	15	0
3	A	4	0	0	1	0
3	B	12	0	0	0	0
3	C	11	0	0	0	0
3	D	7	0	0	0	0
3	E	4	0	0	2	0
3	F	8	0	0	0	0
3	G	6	0	0	1	0
3	H	6	0	0	0	0
3	I	3	0	0	0	0
3	J	2	0	0	0	0
3	L	6	0	0	0	0
3	M	1	0	0	0	0
3	N	6	0	0	0	0
3	O	2	0	0	0	0
3	P	4	0	0	0	0
3	Q	8	0	0	0	0
3	R	5	0	0	0	0
3	S	6	0	0	0	0
3	T	5	0	0	0	0
3	U	9	0	0	0	0
3	V	2	0	0	0	0
3	W	9	0	0	1	0
All	All	53931	0	50890	903	5

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 9.

All (903) 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:D:198:VAL:O	1:D:202:VAL:HG23	1.17	1.27
1:S:217:TRP:CZ2	1:X:430:PRO:HB3	1.88	1.09
1:S:217:TRP:CH2	1:X:430:PRO:HB3	1.94	1.01
1:V:480:LEU:HD22	1:V:484:ARG:HG2	1.40	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:467:MET:HE1	1:G:489:LEU:HD11	1.04	1.00
1:D:198:VAL:O	1:D:202:VAL:CG2	2.10	0.99
1:G:467:MET:CE	1:G:489:LEU:HD11	1.92	0.99
1:B:467:MET:HE1	1:B:489:LEU:HD11	1.44	0.98
1:T:480:LEU:HD22	1:T:484:ARG:HG2	1.49	0.95
1:P:412:THR:HG21	1:P:461:LEU:HD11	1.47	0.94
1:N:239:TRP:CD2	1:N:273:LEU:HD23	2.04	0.93
1:O:198:VAL:O	1:O:202:VAL:HG23	1.70	0.92
1:N:480:LEU:HD22	1:N:484:ARG:HG2	1.52	0.90
1:P:461:LEU:HD23	1:P:464:LEU:HD12	1.51	0.89
1:J:405:LEU:HD22	1:J:464:LEU:HD11	1.51	0.89
1:X:455:LEU:CD2	1:X:465:ALA:HB2	2.02	0.88
1:X:455:LEU:HD22	1:X:465:ALA:HB2	1.55	0.88
1:V:198:VAL:O	1:V:202:VAL:HG23	1.73	0.88
1:D:295:GLU:OE2	1:D:297:HIS:HB3	1.71	0.88
1:B:386:ARG:HB3	1:B:386:ARG:HH11	1.37	0.87
1:O:382:ASP:OD2	1:O:384:GLN:NE2	2.08	0.87
1:N:239:TRP:CE3	1:N:273:LEU:CD2	2.57	0.86
1:D:417:ILE:O	1:D:454:ARG:NH1	2.09	0.86
1:E:467:MET:HE1	1:E:489:LEU:HD11	1.58	0.84
1:N:239:TRP:CE3	1:N:273:LEU:HD23	2.12	0.84
1:T:470:GLU:HG2	1:T:473:TYR:OH	1.76	0.84
1:V:466:GLN:OE1	1:V:469:ARG:NH1	2.09	0.83
1:X:283:GLY:HA2	2:X:600:LDN:CAV	2.08	0.83
1:X:249:VAL:CG1	1:X:251:LEU:HD13	2.09	0.83
1:X:249:VAL:HG12	1:X:251:LEU:HD13	1.59	0.83
1:U:358:GLY:O	1:U:359:SER:O	1.97	0.83
1:E:464:LEU:HD23	1:E:489:LEU:HD21	1.61	0.82
1:S:480:LEU:HD22	1:S:484:ARG:HG2	1.60	0.82
1:G:464:LEU:HD23	1:G:489:LEU:HD21	1.62	0.82
1:C:486:LYS:HG2	1:C:490:GLN:OE1	1.79	0.81
1:B:455:LEU:HD12	1:B:461:LEU:HB3	1.62	0.81
1:F:477:SER:OG	1:J:382:ASP:HB3	1.80	0.80
1:X:480:LEU:HD22	1:X:484:ARG:HG2	1.63	0.80
1:F:480:LEU:HD22	1:F:484:ARG:HG2	1.63	0.80
1:G:467:MET:HE1	1:G:489:LEU:CD1	2.00	0.80
1:U:461:LEU:HD23	1:U:464:LEU:HD22	1.63	0.80
1:B:291:ARG:HH11	2:B:600:LDN:HANA	1.45	0.79
1:I:467:MET:HE1	1:I:489:LEU:HD11	1.62	0.79
1:G:464:LEU:CD2	1:G:489:LEU:HD21	2.12	0.78
1:R:412:THR:HG21	1:R:461:LEU:HD21	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:464:LEU:HD23	1:Q:489:LEU:HD21	1.66	0.78
1:G:464:LEU:CD2	1:G:489:LEU:CD2	2.62	0.78
1:G:464:LEU:HD23	1:G:489:LEU:CD2	2.14	0.77
1:F:467:MET:HE1	1:F:489:LEU:HD11	1.66	0.77
1:Q:198:VAL:HG13	1:Q:221:TRP:CE2	2.19	0.77
1:U:300:LEU:HD13	1:U:460:VAL:HG13	1.65	0.77
1:W:236:GLU:HG2	1:W:273:LEU:HD21	1.67	0.76
1:X:467:MET:CE	1:X:485:ILE:HG23	2.16	0.76
1:T:412:THR:HG21	1:T:461:LEU:HD21	1.68	0.76
1:O:458:ASP:CB	1:O:461:LEU:HD12	2.17	0.75
1:O:252:ARG:NH1	1:T:317:ILE:HD13	2.01	0.75
1:P:195:GLN:HG2	1:P:261:ALA:CB	2.16	0.75
1:E:199:ALA:HB2	1:E:276:ILE:HD11	1.68	0.74
1:R:480:LEU:HD22	1:R:484:ARG:HG2	1.69	0.74
1:G:467:MET:CE	1:G:485:ILE:HG23	2.18	0.74
1:A:381:LEU:HA	1:A:435:PHE:CZ	2.23	0.74
1:A:291:ARG:HD2	1:F:291:ARG:CB	2.18	0.73
1:W:295:GLU:OE1	1:W:297:HIS:HB3	1.87	0.73
1:B:291:ARG:NH1	2:B:600:LDN:HANA	2.03	0.72
1:P:413:ILE:HG23	1:P:416:GLY:HA2	1.72	0.72
1:P:412:THR:HG21	1:P:461:LEU:CD1	2.18	0.72
1:D:293:THR:HB	1:D:413:ILE:HD11	1.70	0.72
1:O:460:VAL:O	1:O:461:LEU:HD23	1.90	0.71
1:N:239:TRP:CD2	1:N:273:LEU:CD2	2.73	0.71
1:X:483:LEU:HD11	1:X:487:LYS:HE3	1.70	0.71
1:E:467:MET:CE	1:E:485:ILE:HG23	2.20	0.71
1:P:461:LEU:CD2	1:P:464:LEU:HD12	2.20	0.71
1:X:480:LEU:HD22	1:X:484:ARG:CG	2.20	0.71
1:M:467:MET:HE1	1:M:489:LEU:HD11	1.72	0.71
1:L:198:VAL:O	1:L:202:VAL:HG23	1.90	0.71
1:P:195:GLN:HG2	1:P:261:ALA:HB1	1.73	0.71
1:X:337:LEU:HD11	2:X:600:LDN:HAJ	1.73	0.71
1:A:480:LEU:HD22	1:A:484:ARG:HG2	1.73	0.70
1:I:414:VAL:HG13	1:I:454:ARG:HD2	1.73	0.70
1:Q:198:VAL:HG13	1:Q:221:TRP:CZ2	2.26	0.70
1:Q:351:LEU:HD21	1:Q:369:ARG:O	1.92	0.70
1:I:295:GLU:CD	1:I:297:HIS:HB3	2.12	0.70
1:P:467:MET:CE	1:P:485:ILE:HG23	2.22	0.70
1:W:454:ARG:HG2	1:W:454:ARG:O	1.90	0.70
1:D:317:ILE:N	1:D:317:ILE:HD12	2.07	0.69
1:E:353:VAL:HB	1:E:362:LEU:HD11	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:222:HIS:O	1:I:224:GLU:OE2	2.10	0.69
1:N:239:TRP:CE2	1:N:273:LEU:HD23	2.27	0.69
1:T:281:GLU:O	2:T:600:LDN:HAQA	1.91	0.69
1:N:206:GLU:OE1	1:N:218:ARG:NH1	2.26	0.69
1:Q:467:MET:CE	1:Q:485:ILE:HG23	2.22	0.69
1:T:374:ARG:NH1	1:T:431:ASN:O	2.26	0.69
1:M:317:ILE:HG21	1:N:252:ARG:HD2	1.75	0.68
1:N:446:GLN:HB2	1:R:395:TRP:HH2	1.58	0.68
1:F:300:LEU:HD12	1:F:460:VAL:HG13	1.75	0.68
1:K:330:ASP:OD1	1:K:372:THR:OG1	2.09	0.68
1:M:236:GLU:HG2	1:M:273:LEU:HD11	1.74	0.68
1:Q:207:CYS:HB2	1:Q:217:TRP:CZ2	2.28	0.68
1:S:460:VAL:HG12	1:S:461:LEU:HD23	1.75	0.68
1:J:386:ARG:NH1	1:J:392:SER:OG	2.27	0.68
1:Q:206:GLU:OE2	1:Q:218:ARG:NH1	2.27	0.67
1:D:239:TRP:CE3	1:D:273:LEU:CD2	2.78	0.67
1:S:217:TRP:CZ2	1:X:430:PRO:CB	2.72	0.67
1:K:332:LYS:HB2	1:K:375:TYR:CE2	2.29	0.67
1:X:405:LEU:HD22	1:X:464:LEU:HD22	1.76	0.67
1:M:321:GLN:O	1:N:252:ARG:NE	2.28	0.67
1:K:199:ALA:HB2	1:K:276:ILE:HD11	1.77	0.67
1:Q:326:ILE:HG12	1:Q:354:MET:HG2	1.77	0.67
1:F:353:VAL:HB	1:F:362:LEU:HD11	1.77	0.67
1:C:239:TRP:CE3	1:C:273:LEU:HD23	2.30	0.66
1:F:293:THR:OG1	1:F:413:ILE:HD11	1.95	0.66
1:W:329:ARG:HE	1:W:353:VAL:HG13	1.60	0.66
1:J:254:ASP:OD1	1:W:490:GLN:HB3	1.94	0.66
1:X:467:MET:SD	1:X:485:ILE:HG23	2.35	0.66
1:B:293:THR:OG1	1:B:413:ILE:HD11	1.95	0.66
1:C:239:TRP:CE3	1:C:273:LEU:CD2	2.79	0.66
1:L:236:GLU:HG2	1:L:273:LEU:HD21	1.76	0.66
1:N:305:SER:HB3	1:N:343:GLN:HG2	1.78	0.66
1:X:337:LEU:HD11	2:X:600:LDN:CAJ	2.25	0.66
1:D:486:LYS:NZ	1:I:254:ASP:OD1	2.28	0.65
1:O:283:GLY:HA2	2:O:600:LDN:CAV	2.26	0.65
1:T:304:VAL:HA	1:T:489:LEU:HD12	1.77	0.65
1:F:422:ARG:HD2	1:F:426:TYR:CD1	2.31	0.65
1:G:427:ASP:OD1	1:G:428:VAL:HG13	1.96	0.65
1:I:236:GLU:HG2	1:I:273:LEU:HD21	1.79	0.65
1:R:434:SER:O	1:R:437:ASP:N	2.29	0.65
1:F:351:LEU:HD21	1:F:369:ARG:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:480:LEU:HD22	1:C:484:ARG:HG2	1.79	0.65
1:G:233:SER:HB2	1:K:210:LYS:C	2.16	0.65
1:X:251:LEU:HD11	1:X:326:ILE:CD1	2.27	0.65
1:L:382:ASP:OD2	1:P:477:SER:OG	2.15	0.65
1:F:467:MET:CE	1:F:485:ILE:HG23	2.26	0.65
1:B:287:ASP:O	1:B:291:ARG:HD3	1.97	0.65
1:H:382:ASP:OD1	1:H:443:CYS:SG	2.54	0.65
1:R:428:VAL:HG23	1:R:429:VAL:HG13	1.78	0.64
1:L:295:GLU:HG2	1:L:296:PRO:HD2	1.80	0.64
1:A:218:ARG:HD2	1:A:279:TYR:CE2	2.33	0.64
1:Q:264:MET:HG3	1:Q:273:LEU:CD2	2.28	0.64
1:U:463:GLY:HA3	1:U:492:ILE:HD11	1.80	0.64
1:K:428:VAL:HG21	1:K:441:VAL:HG11	1.80	0.63
1:E:489:LEU:HA	1:E:492:ILE:HD12	1.79	0.63
1:L:205:VAL:O	1:Q:416:GLY:HA2	1.99	0.63
1:N:461:LEU:HD23	1:N:464:LEU:HD12	1.79	0.63
1:E:464:LEU:CD2	1:E:489:LEU:HD21	2.28	0.63
1:X:315:VAL:O	1:X:323:LYS:NZ	2.31	0.63
1:S:275:LEU:HD13	1:S:277:THR:HG23	1.80	0.62
1:U:455:LEU:HD13	1:U:465:ALA:HB2	1.81	0.62
1:K:347:ALA:HB1	2:K:600:LDN:CAI	2.30	0.62
1:H:428:VAL:HG11	1:H:447:GLN:NE2	2.15	0.62
1:P:355:HIS:HB3	1:P:390:PHE:HB2	1.81	0.62
1:R:251:LEU:HD21	1:R:349:LEU:HD21	1.81	0.62
1:M:464:LEU:HD23	1:M:489:LEU:HD21	1.81	0.62
1:J:412:THR:HG21	1:J:461:LEU:HD11	1.81	0.61
1:I:480:LEU:HD22	1:I:484:ARG:HG2	1.81	0.61
1:J:204:LEU:HD22	1:J:217:TRP:CB	2.30	0.61
1:M:467:MET:CE	1:M:485:ILE:HG23	2.30	0.61
1:U:300:LEU:CD2	1:U:493:SER:HA	2.31	0.61
1:B:405:LEU:HD11	1:B:467:MET:HE3	1.82	0.61
1:D:198:VAL:C	1:D:202:VAL:HG23	2.14	0.61
1:D:239:TRP:CE3	1:D:273:LEU:HD22	2.35	0.61
1:A:458:ASP:O	1:A:462:SER:HB3	2.01	0.61
1:U:198:VAL:HG22	1:U:221:TRP:HZ2	1.66	0.61
1:H:428:VAL:HG11	1:H:447:GLN:HE22	1.64	0.60
1:L:414:VAL:HG12	1:L:454:ARG:HH11	1.65	0.60
1:H:273:LEU:H	1:H:273:LEU:HD22	1.65	0.60
1:P:283:GLY:HA2	2:P:600:LDN:CAF	2.31	0.60
1:T:467:MET:CE	1:T:485:ILE:HG23	2.31	0.60
1:B:386:ARG:HB3	1:B:386:ARG:NH1	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:374:ARG:NH1	1:F:431:ASN:O	2.35	0.59
1:K:199:ALA:HB2	1:K:276:ILE:CD1	2.32	0.59
1:T:315:VAL:HG13	1:T:315:VAL:O	2.02	0.59
1:P:464:LEU:HD21	1:P:489:LEU:HD11	1.82	0.59
1:W:461:LEU:HD23	1:W:464:LEU:HB2	1.84	0.59
1:H:273:LEU:HD22	1:H:273:LEU:N	2.18	0.59
1:J:467:MET:CE	1:J:485:ILE:HG23	2.32	0.59
1:P:355:HIS:HB2	1:P:362:LEU:HD12	1.84	0.59
1:H:250:LEU:HD21	1:H:321:GLN:OE1	2.03	0.59
1:P:206:GLU:CB	1:P:218:ARG:HH12	2.15	0.59
1:S:460:VAL:HG12	1:S:461:LEU:N	2.17	0.59
1:G:450:THR:CG2	1:I:453:ASN:H	2.16	0.58
1:K:381:LEU:HD11	1:K:438:MET:HB3	1.84	0.58
1:U:374:ARG:NH1	1:U:431:ASN:O	2.36	0.58
1:F:474:PRO:HB3	1:J:475:ASN:HB2	1.86	0.58
1:G:467:MET:SD	1:G:485:ILE:HG23	2.42	0.58
1:D:252:ARG:HD3	1:I:321:GLN:O	2.03	0.58
1:F:235:ASP:OD2	1:F:369:ARG:NH2	2.37	0.58
1:W:464:LEU:HD13	1:W:489:LEU:HD21	1.84	0.58
1:B:386:ARG:CB	1:B:386:ARG:HH11	2.14	0.58
1:B:405:LEU:HD11	1:B:467:MET:CE	2.33	0.58
1:I:417:ILE:HG22	1:I:418:VAL:N	2.19	0.58
1:P:465:ALA:HA	1:P:468:MET:HE3	1.86	0.58
1:Q:381:LEU:HA	1:Q:435:PHE:CZ	2.38	0.58
1:R:428:VAL:HG11	1:R:447:GLN:OE1	2.04	0.58
1:C:239:TRP:CD2	1:C:273:LEU:HD23	2.38	0.57
1:S:386:ARG:NH1	1:T:446:GLN:HB2	2.20	0.57
1:J:227:ALA:HB1	2:J:600:LDN:HAD	1.86	0.57
1:O:301:ARG:NH2	1:O:341:ASN:O	2.37	0.57
1:B:409:ALA:HB2	1:B:468:MET:HE2	1.86	0.57
1:Q:207:CYS:HB2	1:Q:217:TRP:CE2	2.39	0.57
1:A:195:GLN:HB3	1:A:261:ALA:HB1	1.87	0.57
1:I:250:LEU:HD11	1:I:252:ARG:NH1	2.20	0.57
1:Q:440:LYS:HA	1:Q:444:VAL:HG23	1.86	0.57
1:S:428:VAL:HG23	1:S:429:VAL:HG13	1.87	0.57
1:B:412:THR:HG21	1:B:461:LEU:HD21	1.85	0.57
1:W:251:LEU:HD21	1:W:349:LEU:HD21	1.85	0.57
1:W:369:ARG:NH2	3:W:142:HOH:O	2.25	0.57
1:X:420:ASP:CB	1:X:422:ARG:HH21	2.17	0.57
1:D:206:GLU:OE1	1:D:218:ARG:NH1	2.38	0.56
1:G:379:GLU:CG	1:G:385:ILE:HG23	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:265:THR:O	1:S:266:SER:OG	2.14	0.56
1:I:317:ILE:HG22	1:I:322:GLY:HA2	1.87	0.56
1:U:373:LYS:HG3	1:U:433:PRO:O	2.04	0.56
1:N:300:LEU:HD21	1:N:493:SER:HB3	1.87	0.56
1:U:358:GLY:O	1:U:359:SER:C	2.44	0.56
1:X:452:PRO:HD2	1:X:455:LEU:HD13	1.86	0.56
1:R:455:LEU:CD2	1:R:465:ALA:HB2	2.35	0.56
1:G:450:THR:HG22	1:I:453:ASN:HB2	1.87	0.56
1:M:405:LEU:HD11	1:M:467:MET:CE	2.35	0.56
1:E:405:LEU:HD22	1:E:464:LEU:HD22	1.86	0.56
1:A:198:VAL:O	1:A:202:VAL:HG23	2.05	0.56
1:G:450:THR:HG21	1:I:452:PRO:HA	1.85	0.56
1:L:236:GLU:HG2	1:L:273:LEU:CD2	2.36	0.56
1:X:405:LEU:HD11	1:X:467:MET:CE	2.36	0.56
1:G:428:VAL:HG23	1:G:429:VAL:HG13	1.87	0.56
1:N:239:TRP:CZ3	1:N:273:LEU:HD23	2.40	0.56
1:T:414:VAL:HG11	1:T:454:ARG:HG3	1.86	0.56
1:U:480:LEU:HD22	1:U:484:ARG:HG2	1.87	0.56
1:F:474:PRO:CB	1:J:475:ASN:HB2	2.36	0.56
1:C:237:GLN:HG2	1:C:366:ASN:O	2.05	0.55
1:R:414:VAL:HG11	1:R:454:ARG:HG2	1.87	0.55
1:S:265:THR:O	1:S:272:GLN:N	2.39	0.55
1:C:293:THR:OG1	1:C:413:ILE:HD11	2.07	0.55
1:E:452:PRO:HD2	1:E:455:LEU:HD13	1.89	0.55
1:F:477:SER:OG	1:J:382:ASP:CB	2.54	0.55
1:V:263:ASP:OD2	1:V:264:MET:N	2.39	0.55
1:X:400:ALA:HA	1:X:403:LEU:HD12	1.87	0.55
1:N:454:ARG:O	1:N:454:ARG:CG	2.54	0.55
1:W:375:TYR:OH	1:W:407:GLU:OE2	2.17	0.55
1:C:239:TRP:CZ3	1:C:273:LEU:HD23	2.41	0.55
1:M:305:SER:HB3	1:M:343:GLN:HG3	1.88	0.55
1:R:414:VAL:HG13	1:R:454:ARG:NH1	2.22	0.55
1:U:412:THR:HG21	1:U:461:LEU:HD21	1.89	0.55
1:P:410:ARG:NH1	1:P:419:GLU:OE2	2.39	0.55
1:X:347:ALA:HB3	2:X:600:LDN:CAB	2.37	0.55
1:C:315:VAL:HG13	1:C:315:VAL:O	2.06	0.55
1:F:464:LEU:HD23	1:F:489:LEU:HD21	1.88	0.55
2:F:600:LDN:HAJ	2:F:600:LDN:CBC	2.36	0.55
1:M:467:MET:SD	1:M:485:ILE:HG23	2.47	0.55
1:T:452:PRO:HD2	1:T:455:LEU:HD13	1.89	0.55
1:X:483:LEU:HD12	1:X:486:LYS:HE2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:251:LEU:HD11	1:M:326:ILE:CD1	2.36	0.55
1:T:285:LEU:O	1:T:289:LEU:HG	2.06	0.55
1:E:298:LEU:HD12	1:E:298:LEU:O	2.07	0.55
1:H:434:SER:OG	1:H:436:GLU:HG2	2.07	0.55
1:H:414:VAL:HG13	1:H:454:ARG:CG	2.37	0.55
1:L:431:ASN:OD1	1:L:432:ASP:N	2.40	0.55
1:Q:329:ARG:HD3	1:Q:393:TYR:CD1	2.41	0.55
1:F:239:TRP:CE3	1:F:273:LEU:HD13	2.41	0.54
1:G:199:ALA:HB2	1:G:276:ILE:HD11	1.88	0.54
1:J:452:PRO:O	1:J:454:ARG:N	2.41	0.54
1:N:295:GLU:HG2	1:N:296:PRO:HD2	1.89	0.54
1:R:283:GLY:HA2	2:R:600:LDN:CAV	2.37	0.54
1:S:414:VAL:HG21	1:S:454:ARG:HG3	1.89	0.54
1:O:315:VAL:HG13	1:O:315:VAL:O	2.06	0.54
1:O:426:TYR:H	1:O:426:TYR:HD2	1.52	0.54
1:E:354:MET:O	1:E:362:LEU:HD12	2.07	0.54
1:G:199:ALA:HB2	1:G:276:ILE:CD1	2.37	0.54
1:N:305:SER:CB	1:N:343:GLN:HG2	2.37	0.54
1:Q:467:MET:SD	1:Q:485:ILE:HG23	2.48	0.54
1:R:198:VAL:O	1:R:202:VAL:HG23	2.07	0.54
1:P:413:ILE:HG23	1:P:416:GLY:CA	2.37	0.54
1:A:291:ARG:NH2	3:A:105:HOH:O	2.41	0.54
1:R:298:LEU:HD12	1:R:298:LEU:O	2.07	0.54
1:Q:195:GLN:OE1	1:Q:262:SER:N	2.39	0.54
1:A:470:GLU:HA	1:A:473:TYR:CE2	2.43	0.53
1:M:403:LEU:HD23	1:M:472:TRP:CZ2	2.43	0.53
1:P:429:VAL:HG13	1:P:441:VAL:HG21	1.91	0.53
1:N:315:VAL:O	1:N:315:VAL:HG13	2.07	0.53
1:U:300:LEU:HD22	1:U:493:SER:HA	1.89	0.53
2:V:600:LDN:CBC	2:V:600:LDN:HAJ	2.38	0.53
1:L:455:LEU:O	1:L:461:LEU:CB	2.56	0.53
1:G:418:VAL:HG13	1:G:418:VAL:O	2.08	0.53
1:K:347:ALA:HB3	2:K:600:LDN:CAA	2.38	0.53
1:X:283:GLY:CA	2:X:600:LDN:CAV	2.86	0.53
1:D:237:GLN:HG2	1:D:367:ASN:HA	1.89	0.53
1:Q:473:TYR:CZ	1:U:446:GLN:OE1	2.62	0.53
1:B:386:ARG:HD2	1:B:389:CYS:HB2	1.90	0.53
1:E:199:ALA:HB2	1:E:276:ILE:CD1	2.38	0.53
1:K:428:VAL:HG23	1:K:429:VAL:HG13	1.91	0.53
1:Q:474:PRO:HB2	1:U:475:ASN:HB2	1.89	0.53
1:T:470:GLU:HG2	1:T:473:TYR:CZ	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:464:LEU:CD2	1:P:489:LEU:HD11	2.39	0.53
1:N:239:TRP:CE3	1:N:273:LEU:HD22	2.41	0.53
1:O:455:LEU:HD13	1:O:465:ALA:HB2	1.89	0.53
1:P:467:MET:HE3	1:P:485:ILE:HG23	1.90	0.53
1:W:381:LEU:HA	1:W:435:PHE:CZ	2.44	0.53
1:G:417:ILE:HG21	1:I:427:ASP:O	2.09	0.52
1:G:434:SER:O	1:G:435:PHE:C	2.47	0.52
1:S:197:THR:O	1:S:199:ALA:N	2.42	0.52
1:L:329:ARG:HD3	1:L:393:TYR:CD1	2.45	0.52
1:O:426:TYR:CD2	1:O:426:TYR:N	2.77	0.52
1:V:315:VAL:O	1:V:315:VAL:HG13	2.08	0.52
1:X:337:LEU:HD21	2:X:600:LDN:CBC	2.38	0.52
1:B:446:GLN:HA	1:B:446:GLN:OE1	2.08	0.52
1:D:239:TRP:CD2	1:D:273:LEU:CD2	2.92	0.52
1:I:410:ARG:NH1	1:I:419:GLU:OE2	2.42	0.52
1:K:473:TYR:CE1	1:K:475:ASN:HB3	2.44	0.52
1:N:300:LEU:CD2	1:N:492:ILE:O	2.57	0.52
1:X:468:MET:O	1:X:472:TRP:CD1	2.62	0.52
1:G:294:LEU:HD22	1:G:298:LEU:HG	1.92	0.52
1:J:412:THR:CG2	1:J:461:LEU:HD11	2.39	0.52
1:Q:422:ARG:HD2	1:Q:426:TYR:CD1	2.45	0.52
1:R:202:VAL:HG22	1:R:221:TRP:HB2	1.91	0.52
1:R:315:VAL:O	1:R:315:VAL:HG13	2.08	0.52
1:D:337:LEU:HD21	2:D:600:LDN:HAJ	1.90	0.52
1:K:428:VAL:HG23	1:K:441:VAL:HG21	1.91	0.52
1:M:422:ARG:HD2	1:M:426:TYR:CD1	2.45	0.52
1:T:251:LEU:HD21	1:T:349:LEU:HD21	1.91	0.52
1:X:249:VAL:HG11	1:X:251:LEU:HD13	1.90	0.52
1:G:375:TYR:OH	1:G:407:GLU:OE2	2.22	0.52
1:O:417:ILE:HG22	1:O:454:ARG:HH11	1.75	0.52
1:C:360:ASP:HA	1:C:361:TYR:C	2.30	0.52
1:C:434:SER:OG	1:C:437:ASP:CG	2.47	0.52
1:O:206:GLU:OE1	1:O:218:ARG:NH1	2.42	0.52
1:U:300:LEU:HD13	1:U:460:VAL:CG1	2.36	0.52
1:B:458:ASP:O	1:B:462:SER:HB2	2.09	0.52
1:N:446:GLN:HB2	1:R:395:TRP:CH2	2.42	0.52
1:C:386:ARG:HB2	1:C:386:ARG:CZ	2.40	0.52
1:O:305:SER:HB3	1:O:343:GLN:HG2	1.91	0.52
1:X:347:ALA:HB3	2:X:600:LDN:CAA	2.39	0.52
1:A:250:LEU:HD13	1:A:321:GLN:OE1	2.10	0.52
1:F:464:LEU:O	1:F:468:MET:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:375:TYR:OH	1:K:407:GLU:OE2	2.22	0.52
1:L:381:LEU:HD11	1:L:438:MET:HB3	1.92	0.52
1:R:376:MET:HG2	1:R:380:VAL:CG1	2.39	0.52
1:X:455:LEU:HD23	1:X:465:ALA:HB2	1.91	0.51
1:I:236:GLU:HG2	1:I:273:LEU:CD2	2.40	0.51
1:I:373:LYS:HA	1:I:376:MET:HG3	1.92	0.51
1:X:241:ARG:NH1	1:X:244:GLU:OE1	2.43	0.51
1:B:460:VAL:HG12	1:B:492:ILE:HG22	1.93	0.51
1:M:328:HIS:O	1:M:329:ARG:HB2	2.10	0.51
1:N:440:LYS:HA	1:N:444:VAL:HG23	1.92	0.51
1:A:298:LEU:O	1:A:298:LEU:HD12	2.10	0.51
1:D:239:TRP:CD2	1:D:273:LEU:HD23	2.45	0.51
1:D:360:ASP:HA	1:D:361:TYR:C	2.30	0.51
1:M:275:LEU:HD13	1:M:277:THR:HG23	1.92	0.51
1:M:305:SER:HB3	1:M:343:GLN:CG	2.41	0.51
1:S:215:GLU:OE2	1:X:431:ASN:HB3	2.10	0.51
1:B:251:LEU:HD21	1:B:326:ILE:CD1	2.41	0.51
1:K:473:TYR:HE1	1:K:475:ASN:HB3	1.76	0.51
1:N:198:VAL:O	1:N:202:VAL:HG23	2.11	0.51
1:Q:315:VAL:HG13	1:Q:315:VAL:O	2.10	0.51
1:U:198:VAL:HG22	1:U:221:TRP:CZ2	2.46	0.51
1:X:399:TRP:NE1	1:X:403:LEU:HD11	2.26	0.51
1:F:477:SER:CB	1:J:382:ASP:HB3	2.41	0.51
1:M:455:LEU:HD22	1:M:461:LEU:HB3	1.93	0.51
1:B:467:MET:HE1	1:B:489:LEU:CD1	2.28	0.51
1:E:414:VAL:HG11	1:E:454:ARG:HG2	1.93	0.51
1:E:480:LEU:HD22	1:E:484:ARG:HG2	1.92	0.51
1:N:239:TRP:CZ3	1:N:273:LEU:CD2	2.93	0.51
1:O:304:VAL:HA	1:O:489:LEU:HD13	1.93	0.51
1:T:315:VAL:CG1	1:T:315:VAL:O	2.59	0.51
1:V:295:GLU:OE2	1:V:297:HIS:HB3	2.10	0.51
1:A:202:VAL:HG22	1:A:221:TRP:HB2	1.93	0.51
1:B:467:MET:SD	1:B:485:ILE:HG23	2.51	0.51
1:C:289:LEU:CD2	1:C:294:LEU:HD11	2.40	0.51
1:O:360:ASP:HA	1:O:361:TYR:C	2.31	0.51
1:R:455:LEU:HD23	1:R:465:ALA:HB2	1.92	0.51
1:R:467:MET:HE1	1:R:489:LEU:HD21	1.92	0.51
1:S:459:PRO:O	1:S:460:VAL:C	2.49	0.51
1:U:351:LEU:HD21	1:U:369:ARG:O	2.10	0.51
1:W:329:ARG:HD3	1:W:393:TYR:CD1	2.45	0.51
1:N:360:ASP:HA	1:N:361:TYR:C	2.31	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:430:PRO:O	1:P:431:ASN:O	2.29	0.50
1:T:206:GLU:OE2	1:T:218:ARG:NH1	2.44	0.50
1:X:283:GLY:HA3	2:X:600:LDN:CAG	2.41	0.50
1:E:415:ASN:O	1:E:417:ILE:HD12	2.11	0.50
1:U:451:ILE:HD12	1:U:469:ARG:HE	1.76	0.50
1:B:317:ILE:HG21	1:C:252:ARG:HD2	1.93	0.50
1:B:412:THR:HG21	1:B:461:LEU:HD11	1.94	0.50
1:S:197:THR:O	1:S:200:ARG:N	2.45	0.50
1:C:295:GLU:HG2	1:C:296:PRO:HD2	1.92	0.50
1:S:460:VAL:HG12	1:S:461:LEU:CD2	2.41	0.50
1:H:250:LEU:HD23	1:H:321:GLN:HA	1.92	0.50
1:G:417:ILE:CG2	1:I:427:ASP:O	2.59	0.50
1:F:315:VAL:O	1:F:315:VAL:HG13	2.11	0.50
1:P:252:ARG:HB3	1:P:252:ARG:CZ	2.42	0.50
1:V:417:ILE:HG22	1:V:454:ARG:HH11	1.77	0.50
1:B:317:ILE:HG21	1:C:252:ARG:CD	2.42	0.50
1:H:428:VAL:HG23	1:H:429:VAL:HG13	1.94	0.50
1:I:417:ILE:CG2	1:I:418:VAL:N	2.75	0.50
1:L:322:GLY:O	1:L:323:LYS:HB3	2.12	0.50
2:T:600:LDN:HAJ	2:T:600:LDN:CBC	2.41	0.50
1:F:289:LEU:HD21	1:F:294:LEU:HD11	1.94	0.50
1:R:434:SER:O	1:R:436:GLU:N	2.45	0.50
1:T:451:ILE:HD11	1:T:472:TRP:HZ3	1.77	0.50
1:I:446:GLN:O	1:I:446:GLN:HG3	2.12	0.49
1:X:235:ASP:OD1	1:X:369:ARG:HD3	2.11	0.49
1:B:386:ARG:CB	1:B:386:ARG:NH1	2.75	0.49
1:C:197:THR:O	1:C:197:THR:HG22	2.11	0.49
1:H:400:ALA:HA	1:H:403:LEU:HD12	1.94	0.49
1:K:337:LEU:HD11	2:K:600:LDN:CAJ	2.42	0.49
1:L:451:ILE:HG23	1:L:455:LEU:HD13	1.94	0.49
1:S:360:ASP:HA	1:S:361:TYR:C	2.32	0.49
1:V:434:SER:OG	1:V:437:ASP:OD2	2.30	0.49
1:C:434:SER:HG	1:C:437:ASP:CG	2.15	0.49
1:M:275:LEU:HD13	1:M:277:THR:CG2	2.43	0.49
1:J:252:ARG:HD3	1:W:486:LYS:NZ	2.26	0.49
1:U:315:VAL:HG13	1:U:315:VAL:O	2.11	0.49
1:X:467:MET:HE3	1:X:485:ILE:HG23	1.94	0.49
1:E:428:VAL:HG23	1:E:429:VAL:HG13	1.94	0.49
1:L:315:VAL:HG13	1:L:315:VAL:O	2.11	0.49
1:S:217:TRP:CH2	1:X:430:PRO:CB	2.84	0.49
1:S:315:VAL:HG13	1:S:315:VAL:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:GLN:O	1:A:493:SER:N	2.38	0.49
1:C:251:LEU:HD11	1:C:326:ILE:CD1	2.42	0.49
1:G:359:SER:O	1:G:361:TYR:N	2.46	0.49
1:T:417:ILE:O	1:T:454:ARG:NH1	2.46	0.49
1:W:315:VAL:O	1:W:315:VAL:HG13	2.12	0.49
1:X:455:LEU:HB3	1:X:465:ALA:HB2	1.94	0.49
2:D:600:LDN:HAJ	2:D:600:LDN:CBC	2.43	0.49
1:W:205:VAL:HG11	1:W:218:ARG:HH22	1.78	0.49
1:C:425:PHE:O	1:C:429:VAL:HG22	2.13	0.49
1:H:386:ARG:NH1	1:I:446:GLN:HB2	2.28	0.49
1:P:412:THR:O	1:P:418:VAL:HG23	2.13	0.49
1:S:452:PRO:HB2	1:S:455:LEU:HD13	1.95	0.49
1:B:452:PRO:HB2	1:B:454:ARG:HB3	1.95	0.48
1:E:205:VAL:HG21	1:E:220:LEU:HG	1.93	0.48
1:M:447:GLN:OE1	1:Q:454:ARG:HA	2.13	0.48
1:X:283:GLY:HA2	2:X:600:LDN:CAF	2.43	0.48
1:A:361:TYR:CZ	1:M:0:MET:HA	2.48	0.48
1:P:206:GLU:CB	1:P:218:ARG:NH1	2.76	0.48
1:R:207:CYS:HB2	1:R:217:TRP:CZ2	2.49	0.48
1:T:197:THR:CG2	1:T:200:ARG:CB	2.92	0.48
1:W:467:MET:CE	1:W:485:ILE:HG23	2.44	0.48
1:B:332:LYS:HE3	1:B:334:ARG:HB2	1.94	0.48
1:L:291:ARG:NH2	2:L:600:LDN:HNAU	2.10	0.48
1:P:315:VAL:HG13	1:P:315:VAL:O	2.13	0.48
1:O:490:GLN:OE1	1:T:341:ASN:ND2	2.47	0.48
1:G:317:ILE:HB	1:G:323:LYS:HG3	1.94	0.48
1:G:452:PRO:HB2	1:G:455:LEU:HD13	1.95	0.48
1:H:265:THR:HG23	1:H:266:SER:N	2.28	0.48
1:H:434:SER:O	1:H:435:PHE:C	2.51	0.48
1:K:198:VAL:HG13	1:K:221:TRP:CZ2	2.48	0.48
1:A:315:VAL:O	1:A:315:VAL:HG13	2.12	0.48
1:K:428:VAL:HG21	1:K:441:VAL:CG1	2.44	0.48
1:M:198:VAL:HG13	1:M:221:TRP:NE1	2.28	0.48
1:P:354:MET:HA	1:P:390:PHE:CE1	2.48	0.48
1:R:403:LEU:HD22	1:R:449:PRO:HG2	1.94	0.48
1:S:456:ALA:HA	1:S:462:SER:OG	2.13	0.48
1:T:250:LEU:HD11	1:T:252:ARG:NH1	2.29	0.48
1:T:418:VAL:O	1:T:418:VAL:HG13	2.14	0.48
1:M:236:GLU:HG2	1:M:273:LEU:CD1	2.41	0.48
1:C:486:LYS:HE2	1:C:490:GLN:HE22	1.78	0.48
1:D:198:VAL:O	1:D:202:VAL:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:362:LEU:HD13	1:Q:390:PHE:HB2	1.96	0.48
1:B:460:VAL:HG12	1:B:492:ILE:CG2	2.44	0.48
2:C:600:LDN:CBC	2:C:600:LDN:HAJ	2.43	0.48
1:D:316:GLU:HG3	1:D:324:PRO:HA	1.95	0.48
1:E:315:VAL:HG13	1:E:315:VAL:O	2.13	0.48
1:G:245:ILE:HG21	1:G:349:LEU:HD23	1.95	0.48
1:T:414:VAL:O	1:T:416:GLY:N	2.47	0.48
1:V:391:GLU:OE2	1:V:394:LYS:NZ	2.43	0.48
1:D:305:SER:HB3	1:D:343:GLN:HG2	1.96	0.48
1:L:325:ALA:N	1:L:355:HIS:O	2.40	0.48
1:N:446:GLN:CD	1:R:395:TRP:HZ3	2.17	0.48
1:Q:264:MET:HG3	1:Q:273:LEU:HD22	1.95	0.48
1:T:245:ILE:HG21	1:T:349:LEU:HD23	1.96	0.48
1:F:207:CYS:HB2	1:F:217:TRP:CZ2	2.48	0.48
1:F:329:ARG:HD3	1:F:393:TYR:CD1	2.49	0.48
1:H:258:GLY:O	1:H:277:THR:HB	2.14	0.48
1:Q:237:GLN:CD	1:Q:368:PRO:HD3	2.34	0.48
1:N:446:GLN:CB	1:R:395:TRP:CH2	2.97	0.48
1:I:432:ASP:O	1:I:433:PRO:C	2.52	0.47
1:I:315:VAL:O	1:I:315:VAL:HG13	2.14	0.47
1:F:237:GLN:CD	1:F:368:PRO:HD3	2.34	0.47
1:H:316:GLU:HG2	1:H:324:PRO:HA	1.96	0.47
1:H:360:ASP:HA	1:H:361:TYR:C	2.35	0.47
1:I:400:ALA:O	1:I:404:VAL:HG23	2.14	0.47
1:L:467:MET:HE1	1:L:489:LEU:HD21	1.95	0.47
1:M:403:LEU:HD22	1:M:449:PRO:HG2	1.95	0.47
1:N:400:ALA:O	1:N:404:VAL:HG23	2.14	0.47
1:T:386:ARG:H	1:T:386:ARG:HE	1.62	0.47
1:U:488:THR:O	1:U:491:LYS:HB2	2.14	0.47
1:V:298:LEU:HD12	1:V:302:LEU:HD13	1.96	0.47
1:B:315:VAL:HG13	1:B:315:VAL:O	2.14	0.47
1:F:467:MET:SD	1:F:485:ILE:HG23	2.54	0.47
1:Q:198:VAL:HG22	1:Q:221:TRP:CZ2	2.49	0.47
1:S:230:ILE:CG2	1:S:272:GLN:OE1	2.62	0.47
1:A:304:VAL:HA	1:A:489:LEU:HD13	1.97	0.47
1:E:455:LEU:HD23	1:E:465:ALA:HB2	1.97	0.47
1:E:467:MET:SD	1:E:485:ILE:HG23	2.55	0.47
1:F:458:ASP:CB	1:F:461:LEU:HD12	2.44	0.47
1:I:467:MET:CE	1:I:485:ILE:HG23	2.44	0.47
1:O:465:ALA:HA	1:O:468:MET:HE3	1.96	0.47
2:U:600:LDN:HAJ	2:U:600:LDN:CBC	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:THR:C	1:C:321:GLN:NE2	2.68	0.47
1:I:491:LYS:O	1:I:492:ILE:C	2.52	0.47
1:N:298:LEU:HD12	1:N:298:LEU:O	2.14	0.47
1:S:381:LEU:HD11	1:S:438:MET:HB3	1.96	0.47
1:T:312:HIS:O	1:T:323:LYS:HE3	2.15	0.47
1:I:446:GLN:NE2	1:I:446:GLN:HA	2.29	0.47
1:O:256:ILE:CD1	1:O:312:HIS:HD1	2.28	0.47
1:A:195:GLN:OE1	1:A:262:SER:N	2.46	0.47
1:B:328:HIS:O	1:B:329:ARG:HB2	2.15	0.47
1:F:332:LYS:HD3	1:F:372:THR:OG1	2.15	0.47
1:J:283:GLY:HA2	2:J:600:LDN:CAM	2.45	0.47
1:K:347:ALA:CB	2:K:600:LDN:CAA	2.93	0.47
1:Q:440:LYS:HA	1:Q:444:VAL:CG2	2.45	0.47
1:R:304:VAL:HA	1:R:489:LEU:HD13	1.97	0.47
1:X:198:VAL:HA	1:X:221:TRP:NE1	2.30	0.47
1:E:283:GLY:HA2	2:E:600:LDN:CAV	2.45	0.47
1:L:467:MET:CE	1:L:489:LEU:HD21	2.45	0.47
1:R:403:LEU:HD23	1:R:472:TRP:NE1	2.30	0.47
1:S:202:VAL:HG22	1:S:221:TRP:HB2	1.97	0.47
1:X:317:ILE:HD12	1:X:323:LYS:HG2	1.95	0.47
1:B:202:VAL:HG22	1:B:221:TRP:HB2	1.97	0.46
1:T:386:ARG:H	1:T:386:ARG:NE	2.13	0.46
1:X:302:LEU:HD22	1:X:344:CYS:SG	2.55	0.46
1:F:241:ARG:HD3	1:F:365:GLY:HA3	1.96	0.46
1:G:447:GLN:OE1	1:I:454:ARG:HA	2.14	0.46
1:K:305:SER:HA	1:K:308:CYS:SG	2.55	0.46
1:C:381:LEU:HD23	1:C:435:PHE:CE1	2.50	0.46
1:G:293:THR:OG1	1:G:413:ILE:HD11	2.15	0.46
1:I:446:GLN:HE21	1:I:446:GLN:HA	1.79	0.46
1:I:467:MET:SD	1:I:485:ILE:HG23	2.55	0.46
1:J:227:ALA:CB	2:J:600:LDN:HAD	2.44	0.46
1:K:332:LYS:HD3	1:K:372:THR:OG1	2.15	0.46
1:P:195:GLN:CG	1:P:261:ALA:CB	2.92	0.46
1:N:446:GLN:CB	1:R:395:TRP:HH2	2.26	0.46
1:T:197:THR:HG23	1:T:200:ARG:CB	2.45	0.46
1:I:332:LYS:HE3	1:I:334:ARG:HB2	1.98	0.46
1:W:464:LEU:CD1	1:W:489:LEU:HD21	2.45	0.46
1:A:364:ILE:HG22	1:A:365:GLY:O	2.15	0.46
1:L:464:LEU:O	1:L:468:MET:HE2	2.16	0.46
1:M:354:MET:HB2	1:M:363:ASP:HB3	1.97	0.46
1:Q:317:ILE:HD12	1:Q:323:LYS:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:428:VAL:HG11	1:S:447:GLN:OE1	2.15	0.46
1:V:418:VAL:HA	1:V:454:ARG:HH12	1.81	0.46
1:G:379:GLU:HG3	1:G:385:ILE:HG23	1.97	0.46
1:O:455:LEU:HD22	1:O:461:LEU:HB3	1.97	0.46
1:R:207:CYS:HB2	1:R:217:TRP:CE2	2.51	0.46
1:R:315:VAL:CG1	1:R:315:VAL:O	2.64	0.46
1:W:403:LEU:HD22	1:W:424:PRO:HB3	1.97	0.46
2:W:600:LDN:CBC	2:W:600:LDN:HAJ	2.46	0.46
1:E:198:VAL:O	1:E:202:VAL:HG23	2.16	0.46
1:E:206:GLU:CB	3:E:113:HOH:O	2.63	0.46
1:H:204:LEU:HD13	1:H:217:TRP:CG	2.51	0.46
1:M:204:LEU:HB3	1:M:217:TRP:CE3	2.50	0.46
1:M:245:ILE:HG21	1:M:349:LEU:HD23	1.98	0.46
1:O:256:ILE:HD12	1:O:312:HIS:HD1	1.80	0.46
1:B:315:VAL:O	1:B:323:LYS:NZ	2.49	0.46
1:B:464:LEU:HD23	1:B:489:LEU:HD21	1.98	0.46
1:B:409:ALA:HB2	1:B:468:MET:CE	2.45	0.46
1:C:315:VAL:CG1	1:C:315:VAL:O	2.63	0.46
1:H:245:ILE:HG21	1:H:349:LEU:HD23	1.97	0.46
1:K:315:VAL:O	1:K:315:VAL:HG13	2.15	0.46
1:N:403:LEU:HD23	1:N:472:TRP:NE1	2.30	0.46
1:N:300:LEU:HD22	1:N:492:ILE:O	2.15	0.46
1:R:251:LEU:HD21	1:R:349:LEU:CD2	2.45	0.46
1:R:414:VAL:HG21	1:R:454:ARG:CG	2.46	0.46
1:B:293:THR:CB	1:B:413:ILE:HD11	2.46	0.46
1:D:315:VAL:HG13	1:D:315:VAL:O	2.15	0.46
1:M:405:LEU:HD11	1:M:467:MET:HE3	1.97	0.46
1:T:315:VAL:O	1:T:323:LYS:NZ	2.48	0.46
1:W:245:ILE:HG21	1:W:349:LEU:HD23	1.98	0.46
1:X:283:GLY:CA	2:X:600:LDN:CAE	2.93	0.46
1:X:483:LEU:CD1	1:X:487:LYS:HE3	2.43	0.46
1:X:281:GLU:O	2:X:600:LDN:HAH	2.16	0.46
1:G:460:VAL:HA	1:G:492:ILE:HG21	1.98	0.46
1:H:414:VAL:CG1	1:H:454:ARG:HG2	2.46	0.46
1:W:420:ASP:OD2	1:W:422:ARG:CZ	2.64	0.46
1:D:317:ILE:N	1:D:317:ILE:CD1	2.75	0.45
1:L:382:ASP:CG	1:P:477:SER:HG	2.17	0.45
1:R:427:ASP:C	1:T:417:ILE:HD12	2.37	0.45
1:X:283:GLY:HA3	2:X:600:LDN:CAE	2.46	0.45
1:X:337:LEU:CD1	2:X:600:LDN:HAJ	2.45	0.45
1:B:305:SER:CB	1:B:343:GLN:HG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:272:GLN:O	1:F:273:LEU:HD23	2.16	0.45
1:F:351:LEU:HG	1:F:369:ARG:HG2	1.97	0.45
1:P:409:ALA:HB1	1:P:455:LEU:HD22	1.97	0.45
1:X:335:ASN:HA	2:X:600:LDN:HAA	1.98	0.45
2:E:600:LDN:CBC	2:E:600:LDN:HAJ	2.46	0.45
1:H:414:VAL:HG13	1:H:454:ARG:HG2	1.98	0.45
1:O:315:VAL:CG1	1:O:315:VAL:O	2.64	0.45
1:F:289:LEU:CD2	1:F:294:LEU:HD11	2.46	0.45
1:F:328:HIS:O	1:F:329:ARG:HB2	2.15	0.45
1:M:305:SER:CB	1:M:343:GLN:CG	2.95	0.45
1:T:317:ILE:HG22	1:T:322:GLY:HA2	1.98	0.45
1:B:467:MET:SD	1:B:489:LEU:HG	2.56	0.45
1:C:293:THR:CB	1:C:413:ILE:HD11	2.47	0.45
1:D:239:TRP:CE2	1:D:273:LEU:HD23	2.50	0.45
1:H:315:VAL:O	1:H:315:VAL:HG13	2.15	0.45
1:F:355:HIS:NE2	1:F:360:ASP:OD2	2.47	0.45
1:J:403:LEU:HD23	1:J:472:TRP:CZ2	2.52	0.45
1:K:199:ALA:CB	1:K:276:ILE:HD11	2.44	0.45
1:M:484:ARG:HA	1:M:484:ARG:HD2	1.77	0.45
1:O:451:ILE:HG23	1:O:455:LEU:HD12	1.98	0.45
1:X:405:LEU:HD11	1:X:467:MET:HE2	1.99	0.45
1:B:435:PHE:CD2	1:B:435:PHE:O	2.70	0.45
1:C:451:ILE:O	1:C:452:PRO:C	2.53	0.45
1:E:320:THR:HG22	1:E:321:GLN:N	2.30	0.45
1:N:315:VAL:CG1	1:N:315:VAL:O	2.64	0.45
1:P:195:GLN:HG2	1:P:261:ALA:CA	2.46	0.45
1:R:357:GLN:O	1:R:358:GLY:C	2.55	0.45
1:R:467:MET:CE	1:R:489:LEU:HD21	2.47	0.45
1:X:455:LEU:HD22	1:X:465:ALA:CB	2.39	0.45
1:O:337:LEU:HD21	2:O:600:LDN:CBC	2.47	0.45
1:T:489:LEU:O	1:T:490:GLN:C	2.55	0.45
1:B:480:LEU:HD22	1:B:484:ARG:HG2	1.99	0.45
1:G:485:ILE:O	1:G:489:LEU:HD12	2.17	0.45
1:A:257:LEU:HD13	1:A:337:LEU:HD13	1.99	0.45
1:D:239:TRP:CD2	1:D:273:LEU:HD22	2.52	0.45
1:K:427:ASP:OD1	1:K:428:VAL:HG13	2.16	0.45
1:N:265:THR:HG21	1:N:274:TRP:CE2	2.52	0.45
1:P:351:LEU:HD21	1:P:369:ARG:O	2.17	0.45
1:E:281:GLU:O	2:E:600:LDN:HAH	2.18	0.44
1:K:375:TYR:HD1	1:K:403:LEU:HD12	1.82	0.44
2:O:600:LDN:CBC	2:O:600:LDN:HAJ	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:600:LDN:HAM	2:P:600:LDN:HAF	1.76	0.44
1:R:414:VAL:HG21	1:R:454:ARG:HG3	1.98	0.44
1:F:252:ARG:O	1:F:252:ARG:HG2	2.16	0.44
1:I:467:MET:HE1	1:I:489:LEU:CD1	2.41	0.44
1:M:381:LEU:HA	1:M:435:PHE:CZ	2.52	0.44
1:Q:251:LEU:HD11	1:Q:326:ILE:CD1	2.48	0.44
1:A:273:LEU:HD22	1:A:273:LEU:N	2.32	0.44
1:N:458:ASP:CB	1:N:461:LEU:HD12	2.47	0.44
1:U:455:LEU:HD22	1:U:461:LEU:HB3	1.99	0.44
1:C:386:ARG:NH1	1:C:386:ARG:HB2	2.33	0.44
1:E:357:GLN:HG2	1:E:357:GLN:O	2.17	0.44
1:E:381:LEU:HD23	1:E:435:PHE:CE1	2.52	0.44
1:O:283:GLY:CA	2:O:600:LDN:CAV	2.94	0.44
1:R:405:LEU:HD11	1:R:467:MET:CE	2.47	0.44
1:S:258:GLY:O	1:S:277:THR:HB	2.17	0.44
1:B:245:ILE:HG21	1:B:349:LEU:HD23	2.00	0.44
1:B:251:LEU:HA	1:B:251:LEU:HD23	1.84	0.44
1:D:239:TRP:CE3	1:D:273:LEU:HD23	2.52	0.44
1:E:467:MET:HE1	1:E:489:LEU:CD1	2.39	0.44
1:H:304:VAL:HA	1:H:489:LEU:HD13	1.99	0.44
1:K:198:VAL:HG13	1:K:221:TRP:CH2	2.52	0.44
1:P:245:ILE:HG21	1:P:349:LEU:HD23	1.99	0.44
1:S:414:VAL:CG1	1:S:461:LEU:HD12	2.47	0.44
1:U:461:LEU:HA	1:U:464:LEU:HD13	1.99	0.44
1:X:245:ILE:HG21	1:X:349:LEU:HD23	2.00	0.44
1:X:315:VAL:HG13	1:X:315:VAL:O	2.17	0.44
1:X:386:ARG:HG2	1:X:388:ASP:OD1	2.17	0.44
1:C:414:VAL:O	1:C:416:GLY:N	2.51	0.44
1:C:431:ASN:OD1	1:C:431:ASN:N	2.51	0.44
1:D:245:ILE:HG21	1:D:349:LEU:HD23	1.99	0.44
1:G:432:ASP:O	1:G:433:PRO:C	2.55	0.44
1:N:205:VAL:HG11	1:N:218:ARG:NH2	2.33	0.44
1:O:198:VAL:O	1:O:202:VAL:CG2	2.55	0.44
1:P:410:ARG:NH2	1:P:426:TYR:OH	2.50	0.44
1:Q:264:MET:HG3	1:Q:273:LEU:HD21	1.99	0.44
1:R:251:LEU:HD11	1:R:326:ILE:CD1	2.48	0.44
1:V:417:ILE:HA	1:V:417:ILE:HD12	1.82	0.44
1:B:337:LEU:HD21	2:B:600:LDN:CBC	2.48	0.44
1:H:414:VAL:HG13	1:H:454:ARG:HD2	2.00	0.44
1:I:312:HIS:O	1:I:323:LYS:NZ	2.44	0.44
1:R:467:MET:CE	1:R:485:ILE:HG23	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:295:GLU:HG2	1:L:296:PRO:CD	2.47	0.44
1:L:480:LEU:HD22	1:L:484:ARG:HG2	2.00	0.44
2:P:600:LDN:HAQA	2:P:600:LDN:HAH	1.82	0.44
1:Q:206:GLU:HG2	1:Q:208:VAL:HG13	2.00	0.44
1:I:422:ARG:HD2	1:I:426:TYR:CD1	2.53	0.43
1:M:315:VAL:O	1:M:315:VAL:HG13	2.17	0.43
1:A:475:ASN:HB2	1:E:474:PRO:HB2	1.99	0.43
1:C:454:ARG:CG	1:C:454:ARG:O	2.66	0.43
1:I:285:LEU:O	1:I:289:LEU:HG	2.18	0.43
1:J:315:VAL:HG13	1:J:315:VAL:O	2.18	0.43
1:M:386:ARG:HG2	1:M:388:ASP:OD1	2.19	0.43
1:L:292:GLN:NE2	2:Q:600:LDN:HAOA	2.33	0.43
1:V:315:VAL:O	1:V:315:VAL:CG1	2.65	0.43
1:X:455:LEU:HB3	1:X:465:ALA:CB	2.48	0.43
1:G:414:VAL:O	1:G:416:GLY:N	2.51	0.43
1:J:401:PHE:O	1:J:404:VAL:HG12	2.18	0.43
1:M:462:SER:O	1:M:465:ALA:HB3	2.18	0.43
1:O:289:LEU:HD11	1:O:408:ILE:HA	1.98	0.43
1:Q:202:VAL:HG22	1:Q:221:TRP:HB2	2.00	0.43
1:R:403:LEU:HD23	1:R:472:TRP:CE2	2.53	0.43
2:A:600:LDN:HAJ	2:A:600:LDN:CBC	2.49	0.43
1:G:239:TRP:CE3	1:G:273:LEU:HD12	2.53	0.43
1:S:275:LEU:HD13	1:S:277:THR:CG2	2.46	0.43
1:W:414:VAL:CG2	1:W:454:ARG:CZ	2.96	0.43
1:W:420:ASP:OD2	1:W:422:ARG:NH2	2.51	0.43
1:X:235:ASP:OD1	1:X:369:ARG:CD	2.67	0.43
1:F:486:LYS:HG2	1:F:490:GLN:HE22	1.83	0.43
1:E:218:ARG:NH1	3:E:113:HOH:O	2.52	0.43
1:E:405:LEU:HD11	1:E:467:MET:CE	2.48	0.43
1:F:454:ARG:CG	1:F:454:ARG:O	2.66	0.43
2:G:600:LDN:HAQA	2:G:600:LDN:HAH	1.77	0.43
1:G:233:SER:OG	1:K:211:GLY:HA2	2.19	0.43
1:L:245:ILE:HG21	1:L:349:LEU:HD23	2.01	0.43
1:N:461:LEU:HD23	1:N:464:LEU:CD1	2.46	0.43
1:Q:244:GLU:O	1:Q:248:THR:HB	2.19	0.43
1:S:443:CYS:O	1:S:446:GLN:OE1	2.36	0.43
1:U:198:VAL:HG13	1:U:221:TRP:CE2	2.53	0.43
1:A:366:ASN:ND2	1:M:263:ASP:OD2	2.52	0.43
1:B:300:LEU:HD23	1:B:489:LEU:HD22	2.00	0.43
1:G:273:LEU:N	1:G:273:LEU:HD22	2.33	0.43
1:E:239:TRP:CE3	1:E:273:LEU:HD13	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:198:VAL:O	1:G:202:VAL:N	2.51	0.43
1:K:381:LEU:HD23	1:K:435:PHE:CE1	2.52	0.43
1:Q:315:VAL:O	1:Q:315:VAL:CG1	2.67	0.43
1:R:316:GLU:CD	1:R:357:GLN:H	2.22	0.43
1:W:332:LYS:HE3	1:W:334:ARG:HB2	2.01	0.43
1:C:239:TRP:CE3	1:C:273:LEU:HD22	2.53	0.43
1:F:283:GLY:HA2	2:F:600:LDN:CAV	2.49	0.43
1:I:451:ILE:HA	1:I:452:PRO:HD2	1.83	0.43
1:N:381:LEU:HA	1:N:435:PHE:CZ	2.53	0.43
1:E:258:GLY:O	1:E:277:THR:HB	2.19	0.43
1:F:237:GLN:OE1	1:F:366:ASN:O	2.36	0.43
1:G:315:VAL:O	1:G:315:VAL:HG13	2.19	0.43
1:H:418:VAL:HA	1:H:454:ARG:NH1	2.34	0.43
1:M:305:SER:CB	1:M:343:GLN:HG3	2.48	0.43
1:T:205:VAL:HG21	1:T:220:LEU:HD23	1.99	0.43
1:U:405:LEU:HD11	1:U:467:MET:HE3	2.01	0.43
1:U:405:LEU:HD11	1:U:467:MET:CE	2.48	0.43
1:D:459:PRO:CD	1:D:460:VAL:H	2.32	0.42
1:E:252:ARG:HB3	1:E:252:ARG:NH1	2.33	0.42
2:F:600:LDN:HAH	2:F:600:LDN:HAQA	1.82	0.42
1:L:364:ILE:HG22	1:L:365:GLY:O	2.18	0.42
1:P:283:GLY:CA	2:P:600:LDN:CAF	2.96	0.42
1:R:431:ASN:O	1:R:433:PRO:HD3	2.18	0.42
1:T:373:LYS:HD3	1:T:433:PRO:O	2.19	0.42
1:W:422:ARG:HD2	1:W:426:TYR:CD1	2.52	0.42
1:H:465:ALA:O	1:H:469:ARG:HG2	2.19	0.42
1:K:245:ILE:HG21	1:K:349:LEU:HD23	2.01	0.42
1:N:205:VAL:HG21	1:N:220:LEU:HG	2.00	0.42
1:A:451:ILE:O	1:A:452:PRO:C	2.56	0.42
1:D:0:MET:O	1:D:196:ARG:N	2.52	0.42
1:E:465:ALA:HA	1:E:468:MET:HE3	2.01	0.42
2:L:600:LDN:HAJ	2:L:600:LDN:CBC	2.48	0.42
1:M:282:HIS:HA	1:M:291:ARG:NH2	2.34	0.42
2:N:600:LDN:HAQA	2:N:600:LDN:HAH	1.75	0.42
1:P:457:ALA:O	1:P:458:ASP:CB	2.67	0.42
1:R:316:GLU:OE1	1:R:357:GLN:HB2	2.20	0.42
1:V:431:ASN:O	1:V:433:PRO:HD3	2.19	0.42
1:A:221:TRP:NE1	1:A:222:HIS:CE1	2.87	0.42
1:G:355:HIS:C	1:G:355:HIS:ND1	2.72	0.42
1:M:205:VAL:HG12	1:M:206:GLU:HG3	2.02	0.42
1:O:283:GLY:HA3	2:O:600:LDN:CAE	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:382:ASP:HB3	1:Q:384:GLN:HG2	2.02	0.42
1:U:289:LEU:CD2	1:U:294:LEU:HD11	2.50	0.42
2:X:600:LDN:HAQA	2:X:600:LDN:HAH	1.91	0.42
1:F:377:ALA:O	1:F:381:LEU:HD12	2.20	0.42
1:J:403:LEU:HD23	1:J:472:TRP:CE2	2.54	0.42
1:J:412:THR:HG21	1:J:461:LEU:HD21	2.00	0.42
1:L:316:GLU:CD	1:L:357:GLN:H	2.23	0.42
1:N:300:LEU:HD21	1:N:492:ILE:O	2.19	0.42
1:O:405:LEU:HD11	1:O:467:MET:CE	2.50	0.42
1:R:258:GLY:O	1:R:277:THR:HB	2.20	0.42
2:W:600:LDN:NAS	2:W:600:LDN:HAJ	2.34	0.42
1:D:466:GLN:O	1:D:470:GLU:HG3	2.20	0.42
1:H:244:GLU:O	1:H:248:THR:HB	2.18	0.42
1:N:237:GLN:HG2	1:N:367:ASN:HA	2.01	0.42
1:U:245:ILE:HG21	1:U:349:LEU:HD23	2.00	0.42
1:A:315:VAL:O	1:A:315:VAL:CG1	2.68	0.42
1:I:467:MET:CE	1:I:489:LEU:HD21	2.49	0.42
1:M:312:HIS:O	1:M:323:LYS:CE	2.67	0.42
1:L:475:ASN:HB2	1:P:474:PRO:HB3	2.01	0.42
1:R:360:ASP:N	1:R:360:ASP:OD1	2.48	0.42
1:N:473:TYR:CE1	1:R:384:GLN:NE2	2.88	0.42
2:D:600:LDN:HAF	2:D:600:LDN:HAM	1.80	0.42
1:H:373:LYS:HA	1:H:376:MET:HG3	2.01	0.42
1:Q:328:HIS:O	1:Q:329:ARG:HB2	2.20	0.42
1:S:315:VAL:CG1	1:S:315:VAL:O	2.68	0.42
1:T:386:ARG:NE	1:T:392:SER:OG	2.52	0.42
1:T:425:PHE:O	1:T:429:VAL:HG22	2.19	0.42
1:A:295:GLU:HG2	1:A:296:PRO:HD2	2.02	0.42
1:A:452:PRO:C	1:A:454:ARG:H	2.23	0.42
1:G:244:GLU:O	1:G:248:THR:HB	2.19	0.42
1:G:484:ARG:NH1	3:G:10:HOH:O	2.51	0.42
1:D:252:ARG:NH1	1:I:317:ILE:HD13	2.35	0.42
1:J:337:LEU:HD22	2:J:600:LDN:NAT	2.34	0.42
1:U:246:TYR:CD1	1:U:259:PHE:HB2	2.55	0.42
1:W:467:MET:SD	1:W:489:LEU:HG	2.60	0.42
1:B:300:LEU:HD11	1:B:493:SER:HA	2.02	0.42
2:P:600:LDN:HAJ	2:P:600:LDN:CBC	2.49	0.42
1:S:257:LEU:HD13	1:S:337:LEU:HD13	2.01	0.42
1:W:202:VAL:HG22	1:W:221:TRP:HB2	2.02	0.42
1:L:282:HIS:O	1:L:291:ARG:NH2	2.53	0.41
1:L:475:ASN:HB2	1:P:474:PRO:CB	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:409:ALA:HB1	1:P:455:LEU:CD2	2.50	0.41
1:P:422:ARG:CB	1:P:426:TYR:CD1	3.03	0.41
1:R:376:MET:HG2	1:R:380:VAL:HG11	2.01	0.41
1:R:434:SER:O	1:R:435:PHE:C	2.58	0.41
1:U:315:VAL:CG1	1:U:315:VAL:O	2.68	0.41
1:J:252:ARG:HD3	1:W:486:LYS:CE	2.50	0.41
1:E:245:ILE:HG21	1:E:349:LEU:HD23	2.02	0.41
1:E:252:ARG:CZ	1:E:252:ARG:HB3	2.50	0.41
1:J:280:HIS:O	2:J:600:LDN:HAM	2.20	0.41
1:L:251:LEU:HD21	1:L:349:LEU:HD21	2.02	0.41
1:R:427:ASP:OD1	1:R:428:VAL:HG13	2.21	0.41
1:S:245:ILE:HG21	1:S:349:LEU:HD23	2.00	0.41
1:S:275:LEU:CD1	1:S:277:THR:CG2	2.98	0.41
1:V:245:ILE:HG21	1:V:349:LEU:HD23	2.03	0.41
1:W:315:VAL:CG1	1:W:315:VAL:O	2.68	0.41
1:C:239:TRP:CD2	1:C:273:LEU:CD2	3.02	0.41
1:D:236:GLU:HG2	1:D:273:LEU:HD13	2.01	0.41
1:K:381:LEU:HD11	1:K:438:MET:CB	2.50	0.41
1:R:434:SER:C	1:R:436:GLU:N	2.73	0.41
1:L:315:VAL:O	1:L:315:VAL:CG1	2.69	0.41
1:Q:415:ASN:O	1:Q:417:ILE:HD12	2.20	0.41
1:Q:467:MET:HE3	1:Q:485:ILE:HG23	2.02	0.41
2:V:600:LDN:NAS	2:V:600:LDN:HAJ	2.35	0.41
1:X:204:LEU:HD22	1:X:217:TRP:CB	2.49	0.41
1:B:455:LEU:HD12	1:B:461:LEU:CB	2.43	0.41
1:B:300:LEU:HD11	1:B:493:SER:CA	2.50	0.41
1:E:486:LYS:O	1:E:490:GLN:HG3	2.20	0.41
1:F:258:GLY:O	1:F:277:THR:HB	2.21	0.41
1:F:315:VAL:CG1	1:F:315:VAL:O	2.68	0.41
1:I:246:TYR:CD1	1:I:259:PHE:HB2	2.55	0.41
1:L:331:PHE:O	1:L:400:ALA:HB1	2.21	0.41
1:P:195:GLN:CG	1:P:261:ALA:HB1	2.45	0.41
1:Q:362:LEU:HA	1:Q:362:LEU:HD12	1.90	0.41
1:B:315:VAL:CG1	1:B:315:VAL:O	2.69	0.41
1:B:348:ASP:HB2	2:B:600:LDN:HAI	2.03	0.41
1:C:0:MET:CB	1:C:197:THR:HB	2.50	0.41
1:C:198:VAL:O	1:C:202:VAL:HG23	2.20	0.41
1:E:464:LEU:CD2	1:E:489:LEU:CD2	2.98	0.41
1:H:414:VAL:HG13	1:H:454:ARG:CD	2.50	0.41
1:I:414:VAL:CG1	1:I:454:ARG:HD2	2.48	0.41
1:J:245:ILE:HG21	1:J:349:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:460:VAL:CG1	1:S:461:LEU:HD23	2.45	0.41
1:T:414:VAL:C	1:T:416:GLY:N	2.74	0.41
1:F:405:LEU:HD11	1:F:467:MET:CE	2.50	0.41
1:M:251:LEU:HD11	1:M:326:ILE:HD12	2.02	0.41
1:Q:206:GLU:HG2	1:Q:208:VAL:CG1	2.51	0.41
1:T:357:GLN:O	1:T:358:GLY:C	2.59	0.41
1:U:289:LEU:HD21	1:U:294:LEU:HD11	2.02	0.41
2:W:600:LDN:HAH	2:W:600:LDN:HAQA	1.81	0.41
1:D:289:LEU:HD11	1:D:408:ILE:HA	2.03	0.41
1:E:315:VAL:O	1:E:315:VAL:CG1	2.69	0.41
1:E:490:GLN:O	1:E:493:SER:N	2.52	0.41
1:G:405:LEU:HD11	1:G:467:MET:CE	2.50	0.41
1:H:386:ARG:NH2	1:I:446:GLN:OE1	2.54	0.41
1:O:244:GLU:O	1:O:248:THR:HB	2.20	0.41
1:S:304:VAL:HA	1:S:489:LEU:HD13	2.02	0.41
1:V:252:ARG:HG2	1:V:252:ARG:HH11	1.86	0.41
1:W:286:TYR:HB2	1:W:334:ARG:HG2	2.02	0.41
1:X:329:ARG:HH11	1:X:353:VAL:CG1	2.34	0.41
1:J:467:MET:HE1	1:J:485:ILE:HG23	2.03	0.41
1:L:220:LEU:HD12	1:L:224:GLU:O	2.21	0.41
1:L:467:MET:HE1	1:L:489:LEU:HD11	2.03	0.41
1:O:239:TRP:CE3	1:O:273:LEU:HD23	2.56	0.41
1:P:246:TYR:CD1	1:P:259:PHE:HB2	2.55	0.41
1:Q:470:GLU:HG2	1:Q:473:TYR:OH	2.21	0.41
1:T:456:ALA:O	1:T:458:ASP:N	2.54	0.41
1:L:458:ASP:O	1:L:462:SER:HB2	2.21	0.41
1:S:244:GLU:O	1:S:248:THR:HB	2.20	0.41
1:S:230:ILE:HG21	1:S:272:GLN:OE1	2.21	0.41
1:S:386:ARG:NH1	1:T:446:GLN:CB	2.84	0.41
1:X:258:GLY:O	1:X:277:THR:HB	2.21	0.41
1:X:454:ARG:O	1:X:454:ARG:HG3	2.21	0.41
1:X:480:LEU:HD22	1:X:484:ARG:HG3	1.99	0.41
1:B:460:VAL:HA	1:B:492:ILE:HG21	2.03	0.41
1:D:315:VAL:CG1	1:D:315:VAL:O	2.69	0.41
1:F:355:HIS:NE2	1:F:360:ASP:HA	2.36	0.41
1:F:386:ARG:HG2	1:F:392:SER:OG	2.21	0.41
1:I:317:ILE:HD12	1:I:323:LYS:HD3	2.03	0.41
2:I:600:LDN:CBC	2:I:600:LDN:HAJ	2.50	0.41
1:J:246:TYR:CD1	1:J:259:PHE:HB2	2.56	0.41
1:S:418:VAL:HG13	1:S:418:VAL:O	2.21	0.41
1:B:451:ILE:O	1:B:452:PRO:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:403:LEU:HD23	1:R:472:TRP:CZ2	2.56	0.40
1:V:294:LEU:CD1	1:V:411:ARG:HB3	2.51	0.40
1:A:487:LYS:O	1:A:491:LYS:HG3	2.21	0.40
1:B:298:LEU:HD12	1:B:298:LEU:O	2.20	0.40
1:C:431:ASN:O	1:C:433:PRO:CD	2.69	0.40
1:D:459:PRO:HD2	1:D:460:VAL:HG23	2.02	0.40
1:G:195:GLN:O	1:G:196:ARG:C	2.59	0.40
2:G:600:LDN:HAF	2:G:600:LDN:HAM	1.84	0.40
1:H:230:ILE:CG2	1:H:272:GLN:OE1	2.70	0.40
1:I:295:GLU:HG2	1:I:297:HIS:H	1.86	0.40
1:M:376:MET:HG2	1:M:380:VAL:HG11	2.04	0.40
1:N:328:HIS:O	1:N:329:ARG:HB2	2.21	0.40
1:O:246:TYR:CD1	1:O:259:PHE:HB2	2.56	0.40
1:S:304:VAL:HG13	1:S:305:SER:N	2.36	0.40
1:E:414:VAL:HG11	1:E:454:ARG:CG	2.51	0.40
1:I:295:GLU:HG2	1:I:297:HIS:N	2.36	0.40
1:N:464:LEU:HD23	1:N:464:LEU:N	2.34	0.40
2:V:600:LDN:HAP	2:V:600:LDN:HAG	1.84	0.40
1:X:207:CYS:HB2	1:X:217:TRP:CE2	2.56	0.40
1:X:468:MET:O	1:X:472:TRP:NE1	2.54	0.40
1:B:305:SER:HB3	1:B:343:GLN:CG	2.52	0.40
1:G:464:LEU:HD21	1:G:489:LEU:CD2	2.45	0.40
1:J:241:ARG:HE	1:J:245:ILE:HD11	1.86	0.40
1:M:305:SER:CB	1:M:343:GLN:HG2	2.51	0.40
1:N:440:LYS:HA	1:N:444:VAL:CG2	2.51	0.40
1:O:239:TRP:CE3	1:O:273:LEU:CD2	3.04	0.40
1:R:355:HIS:C	1:R:355:HIS:ND1	2.74	0.40
1:R:433:PRO:HB2	1:R:438:MET:HG2	2.03	0.40
1:U:412:THR:HG21	1:U:461:LEU:CD2	2.50	0.40
2:W:600:LDN:HAF	2:W:600:LDN:HAM	1.80	0.40
1:A:252:ARG:HE	1:A:253:HIS:N	2.19	0.40
1:B:464:LEU:HD23	1:B:464:LEU:HA	1.94	0.40
1:C:434:SER:OG	1:C:437:ASP:OD2	2.39	0.40
1:F:490:GLN:HE21	1:F:490:GLN:HB2	1.57	0.40
1:G:205:VAL:HG11	1:G:218:ARG:NH2	2.37	0.40
1:L:258:GLY:O	1:L:277:THR:HB	2.21	0.40
2:L:600:LDN:HAH	2:L:600:LDN:HAQA	1.87	0.40
1:M:249:VAL:HG12	1:M:251:LEU:HD13	2.02	0.40

All (5) 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:E:416:GLY:CA	1:H:205:VAL:O[1_445]	2.08	0.12
1:Q:252:ARG:NH2	1:S:252:ARG:O[1_665]	2.08	0.12
1:B:386:ARG:NH2	1:K:382:ASP:O[1_655]	2.10	0.10
1:G:416:GLY:O	1:J:207:CYS:N[1_455]	2.12	0.08
1:U:291:ARG:O	2:R:600:LDN:NAU[1_655]	2.14	0.06

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	292/305 (96%)	279 (96%)	12 (4%)	1 (0%)	41	56
1	B	291/305 (95%)	277 (95%)	11 (4%)	3 (1%)	15	23
1	C	297/305 (97%)	277 (93%)	18 (6%)	2 (1%)	22	33
1	D	296/305 (97%)	277 (94%)	17 (6%)	2 (1%)	22	33
1	E	290/305 (95%)	272 (94%)	15 (5%)	3 (1%)	15	23
1	F	290/305 (95%)	276 (95%)	10 (3%)	4 (1%)	11	16
1	G	290/305 (95%)	272 (94%)	14 (5%)	4 (1%)	11	16
1	H	290/305 (95%)	270 (93%)	20 (7%)	0	100	100
1	I	289/305 (95%)	271 (94%)	17 (6%)	1 (0%)	41	56
1	J	240/305 (79%)	231 (96%)	7 (3%)	2 (1%)	19	29
1	K	249/305 (82%)	242 (97%)	6 (2%)	1 (0%)	34	48
1	L	292/305 (96%)	279 (96%)	12 (4%)	1 (0%)	41	56
1	M	294/305 (96%)	280 (95%)	12 (4%)	2 (1%)	22	33
1	N	298/305 (98%)	277 (93%)	17 (6%)	4 (1%)	12	18
1	O	295/305 (97%)	278 (94%)	16 (5%)	1 (0%)	41	56
1	P	284/305 (93%)	260 (92%)	15 (5%)	9 (3%)	4	5
1	Q	290/305 (95%)	279 (96%)	10 (3%)	1 (0%)	41	56
1	R	290/305 (95%)	275 (95%)	13 (4%)	2 (1%)	22	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	290/305 (95%)	270 (93%)	15 (5%)	5 (2%)	9	13
1	T	288/305 (94%)	274 (95%)	9 (3%)	5 (2%)	9	13
1	U	277/305 (91%)	267 (96%)	8 (3%)	2 (1%)	22	33
1	V	274/305 (90%)	258 (94%)	14 (5%)	2 (1%)	22	33
1	W	273/305 (90%)	261 (96%)	11 (4%)	1 (0%)	34	48
1	X	245/305 (80%)	239 (98%)	6 (2%)	0	100	100
All	All	6804/7320 (93%)	6441 (95%)	305 (4%)	58 (1%)	17	26

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	359	SER
1	G	415	ASN
1	J	453	ASN
1	P	373	LYS
1	P	431	ASN
1	P	433	PRO
1	U	359	SER
1	D	195	GLN
1	F	320	THR
1	F	453	ASN
1	L	462	SER
1	N	492	ILE
1	P	454	ARG
1	S	198	VAL
1	S	459	PRO
1	S	460	VAL
1	T	358	GLY
1	T	415	ASN
1	T	457	ALA
1	A	459	PRO
1	B	357	GLN
1	B	360	ASP
1	C	269	SER
1	D	269	SER
1	E	198	VAL
1	E	361	TYR
1	G	456	ALA
1	J	454	ARG
1	N	269	SER

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Mol	Chain	Res	Type
1	O	269	SER
1	P	355	HIS
1	R	435	PHE
1	T	196	ARG
1	F	365	GLY
1	I	357	GLN
1	M	415	ASN
1	M	454	ARG
1	P	453	ASN
1	P	460	VAL
1	R	456	ALA
1	S	435	PHE
1	T	456	ALA
1	V	431	ASN
1	W	453	ASN
1	B	459	PRO
1	C	415	ASN
1	F	431	ASN
1	N	196	ARG
1	N	454	ARG
1	P	435	PHE
1	U	459	PRO
1	K	433	PRO
1	Q	460	VAL
1	P	458	ASP
1	S	414	VAL
1	V	414	VAL
1	E	364	ILE
1	G	432	ASP

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	236/267 (88%)	226 (96%)	10 (4%)	30	45
1	B	240/267 (90%)	226 (94%)	14 (6%)	20	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	231/267 (86%)	225 (97%)	6 (3%)	46	64
1	D	232/267 (87%)	223 (96%)	9 (4%)	32	48
1	E	228/267 (85%)	220 (96%)	8 (4%)	36	52
1	F	222/267 (83%)	210 (95%)	12 (5%)	22	34
1	G	234/267 (88%)	221 (94%)	13 (6%)	21	33
1	H	222/267 (83%)	212 (96%)	10 (4%)	27	42
1	I	238/267 (89%)	221 (93%)	17 (7%)	14	22
1	J	185/267 (69%)	176 (95%)	9 (5%)	25	38
1	K	180/267 (67%)	173 (96%)	7 (4%)	32	48
1	L	240/267 (90%)	231 (96%)	9 (4%)	33	49
1	M	243/267 (91%)	235 (97%)	8 (3%)	38	54
1	N	234/267 (88%)	227 (97%)	7 (3%)	41	59
1	O	231/267 (86%)	223 (96%)	8 (4%)	36	52
1	P	198/267 (74%)	193 (98%)	5 (2%)	47	66
1	Q	228/267 (85%)	216 (95%)	12 (5%)	22	35
1	R	231/267 (86%)	220 (95%)	11 (5%)	25	39
1	S	224/267 (84%)	218 (97%)	6 (3%)	44	63
1	T	233/267 (87%)	218 (94%)	15 (6%)	17	27
1	U	212/267 (79%)	206 (97%)	6 (3%)	43	61
1	V	207/267 (78%)	202 (98%)	5 (2%)	49	67
1	W	231/267 (86%)	225 (97%)	6 (3%)	46	64
1	X	194/267 (73%)	190 (98%)	4 (2%)	53	72
All	All	5354/6408 (84%)	5137 (96%)	217 (4%)	30	46

All (217) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	233	SER
1	A	252	ARG
1	A	271	THR
1	A	272	GLN
1	A	273	LEU
1	A	323	LYS
1	A	360	ASP

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Mol	Chain	Res	Type
1	A	361	TYR
1	A	420	ASP
1	A	432	ASP
1	B	201	GLN
1	B	233	SER
1	B	263	ASP
1	B	291	ARG
1	B	297	HIS
1	B	300	LEU
1	B	323	LYS
1	B	343	GLN
1	B	359	SER
1	B	369	ARG
1	B	386	ARG
1	B	418	VAL
1	B	446	GLN
1	B	491	LYS
1	C	265	THR
1	C	291	ARG
1	C	295	GLU
1	C	300	LEU
1	C	475	ASN
1	C	484	ARG
1	D	233	SER
1	D	252	ARG
1	D	273	LEU
1	D	292	GLN
1	D	295	GLU
1	D	321	GLN
1	D	343	GLN
1	D	413	ILE
1	D	484	ARG
1	E	224	GLU
1	E	291	ARG
1	E	323	LYS
1	E	355	HIS
1	E	361	TYR
1	E	382	ASP
1	E	432	ASP
1	E	483	LEU
1	F	252	ARG
1	F	264	MET

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Mol	Chain	Res	Type
1	F	354	MET
1	F	360	ASP
1	F	361	TYR
1	F	362	LEU
1	F	386	ARG
1	F	415	ASN
1	F	418	VAL
1	F	428	VAL
1	F	484	ARG
1	F	490	GLN
1	G	220	LEU
1	G	263	ASP
1	G	273	LEU
1	G	275	LEU
1	G	323	LYS
1	G	360	ASP
1	G	361	TYR
1	G	370	VAL
1	G	382	ASP
1	G	385	ILE
1	G	446	GLN
1	G	447	GLN
1	G	450	THR
1	H	222	HIS
1	H	250	LEU
1	H	273	LEU
1	H	316	GLU
1	H	386	ARG
1	H	414	VAL
1	H	432	ASP
1	H	451	ILE
1	H	458	ASP
1	H	469	ARG
1	I	197	THR
1	I	218	ARG
1	I	237	GLN
1	I	273	LEU
1	I	291	ARG
1	I	292	GLN
1	I	295	GLU
1	I	300	LEU
1	I	323	LYS

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Mol	Chain	Res	Type
1	I	361	TYR
1	I	386	ARG
1	I	431	ASN
1	I	432	ASP
1	I	455	LEU
1	I	475	ASN
1	I	484	ARG
1	I	492	ILE
1	J	252	ARG
1	J	275	LEU
1	J	297	HIS
1	J	300	LEU
1	J	308	CYS
1	J	381	LEU
1	J	404	VAL
1	J	412	THR
1	J	462	SER
1	K	197	THR
1	K	252	ARG
1	K	271	THR
1	K	297	HIS
1	K	301	ARG
1	K	382	ASP
1	K	412	THR
1	L	252	ARG
1	L	273	LEU
1	L	292	GLN
1	L	360	ASP
1	L	361	TYR
1	L	432	ASP
1	L	454	ARG
1	L	455	LEU
1	L	468	MET
1	M	265	THR
1	M	343	GLN
1	M	354	MET
1	M	360	ASP
1	M	361	TYR
1	M	431	ASN
1	M	475	ASN
1	M	484	ARG
1	N	265	THR

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Mol	Chain	Res	Type
1	N	272	GLN
1	N	291	ARG
1	N	382	ASP
1	N	432	ASP
1	N	446	GLN
1	N	454	ARG
1	O	220	LEU
1	O	237	GLN
1	O	265	THR
1	O	291	ARG
1	O	334	ARG
1	O	426	TYR
1	O	435	PHE
1	O	483	LEU
1	P	342	LEU
1	P	366	ASN
1	P	415	ASN
1	P	419	GLU
1	P	426	TYR
1	Q	233	SER
1	Q	234	ARG
1	Q	252	ARG
1	Q	264	MET
1	Q	291	ARG
1	Q	300	LEU
1	Q	359	SER
1	Q	413	ILE
1	Q	414	VAL
1	Q	439	LYS
1	Q	454	ARG
1	Q	493	SER
1	R	295	GLU
1	R	300	LEU
1	R	360	ASP
1	R	361	TYR
1	R	376	MET
1	R	384	GLN
1	R	414	VAL
1	R	417	ILE
1	R	420	ASP
1	R	447	GLN
1	R	484	ARG

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Mol	Chain	Res	Type
1	S	250	LEU
1	S	382	ASP
1	S	412	THR
1	S	414	VAL
1	S	458	ASP
1	S	469	ARG
1	T	197	THR
1	T	202	VAL
1	T	222	HIS
1	T	272	GLN
1	T	300	LEU
1	T	323	LYS
1	T	360	ASP
1	T	361	TYR
1	T	366	ASN
1	T	386	ARG
1	T	412	THR
1	T	431	ASN
1	T	446	GLN
1	T	454	ARG
1	T	484	ARG
1	U	197	THR
1	U	250	LEU
1	U	297	HIS
1	U	373	LYS
1	U	454	ARG
1	U	492	ILE
1	V	294	LEU
1	V	300	LEU
1	V	417	ILE
1	V	461	LEU
1	V	493	SER
1	W	244	GLU
1	W	273	LEU
1	W	291	ARG
1	W	354	MET
1	W	454	ARG
1	W	462	SER
1	X	201	GLN
1	X	265	THR
1	X	431	ASN
1	X	472	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	HIS
1	A	282	HIS
1	B	282	HIS
1	C	282	HIS
1	C	321	GLN
1	D	282	HIS
1	F	490	GLN
1	H	247	ASN
1	L	292	GLN
1	O	384	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

24 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	$\# Z  > 2$
2	LDN	E	600	-	31,36,36	1.20	3 (9%)	40,51,51	2.10	6 (15%)
2	LDN	G	600	-	31,36,36	1.14	3 (9%)	40,51,51	2.21	9 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	LDN	M	600	-	31,36,36	1.38	5 (16%)	40,51,51	2.24	11 (27%)
2	LDN	C	600	-	31,36,36	1.31	3 (9%)	40,51,51	2.47	10 (25%)
2	LDN	T	600	-	31,36,36	1.29	3 (9%)	40,51,51	2.36	12 (30%)
2	LDN	X	600	-	31,36,36	1.22	3 (9%)	40,51,51	2.28	10 (25%)
2	LDN	F	600	-	31,36,36	1.36	3 (9%)	40,51,51	2.19	8 (20%)
2	LDN	B	600	-	31,36,36	1.12	2 (6%)	40,51,51	2.27	8 (20%)
2	LDN	J	600	-	31,36,36	1.18	3 (9%)	40,51,51	2.56	11 (27%)
2	LDN	U	600	-	31,36,36	1.32	2 (6%)	40,51,51	2.01	9 (22%)
2	LDN	K	600	-	31,36,36	1.43	7 (22%)	40,51,51	2.27	10 (25%)
2	LDN	W	600	-	31,36,36	1.27	3 (9%)	40,51,51	2.32	11 (27%)
2	LDN	P	600	-	31,36,36	1.31	4 (12%)	40,51,51	2.34	7 (17%)
2	LDN	S	600	-	31,36,36	1.16	3 (9%)	40,51,51	2.12	7 (17%)
2	LDN	N	600	-	31,36,36	1.33	4 (12%)	40,51,51	2.26	11 (27%)
2	LDN	I	600	-	31,36,36	1.39	5 (16%)	40,51,51	2.47	9 (22%)
2	LDN	L	600	-	31,36,36	1.34	4 (12%)	40,51,51	2.43	7 (17%)
2	LDN	O	600	-	31,36,36	1.37	5 (16%)	40,51,51	2.23	7 (17%)
2	LDN	V	600	-	31,36,36	1.08	2 (6%)	40,51,51	2.03	6 (15%)
2	LDN	Q	600	-	31,36,36	1.23	2 (6%)	40,51,51	2.33	8 (20%)
2	LDN	R	600	-	31,36,36	1.21	4 (12%)	40,51,51	2.31	10 (25%)
2	LDN	A	600	-	31,36,36	1.29	5 (16%)	40,51,51	2.28	9 (22%)
2	LDN	D	600	-	31,36,36	1.33	3 (9%)	40,51,51	2.14	9 (22%)
2	LDN	H	600	-	31,36,36	1.21	3 (9%)	40,51,51	2.09	11 (27%)

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
2	LDN	E	600	-	-	0/12/20/20	0/6/6/6
2	LDN	G	600	-	-	0/12/20/20	0/6/6/6
2	LDN	M	600	-	-	0/12/20/20	0/6/6/6
2	LDN	C	600	-	-	0/12/20/20	0/6/6/6
2	LDN	T	600	-	-	0/12/20/20	0/6/6/6
2	LDN	X	600	-	-	0/12/20/20	1/6/6/6
2	LDN	F	600	-	-	0/12/20/20	0/6/6/6
2	LDN	B	600	-	-	4/12/20/20	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LDN	J	600	-	-	1/12/20/20	0/6/6/6
2	LDN	U	600	-	-	0/12/20/20	0/6/6/6
2	LDN	K	600	-	-	1/12/20/20	0/6/6/6
2	LDN	W	600	-	-	0/12/20/20	0/6/6/6
2	LDN	P	600	-	-	0/12/20/20	0/6/6/6
2	LDN	S	600	-	-	0/12/20/20	0/6/6/6
2	LDN	N	600	-	-	0/12/20/20	0/6/6/6
2	LDN	I	600	-	-	0/12/20/20	0/6/6/6
2	LDN	L	600	-	-	0/12/20/20	0/6/6/6
2	LDN	O	600	-	-	0/12/20/20	0/6/6/6
2	LDN	V	600	-	-	0/12/20/20	0/6/6/6
2	LDN	Q	600	-	-	1/12/20/20	0/6/6/6
2	LDN	R	600	-	-	0/12/20/20	0/6/6/6
2	LDN	A	600	-	-	0/12/20/20	0/6/6/6
2	LDN	D	600	-	-	1/12/20/20	0/6/6/6
2	LDN	H	600	-	-	0/12/20/20	0/6/6/6

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	600	LDN	CAW-CAV	-3.98	1.39	1.49
2	F	600	LDN	CAW-CAV	-3.79	1.39	1.49
2	H	600	LDN	CAW-CAV	-3.67	1.39	1.49
2	W	600	LDN	CAW-CAV	-3.66	1.39	1.49
2	X	600	LDN	CAW-CAV	-3.63	1.40	1.49
2	N	600	LDN	CAW-CAV	-3.51	1.40	1.49
2	L	600	LDN	CAW-CAV	-3.45	1.40	1.49
2	A	600	LDN	CAW-CAV	-3.43	1.40	1.49
2	U	600	LDN	CAW-CAV	-3.41	1.40	1.49
2	J	600	LDN	CAW-CAV	-3.40	1.40	1.49
2	I	600	LDN	CAW-CAV	-3.39	1.40	1.49
2	S	600	LDN	CAW-CAV	-3.37	1.40	1.49
2	T	600	LDN	CAW-CAV	-3.35	1.40	1.49
2	Q	600	LDN	CAW-CAV	-3.35	1.40	1.49
2	C	600	LDN	CAW-CAV	-3.32	1.40	1.49
2	B	600	LDN	CAW-CAV	-3.31	1.40	1.49
2	I	600	LDN	CAZ-CAY	-3.27	1.38	1.49
2	G	600	LDN	CAW-CAV	-3.26	1.40	1.49
2	M	600	LDN	CAW-CAV	-3.24	1.41	1.49
2	P	600	LDN	CAW-CAV	-3.13	1.41	1.49
2	M	600	LDN	CAP-NBD	3.11	1.51	1.46
2	W	600	LDN	CAZ-CAY	-3.09	1.39	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	600	LDN	CAW-CAV	-3.08	1.41	1.49
2	X	600	LDN	CAZ-CAY	-3.05	1.39	1.49
2	C	600	LDN	CAZ-CAY	-3.04	1.39	1.49
2	I	600	LDN	CBA-NAR	-2.92	1.32	1.37
2	V	600	LDN	CAW-CAV	-2.90	1.41	1.49
2	J	600	LDN	CAZ-CAY	-2.89	1.39	1.49
2	M	600	LDN	CAZ-CAY	-2.89	1.39	1.49
2	P	600	LDN	CAZ-CAY	-2.84	1.40	1.49
2	E	600	LDN	CAW-CAV	-2.78	1.42	1.49
2	F	600	LDN	CAZ-CAY	-2.78	1.40	1.49
2	H	600	LDN	CBA-NAR	-2.77	1.32	1.37
2	U	600	LDN	CAZ-CAY	-2.74	1.40	1.49
2	K	600	LDN	CAZ-CAY	-2.73	1.40	1.49
2	A	600	LDN	CAZ-CAY	-2.72	1.40	1.49
2	R	600	LDN	CAW-CAV	-2.70	1.42	1.49
2	K	600	LDN	CAX-NBD	2.69	1.46	1.38
2	R	600	LDN	CAZ-CAY	-2.66	1.40	1.49
2	V	600	LDN	CAZ-CAY	-2.65	1.40	1.49
2	O	600	LDN	CAQ-NBD	2.65	1.50	1.46
2	D	600	LDN	CAZ-CAY	-2.61	1.40	1.49
2	G	600	LDN	CAZ-CAY	-2.60	1.40	1.49
2	T	600	LDN	CAZ-CAY	-2.59	1.40	1.49
2	K	600	LDN	CAQ-NBD	2.59	1.50	1.46
2	Q	600	LDN	CAZ-CAY	-2.55	1.41	1.49
2	N	600	LDN	CAZ-CAY	-2.55	1.41	1.49
2	E	600	LDN	CAZ-CAY	-2.54	1.41	1.49
2	L	600	LDN	CAZ-CAY	-2.51	1.41	1.49
2	K	600	LDN	CAQ-CAO	2.51	1.57	1.51
2	L	600	LDN	CBB-CBA	-2.51	1.38	1.42
2	H	600	LDN	CAZ-CAY	-2.50	1.41	1.49
2	O	600	LDN	CAZ-CAY	-2.49	1.41	1.49
2	E	600	LDN	CAP-NBD	2.49	1.50	1.46
2	S	600	LDN	CAZ-CAY	-2.49	1.41	1.49
2	F	600	LDN	CAP-NBD	2.45	1.50	1.46
2	N	600	LDN	CAP-CAN	2.44	1.57	1.51
2	N	600	LDN	CAQ-CAO	2.40	1.57	1.51
2	A	600	LDN	CAP-NBD	2.37	1.50	1.46
2	I	600	LDN	CAX-NBD	2.37	1.45	1.38
2	P	600	LDN	CAQ-NBD	2.37	1.50	1.46
2	K	600	LDN	CAK-NAS	2.36	1.35	1.31
2	M	600	LDN	CAQ-NBD	2.34	1.50	1.46
2	O	600	LDN	CAP-NBD	2.30	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	LDN	CAZ-CAY	-2.26	1.42	1.49
2	R	600	LDN	CAP-NBD	2.21	1.50	1.46
2	T	600	LDN	CAI-CBA	-2.21	1.38	1.41
2	M	600	LDN	CAQ-CAO	2.20	1.56	1.51
2	K	600	LDN	CAP-NBD	2.20	1.50	1.46
2	J	600	LDN	CBB-CBA	-2.18	1.38	1.42
2	C	600	LDN	CAQ-NBD	2.16	1.50	1.46
2	K	600	LDN	CAW-CAV	-2.15	1.43	1.49
2	W	600	LDN	CBB-CBA	-2.15	1.39	1.42
2	I	600	LDN	CAQ-NBD	2.12	1.50	1.46
2	A	600	LDN	CBB-CBA	-2.11	1.39	1.42
2	R	600	LDN	CAQ-NBD	2.11	1.50	1.46
2	S	600	LDN	CAP-NBD	2.10	1.50	1.46
2	O	600	LDN	CBA-NAR	-2.06	1.33	1.37
2	A	600	LDN	CBA-NAR	-2.04	1.33	1.37
2	X	600	LDN	CAQ-NBD	2.04	1.49	1.46
2	L	600	LDN	CAQ-NBD	2.04	1.49	1.46
2	D	600	LDN	CAD-CAY	2.03	1.42	1.38
2	P	600	LDN	CAA-CAI	2.02	1.41	1.36
2	G	600	LDN	CBA-NAR	-2.02	1.33	1.37

All (216) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	600	LDN	CAL-NAT-NBE	10.33	111.22	103.70
2	P	600	LDN	CAL-NAT-NBE	10.21	111.13	103.70
2	Q	600	LDN	CAL-NAT-NBE	10.16	111.09	103.70
2	V	600	LDN	CAL-NAT-NBE	10.09	111.04	103.70
2	C	600	LDN	CAL-NAT-NBE	10.02	111.00	103.70
2	J	600	LDN	CAL-NAT-NBE	9.97	110.95	103.70
2	L	600	LDN	CAL-NAT-NBE	9.70	110.76	103.70
2	E	600	LDN	CAL-NAT-NBE	9.66	110.73	103.70
2	R	600	LDN	CAL-NAT-NBE	9.54	110.64	103.70
2	O	600	LDN	CAL-NAT-NBE	9.49	110.60	103.70
2	X	600	LDN	CAL-NAT-NBE	9.20	110.39	103.70
2	W	600	LDN	CAL-NAT-NBE	9.20	110.39	103.70
2	N	600	LDN	CAL-NAT-NBE	9.13	110.35	103.70
2	A	600	LDN	CAL-NAT-NBE	9.08	110.31	103.70
2	K	600	LDN	CAL-NAT-NBE	9.05	110.29	103.70
2	F	600	LDN	CAL-NAT-NBE	8.70	110.03	103.70
2	S	600	LDN	CAL-NAT-NBE	8.69	110.02	103.70
2	T	600	LDN	CAL-NAT-NBE	8.67	110.01	103.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	600	LDN	CAL-NAT-NBE	8.66	110.00	103.70
2	B	600	LDN	CAL-NAT-NBE	8.62	109.97	103.70
2	D	600	LDN	CAL-NAT-NBE	8.44	109.84	103.70
2	H	600	LDN	CAL-NAT-NBE	8.02	109.53	103.70
2	U	600	LDN	CAL-NAT-NBE	7.68	109.29	103.70
2	G	600	LDN	CAL-NAT-NBE	7.25	108.97	103.70
2	J	600	LDN	CAW-CAK-NAS	-6.76	119.29	125.55
2	A	600	LDN	CAW-CAK-NAS	-6.04	119.95	125.55
2	C	600	LDN	CAW-CAK-NAS	-5.92	120.07	125.55
2	I	600	LDN	CAW-CAK-NAS	-5.85	120.14	125.55
2	F	600	LDN	CAW-CAK-NAS	-5.72	120.26	125.55
2	L	600	LDN	CAW-CAK-NAS	-5.69	120.28	125.55
2	B	600	LDN	CAW-CAK-NAS	-5.61	120.36	125.55
2	P	600	LDN	CAW-CAK-NAS	-5.53	120.43	125.55
2	T	600	LDN	CAW-CAK-NAS	-5.39	120.56	125.55
2	W	600	LDN	CAW-CAK-NAS	-5.38	120.57	125.55
2	R	600	LDN	CAQ-NBD-CAP	5.21	123.03	111.52
2	Q	600	LDN	CAW-CAK-NAS	-5.21	120.73	125.55
2	X	600	LDN	CAW-CAK-NAS	-5.16	120.77	125.55
2	D	600	LDN	CAW-CAK-NAS	-5.15	120.79	125.55
2	G	600	LDN	CAW-CAK-NAS	-5.10	120.82	125.55
2	L	600	LDN	CAQ-NBD-CAP	4.98	122.50	111.52
2	B	600	LDN	CAQ-NBD-CAP	4.91	122.37	111.52
2	N	600	LDN	CAW-CAK-NAS	-4.89	121.02	125.55
2	P	600	LDN	CAK-NAS-CBC	4.89	122.97	116.73
2	S	600	LDN	CAQ-NBD-CAP	4.86	122.25	111.52
2	I	600	LDN	CAQ-NBD-CAP	4.84	122.21	111.52
2	T	600	LDN	CAK-NAS-CBC	4.83	122.89	116.73
2	L	600	LDN	CAK-NAS-CBC	4.76	122.81	116.73
2	C	600	LDN	CAQ-NBD-CAP	4.74	121.99	111.52
2	O	600	LDN	CAY-CBB-CBA	4.68	119.96	117.44
2	O	600	LDN	CAQ-NBD-CAP	4.68	121.84	111.52
2	Q	600	LDN	CAK-NAS-CBC	4.64	122.65	116.73
2	G	600	LDN	CAK-NAS-CBC	4.63	122.64	116.73
2	U	600	LDN	CAW-CAK-NAS	-4.56	121.33	125.55
2	D	600	LDN	CAK-NAS-CBC	4.54	122.52	116.73
2	G	600	LDN	CAY-CBB-CBA	4.51	119.87	117.44
2	H	600	LDN	CAW-CAK-NAS	-4.49	121.39	125.55
2	S	600	LDN	CAW-CAK-NAS	-4.49	121.39	125.55
2	L	600	LDN	CAY-CBB-CBA	4.42	119.82	117.44
2	B	600	LDN	CAK-NAS-CBC	4.39	122.34	116.73
2	M	600	LDN	CAG-CAX-NBD	-4.31	115.44	121.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	600	LDN	CAW-CAK-NAS	-4.27	121.59	125.55
2	R	600	LDN	CAK-NAS-CBC	4.22	122.12	116.73
2	K	600	LDN	CAK-NAS-CBC	4.19	122.08	116.73
2	H	600	LDN	CAQ-NBD-CAP	4.18	120.75	111.52
2	R	600	LDN	CAW-CAK-NAS	-4.15	121.71	125.55
2	J	600	LDN	CAK-NAS-CBC	4.15	122.02	116.73
2	F	600	LDN	CAK-NAS-CBC	4.12	121.99	116.73
2	N	600	LDN	CAK-NAS-CBC	4.12	121.99	116.73
2	A	600	LDN	CAK-NAS-CBC	4.06	121.91	116.73
2	I	600	LDN	CAK-NAS-CBC	4.05	121.91	116.73
2	C	600	LDN	CAK-NAS-CBC	4.05	121.90	116.73
2	M	600	LDN	CAW-CAK-NAS	-4.02	121.83	125.55
2	B	600	LDN	CAY-CBB-CBA	3.93	119.56	117.44
2	J	600	LDN	CAC-NAR-CBA	3.88	122.94	116.93
2	J	600	LDN	CAD-CAC-NAR	-3.82	118.66	124.58
2	E	600	LDN	CAW-CAK-NAS	-3.81	122.02	125.55
2	R	600	LDN	CAY-CBB-CBA	3.80	119.49	117.44
2	K	600	LDN	CAK-CAW-CAV	3.75	128.24	121.69
2	M	600	LDN	CAC-NAR-CBA	3.74	122.72	116.93
2	S	600	LDN	CAK-NAS-CBC	3.74	121.51	116.73
2	F	600	LDN	CAY-CBB-CBA	3.74	119.45	117.44
2	G	600	LDN	CAZ-CAY-CBB	3.71	127.67	121.45
2	X	600	LDN	CAK-NAS-CBC	3.70	121.45	116.73
2	M	600	LDN	CAK-NAS-CBC	3.68	121.43	116.73
2	K	600	LDN	CAZ-CAY-CBB	3.66	127.59	121.45
2	W	600	LDN	CAC-NAR-CBA	3.63	122.55	116.93
2	E	600	LDN	CAY-CBB-CBA	3.58	119.37	117.44
2	Q	600	LDN	CAQ-NBD-CAP	3.57	119.41	111.52
2	E	600	LDN	CAQ-NBD-CAP	3.56	119.38	111.52
2	T	600	LDN	CAH-CAX-NBD	-3.52	116.53	121.38
2	N	600	LDN	CAY-CBB-CBA	3.51	119.33	117.44
2	X	600	LDN	CAZ-CAY-CBB	3.49	127.31	121.45
2	D	600	LDN	CAQ-NBD-CAP	3.47	119.18	111.52
2	M	600	LDN	CAD-CAC-NAR	-3.45	119.24	124.58
2	V	600	LDN	CAW-CAK-NAS	-3.44	122.36	125.55
2	G	600	LDN	CAQ-NBD-CAP	3.42	119.06	111.52
2	O	600	LDN	CAW-CAK-NAS	-3.41	122.39	125.55
2	U	600	LDN	CAK-NAS-CBC	3.40	121.08	116.73
2	W	600	LDN	CAQ-NBD-CAP	3.40	119.02	111.52
2	U	600	LDN	CAC-NAR-CBA	3.40	122.19	116.93
2	A	600	LDN	CAQ-NBD-CAP	3.35	118.90	111.52
2	H	600	LDN	CAC-NAR-CBA	3.33	122.09	116.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	600	LDN	CAC-NAR-CBA	3.32	122.07	116.93
2	W	600	LDN	CAN-CAP-NBD	-3.30	103.34	110.48
2	X	600	LDN	CAC-NAR-CBA	3.29	122.03	116.93
2	I	600	LDN	CAC-NAR-CBA	3.29	122.03	116.93
2	M	600	LDN	CAQ-NBD-CAP	3.29	118.77	111.52
2	E	600	LDN	CAK-NAS-CBC	3.28	120.92	116.73
2	Q	600	LDN	CAZ-CAY-CBB	3.24	126.88	121.45
2	O	600	LDN	CAK-NAS-CBC	3.20	120.81	116.73
2	J	600	LDN	CAO-CAQ-NBD	-3.20	103.56	110.48
2	N	600	LDN	CAQ-NBD-CAP	3.19	118.57	111.52
2	A	600	LDN	CAO-CAQ-NBD	-3.18	103.59	110.48
2	U	600	LDN	CAQ-NBD-CAP	3.18	118.54	111.52
2	J	600	LDN	CAQ-NBD-CAP	3.17	118.53	111.52
2	U	600	LDN	CAY-CBB-CBA	3.17	119.15	117.44
2	G	600	LDN	CAC-NAR-CBA	3.15	121.81	116.93
2	D	600	LDN	CAC-NAR-CBA	3.14	121.79	116.93
2	T	600	LDN	CAQ-NBD-CAP	3.12	118.41	111.52
2	N	600	LDN	CAH-CAX-NBD	-3.08	117.13	121.38
2	H	600	LDN	CAZ-CAY-CBB	3.07	126.61	121.45
2	S	600	LDN	CAY-CBB-CBA	3.07	119.09	117.44
2	W	600	LDN	CAD-CAC-NAR	-3.06	119.84	124.58
2	F	600	LDN	CAQ-NBD-CAP	3.05	118.25	111.52
2	C	600	LDN	CAH-CAX-NBD	-3.05	117.18	121.38
2	X	600	LDN	CAQ-NBD-CAP	3.05	118.24	111.52
2	P	600	LDN	CAQ-NBD-CAP	3.02	118.19	111.52
2	X	600	LDN	CAD-CAC-NAR	-3.01	119.92	124.58
2	V	600	LDN	CAK-NAS-CBC	3.01	120.58	116.73
2	D	600	LDN	CAD-CAC-NAR	-3.00	119.94	124.58
2	A	600	LDN	CAC-NAR-CBA	2.99	121.56	116.93
2	J	600	LDN	CAM-CAW-CAK	2.99	120.04	115.38
2	T	600	LDN	CAD-CAC-NAR	-2.92	120.07	124.58
2	Q	600	LDN	CAY-CBB-CBA	2.91	119.00	117.44
2	T	600	LDN	CAK-CAW-CAV	2.89	126.73	121.69
2	W	600	LDN	CAK-NAS-CBC	2.85	120.37	116.73
2	T	600	LDN	CAY-CBB-CBA	2.84	118.97	117.44
2	I	600	LDN	CAC-CAD-CAY	-2.83	117.87	120.00
2	A	600	LDN	CAY-CBB-CBA	2.79	118.94	117.44
2	G	600	LDN	CBB-CBA-NAR	-2.78	119.87	122.83
2	B	600	LDN	CAD-CAC-NAR	-2.74	120.34	124.58
2	C	600	LDN	CAD-CAC-NAR	-2.74	120.34	124.58
2	V	600	LDN	CAY-CBB-CBA	2.73	118.91	117.44
2	L	600	LDN	CAD-CAC-NAR	-2.73	120.36	124.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	600	LDN	CAY-CBB-CBA	2.72	118.91	117.44
2	W	600	LDN	CAM-CAW-CAK	2.71	119.61	115.38
2	I	600	LDN	CBB-CBA-NAR	-2.71	119.95	122.83
2	P	600	LDN	CAD-CAC-NAR	-2.70	120.40	124.58
2	A	600	LDN	CAM-CAW-CAK	2.69	119.57	115.38
2	X	600	LDN	CAN-CAP-NBD	-2.66	104.72	110.48
2	B	600	LDN	CAC-NAR-CBA	2.63	121.00	116.93
2	L	600	LDN	CAC-NAR-CBA	2.63	121.00	116.93
2	H	600	LDN	CAK-NAS-CBC	2.62	120.08	116.73
2	T	600	LDN	CAF-CAV-CAW	-2.61	116.83	121.36
2	F	600	LDN	CAC-NAR-CBA	2.61	120.97	116.93
2	R	600	LDN	CAC-NAR-CBA	2.60	120.96	116.93
2	N	600	LDN	CAC-NAR-CBA	2.57	120.91	116.93
2	F	600	LDN	CAM-CAW-CAK	2.57	119.39	115.38
2	Q	600	LDN	CAD-CAC-NAR	-2.56	120.61	124.58
2	U	600	LDN	CAD-CAC-NAR	-2.56	120.62	124.58
2	A	600	LDN	CAD-CAC-NAR	-2.56	120.62	124.58
2	U	600	LDN	CBB-CBA-NAR	-2.55	120.11	122.83
2	D	600	LDN	CAY-CBB-CBA	2.54	118.80	117.44
2	X	600	LDN	CAM-CAW-CAK	2.53	119.32	115.38
2	M	600	LDN	CAH-CAX-NBD	2.53	124.86	121.38
2	K	600	LDN	CAY-CBB-CBA	2.52	118.80	117.44
2	H	600	LDN	CAY-CBB-CBA	2.51	118.79	117.44
2	H	600	LDN	CAD-CAC-NAR	-2.51	120.70	124.58
2	P	600	LDN	CAC-NAR-CBA	2.50	120.80	116.93
2	N	600	LDN	CAM-CAW-CAK	2.48	119.25	115.38
2	C	600	LDN	CAM-CAW-CAK	2.47	119.23	115.38
2	M	600	LDN	CBB-CBA-NAR	-2.38	120.29	122.83
2	H	600	LDN	CAM-CAW-CAK	2.38	119.10	115.38
2	N	600	LDN	CAG-CAX-NBD	2.38	124.66	121.38
2	B	600	LDN	CAZ-CAY-CBB	2.37	125.43	121.45
2	D	600	LDN	CAQ-NBD-CAX	2.36	124.48	118.09
2	U	600	LDN	CAM-CAW-CAK	2.36	119.06	115.38
2	K	600	LDN	CAC-NAR-CBA	2.36	120.58	116.93
2	T	600	LDN	CAM-CAW-CAV	-2.35	115.48	120.53
2	X	600	LDN	CAD-CAY-CAZ	-2.34	113.90	119.12
2	K	600	LDN	CAE-CAV-CAW	2.34	125.42	121.36
2	C	600	LDN	CAY-CBB-CBA	2.34	118.70	117.44
2	Q	600	LDN	CAC-NAR-CBA	2.34	120.55	116.93
2	R	600	LDN	CAC-CAD-CAY	-2.33	118.25	120.00
2	W	600	LDN	CAH-CAX-NBD	-2.31	118.20	121.38
2	T	600	LDN	CAC-NAR-CBA	2.30	120.50	116.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	600	LDN	CAD-CAC-NAR	-2.30	121.02	124.58
2	K	600	LDN	CAD-CAC-NAR	-2.30	121.02	124.58
2	M	600	LDN	CAY-CBB-CBA	2.29	118.67	117.44
2	C	600	LDN	CBB-CBA-NAR	-2.29	120.40	122.83
2	W	600	LDN	CAM-CAW-CAV	-2.26	115.66	120.53
2	P	600	LDN	CAH-CAX-NBD	-2.26	118.26	121.38
2	N	600	LDN	CAD-CAC-NAR	-2.23	121.12	124.58
2	S	600	LDN	CAD-CAC-NAR	-2.23	121.13	124.58
2	R	600	LDN	CBB-CBA-NAR	-2.22	120.47	122.83
2	G	600	LDN	CAB-CAA-CAI	-2.22	117.33	120.44
2	H	600	LDN	CAI-CBA-CBB	2.20	121.65	119.13
2	K	600	LDN	CAM-CAW-CAV	-2.19	115.81	120.53
2	T	600	LDN	CAJ-CBB-CBA	2.19	120.77	118.33
2	J	600	LDN	CBB-CBA-NAR	-2.18	120.51	122.83
2	V	600	LDN	CAC-NAR-CBA	2.17	120.28	116.93
2	V	600	LDN	CAD-CAC-NAR	-2.16	121.23	124.58
2	S	600	LDN	CAC-NAR-CBA	2.12	120.22	116.93
2	R	600	LDN	CAP-CAN-NAU	-2.11	105.64	111.12
2	W	600	LDN	CBB-CBA-NAR	-2.11	120.58	122.83
2	N	600	LDN	CAF-CAV-CAW	-2.10	117.71	121.36
2	O	600	LDN	CAM-CAW-CAK	2.10	118.65	115.38
2	D	600	LDN	CAM-CAW-CAK	2.09	118.64	115.38
2	R	600	LDN	CAZ-CAY-CBB	2.07	124.93	121.45
2	F	600	LDN	CAD-CAC-NAR	-2.06	121.39	124.58
2	H	600	LDN	CBB-CBA-NAR	-2.06	120.64	122.83
2	J	600	LDN	CAN-CAP-NBD	-2.05	106.04	110.48
2	I	600	LDN	CAM-CAW-CAK	2.04	118.56	115.38
2	J	600	LDN	CAY-CBB-CBA	2.04	118.53	117.44
2	M	600	LDN	CAQ-NBD-CAX	2.03	123.58	118.09
2	O	600	LDN	CAG-CAX-NBD	-2.03	118.58	121.38

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	600	LDN	CAH-CAX-NBD-CAP
2	B	600	LDN	CAH-CAX-NBD-CAQ
2	B	600	LDN	CAG-CAX-NBD-CAP
2	B	600	LDN	CAG-CAX-NBD-CAQ
2	K	600	LDN	CBB-CAY-CAZ-CBC
2	D	600	LDN	CAH-CAX-NBD-CAP
2	Q	600	LDN	CAF-CAV-CAW-CAK

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Mol	Chain	Res	Type	Atoms
2	J	600	LDN	CAD-CAY-CAZ-CAL

All (1) ring outliers are listed below:

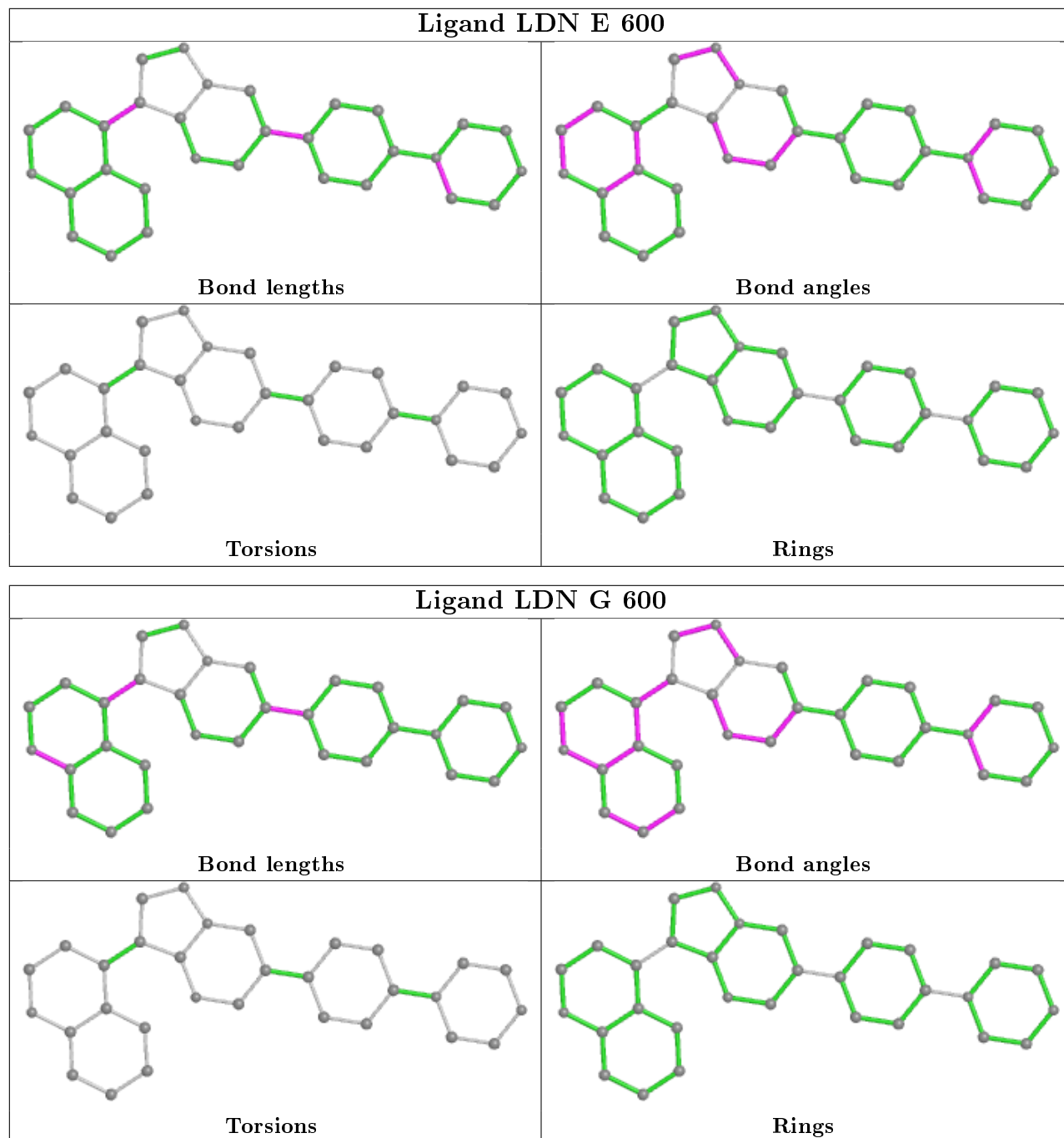
Mol	Chain	Res	Type	Atoms
2	X	600	LDN	CAN-CAO-CAP-CAQ-NAU-NBD

21 monomers are involved in 69 short contacts:

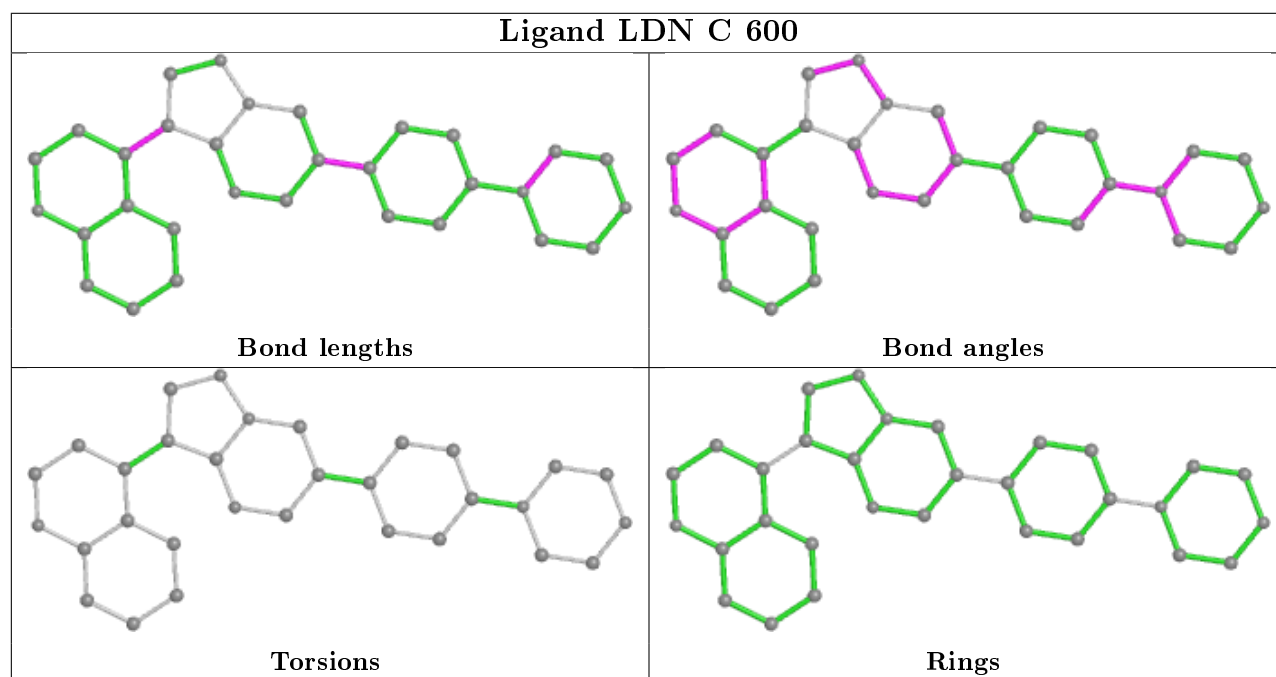
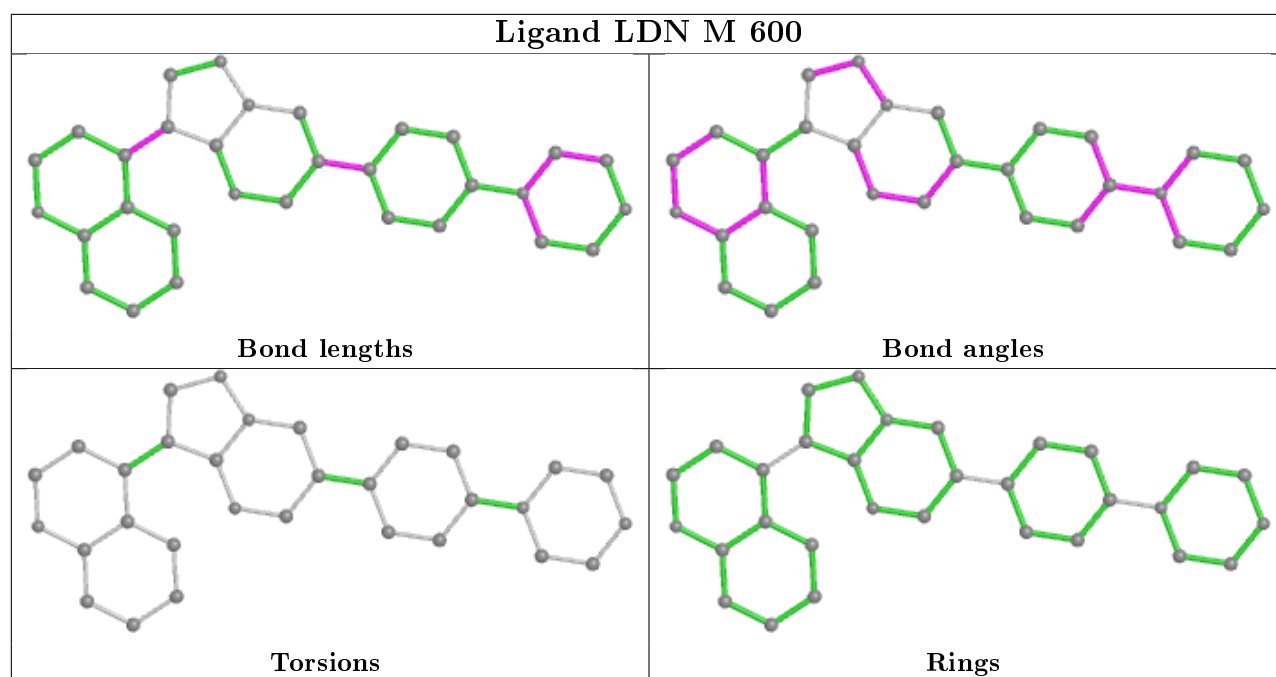
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	600	LDN	3	0
2	G	600	LDN	2	0
2	C	600	LDN	1	0
2	T	600	LDN	2	0
2	X	600	LDN	15	0
2	F	600	LDN	3	0
2	B	600	LDN	4	0
2	J	600	LDN	5	0
2	U	600	LDN	1	0
2	K	600	LDN	4	0
2	W	600	LDN	4	0
2	P	600	LDN	5	0
2	N	600	LDN	1	0
2	I	600	LDN	1	0
2	L	600	LDN	3	0
2	O	600	LDN	5	0
2	V	600	LDN	3	0
2	Q	600	LDN	1	0
2	R	600	LDN	1	1
2	A	600	LDN	1	0
2	D	600	LDN	3	0

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

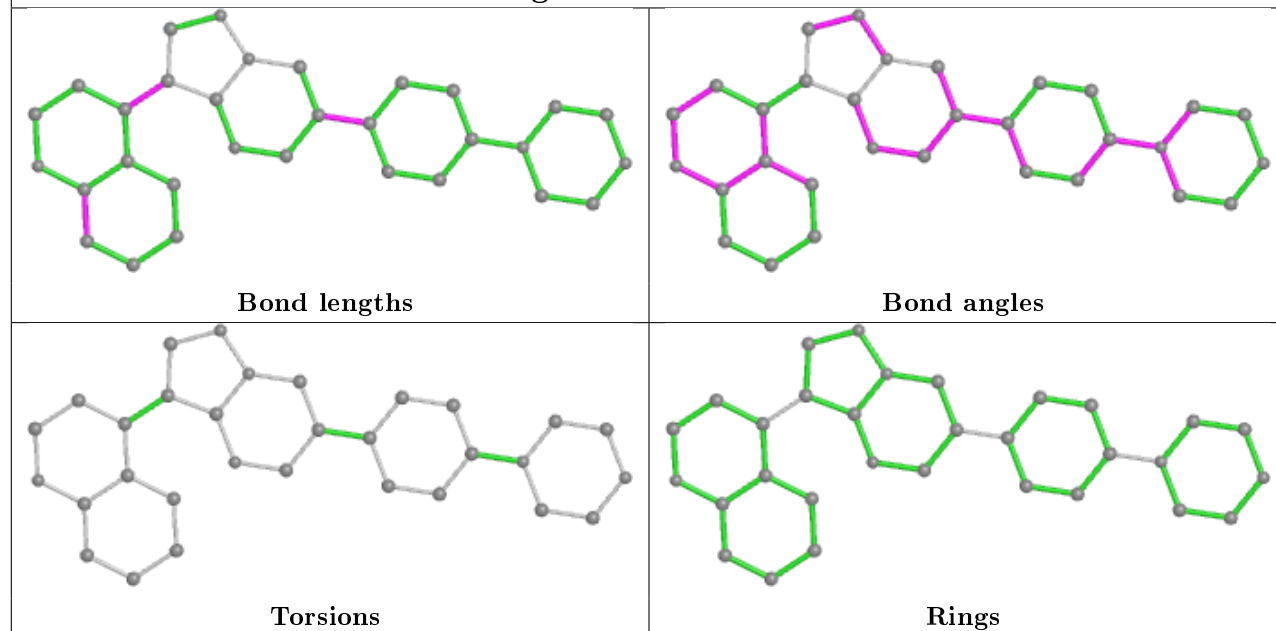
equivalents in the CSD to analyse the geometry.



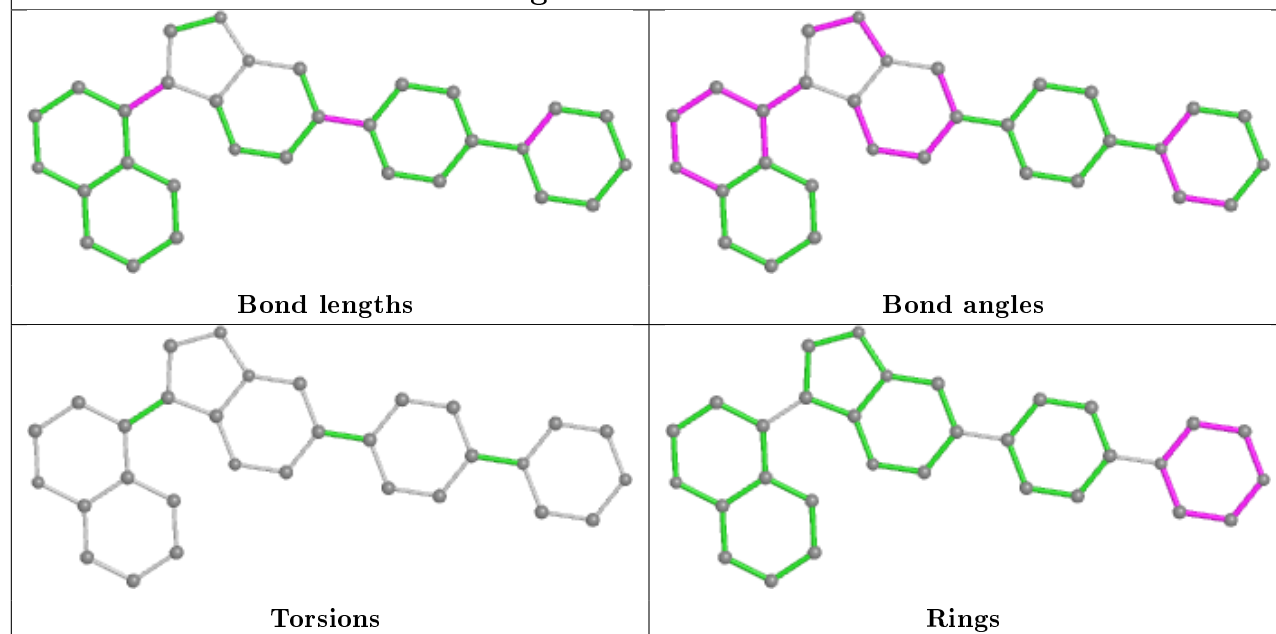




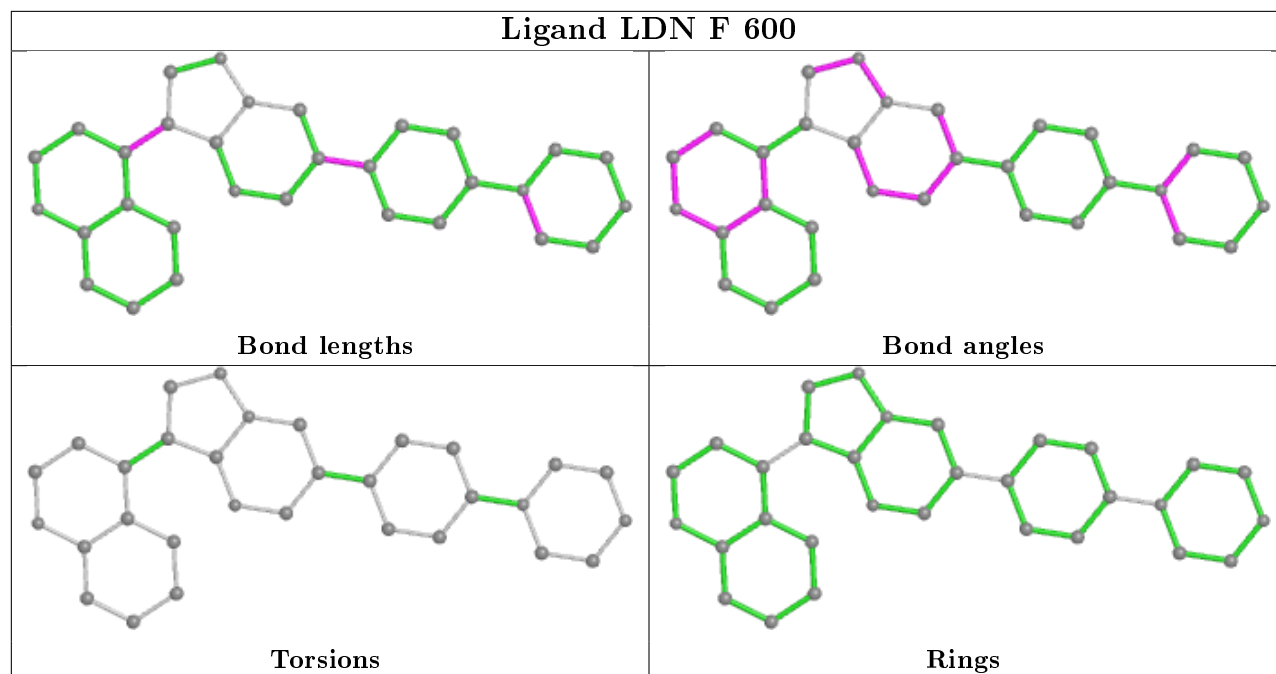
## Ligand LDN T 600



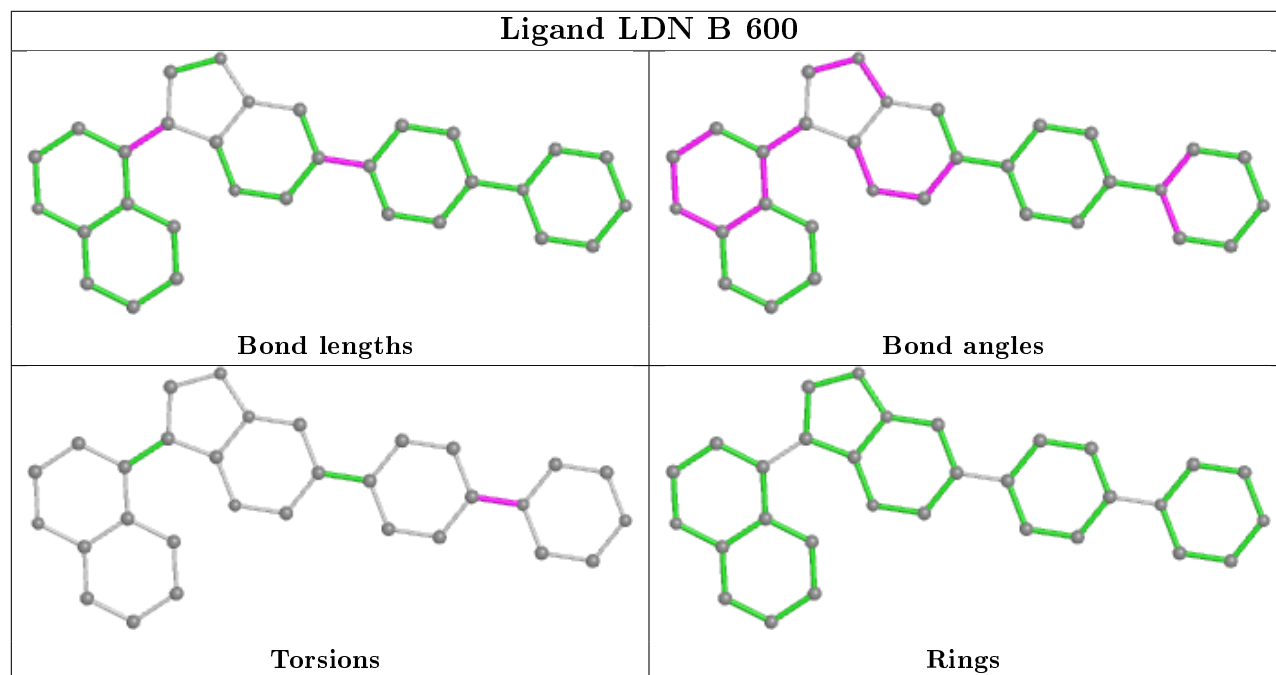
## Ligand LDN X 600



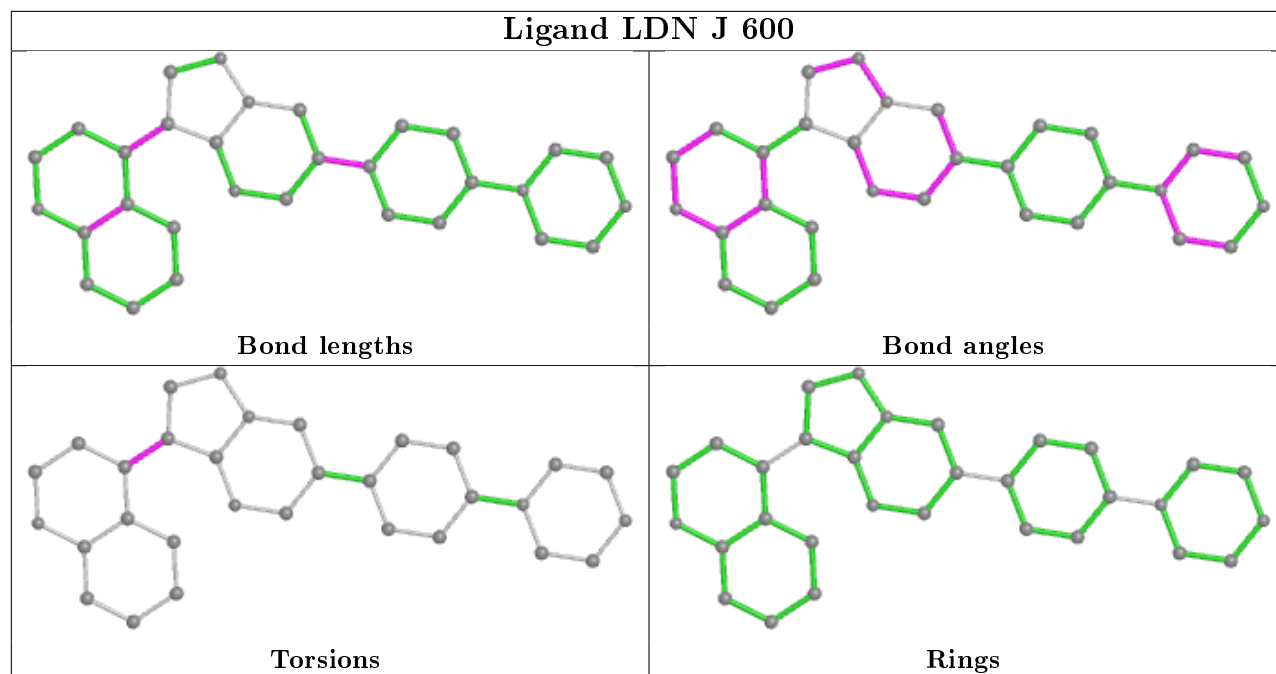
## Ligand LDN F 600



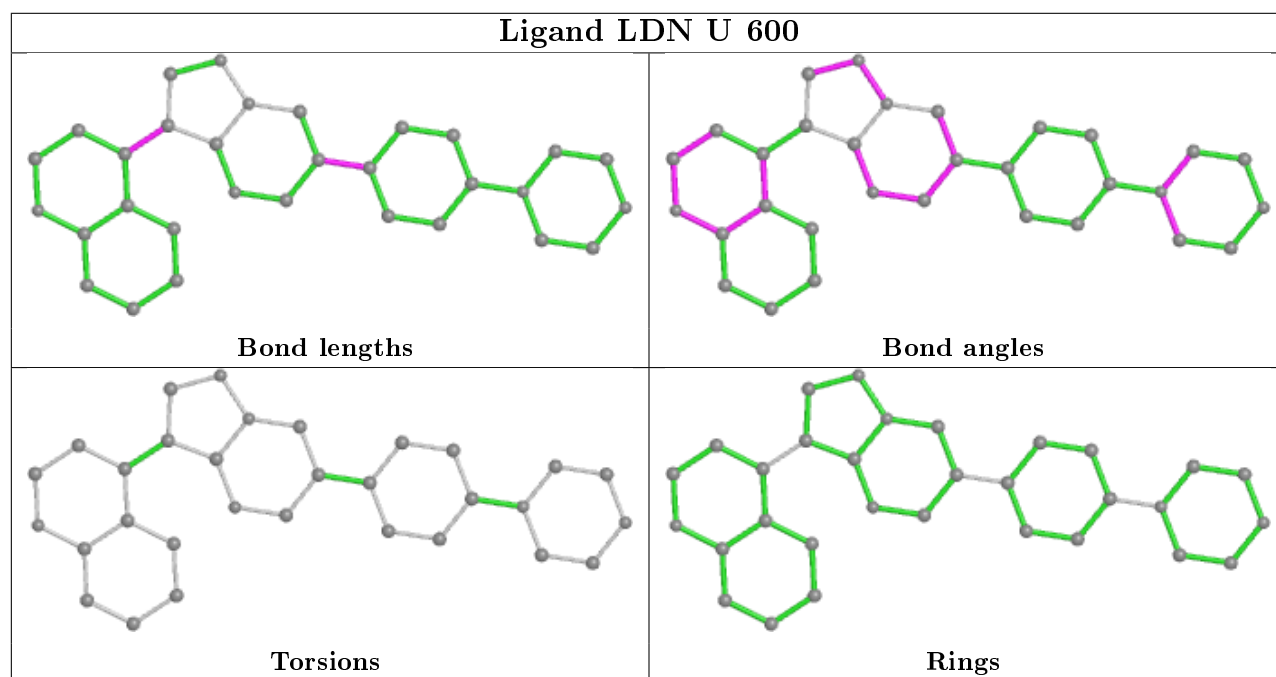
## Ligand LDN B 600

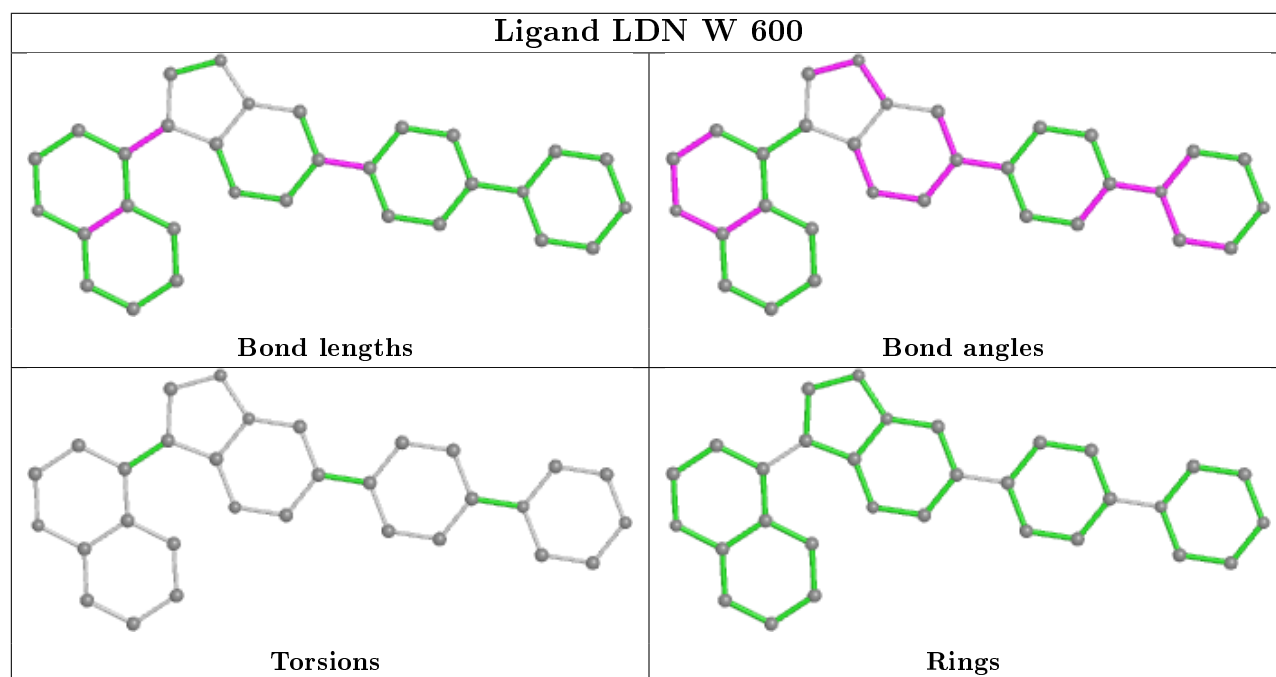
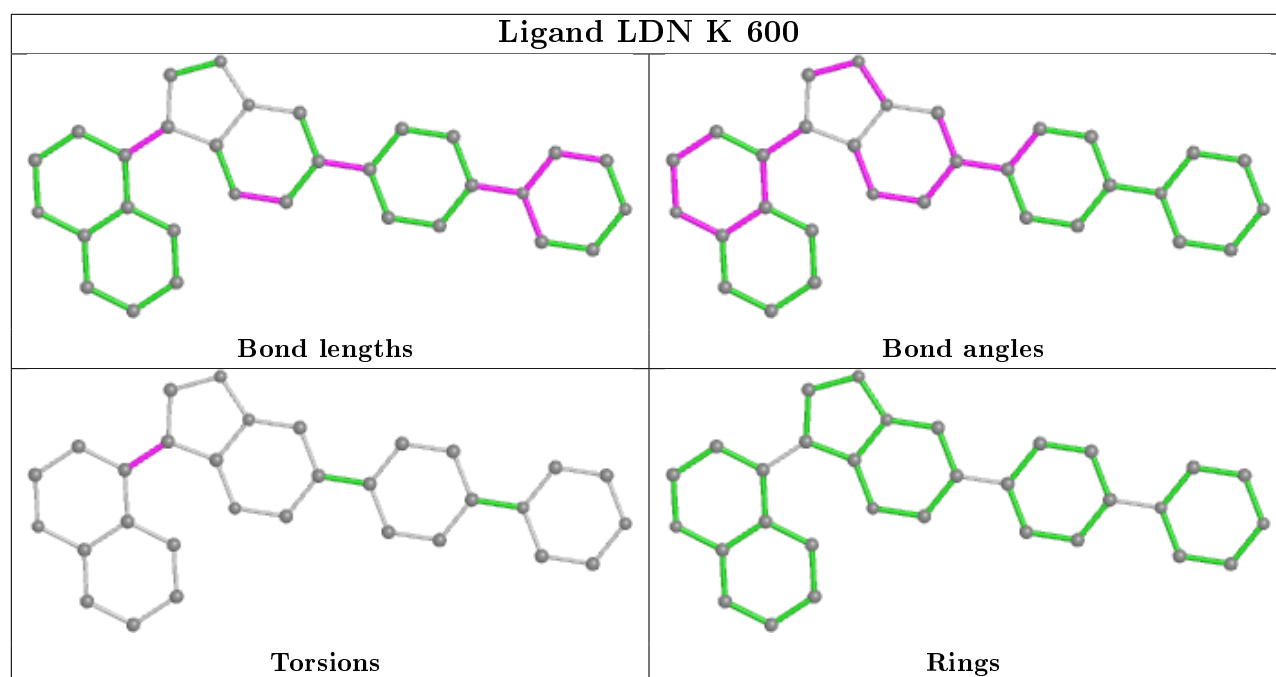


## Ligand LDN J 600

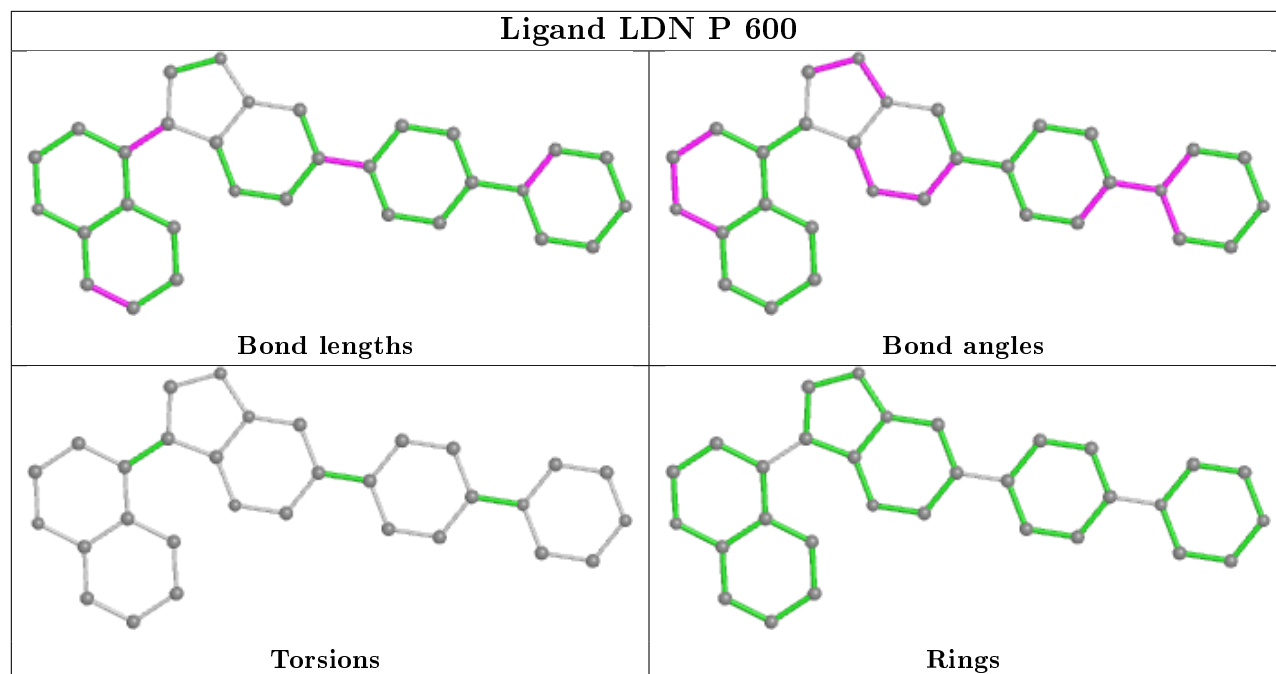


## Ligand LDN U 600

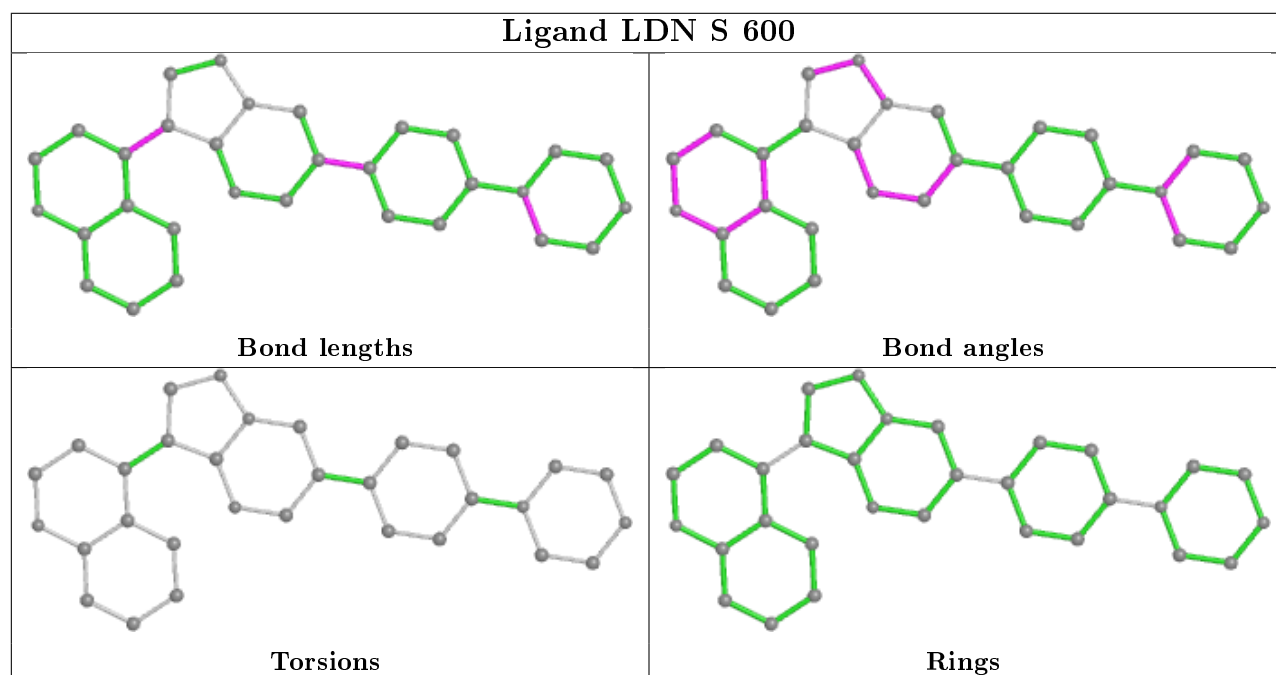


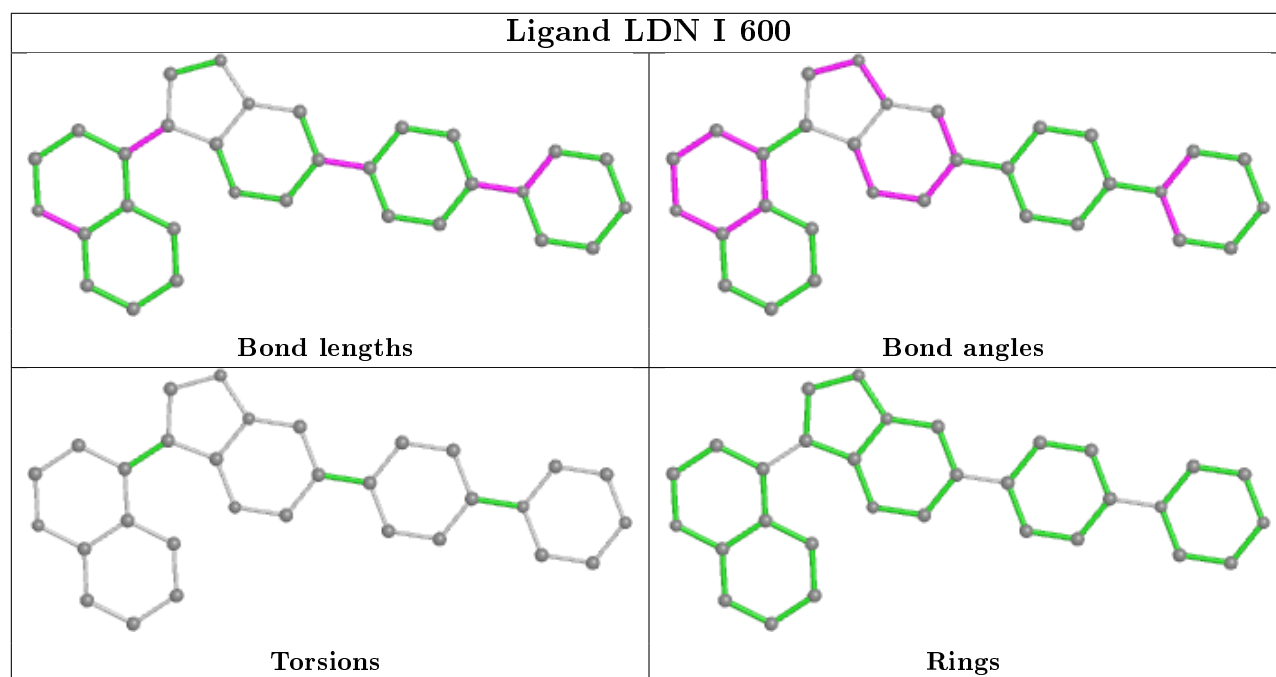
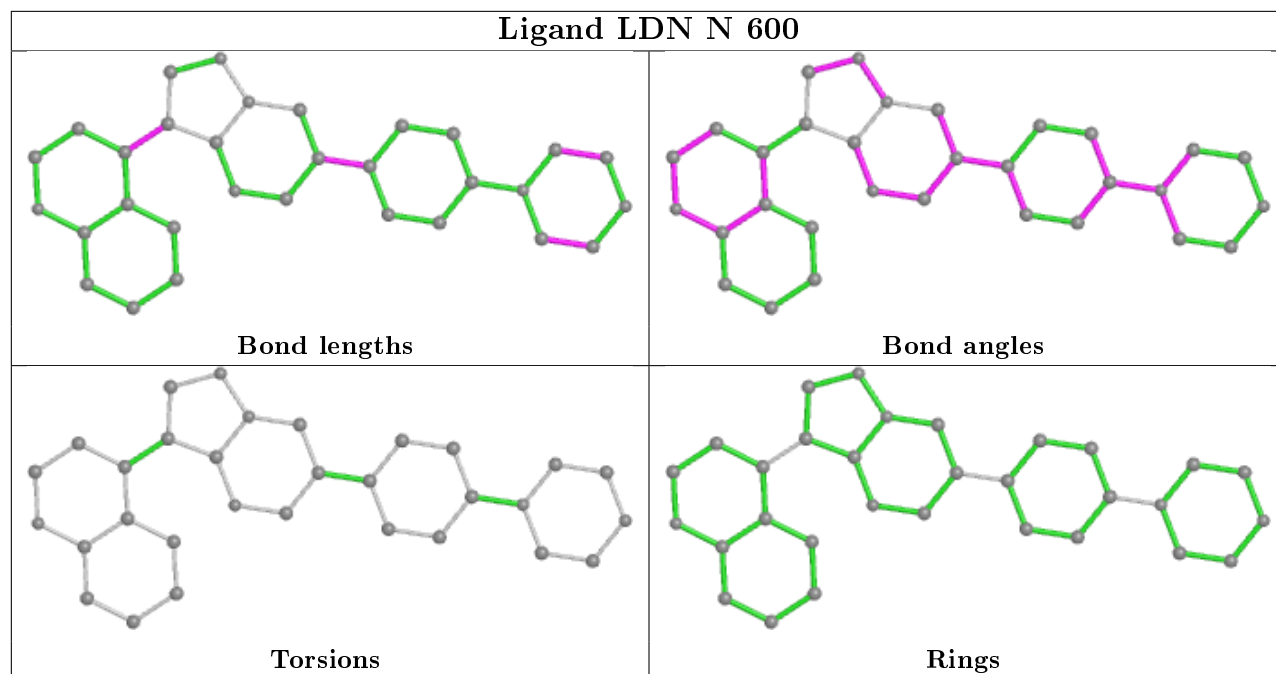


## Ligand LDN P 600

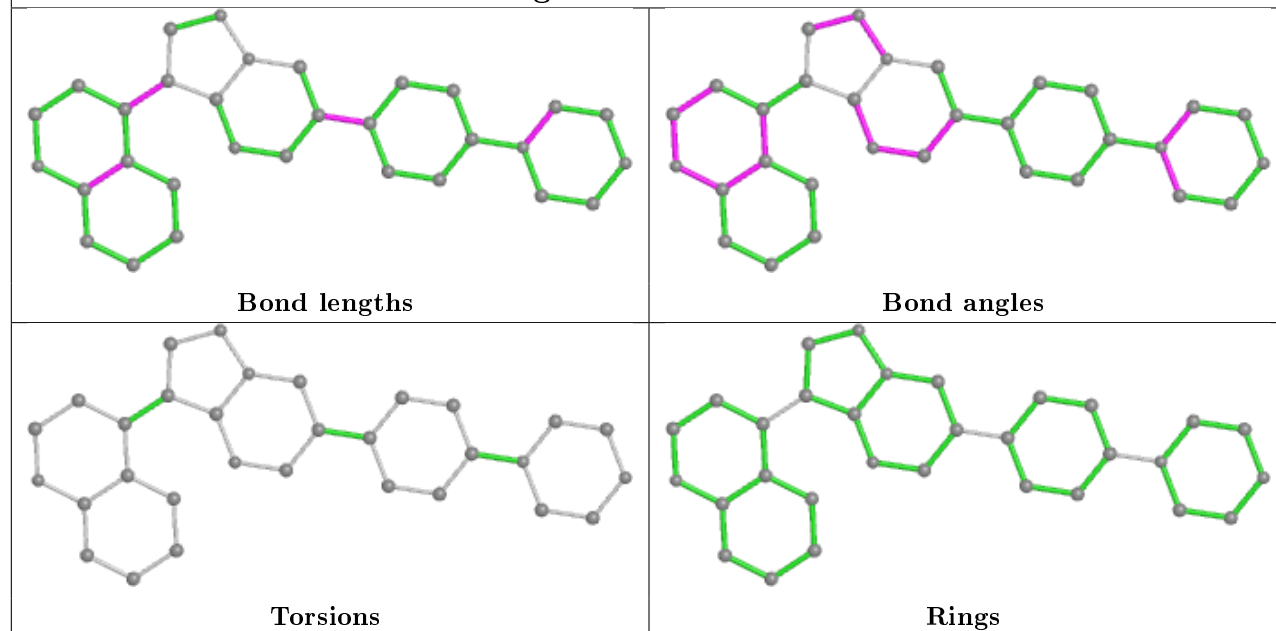


## Ligand LDN S 600

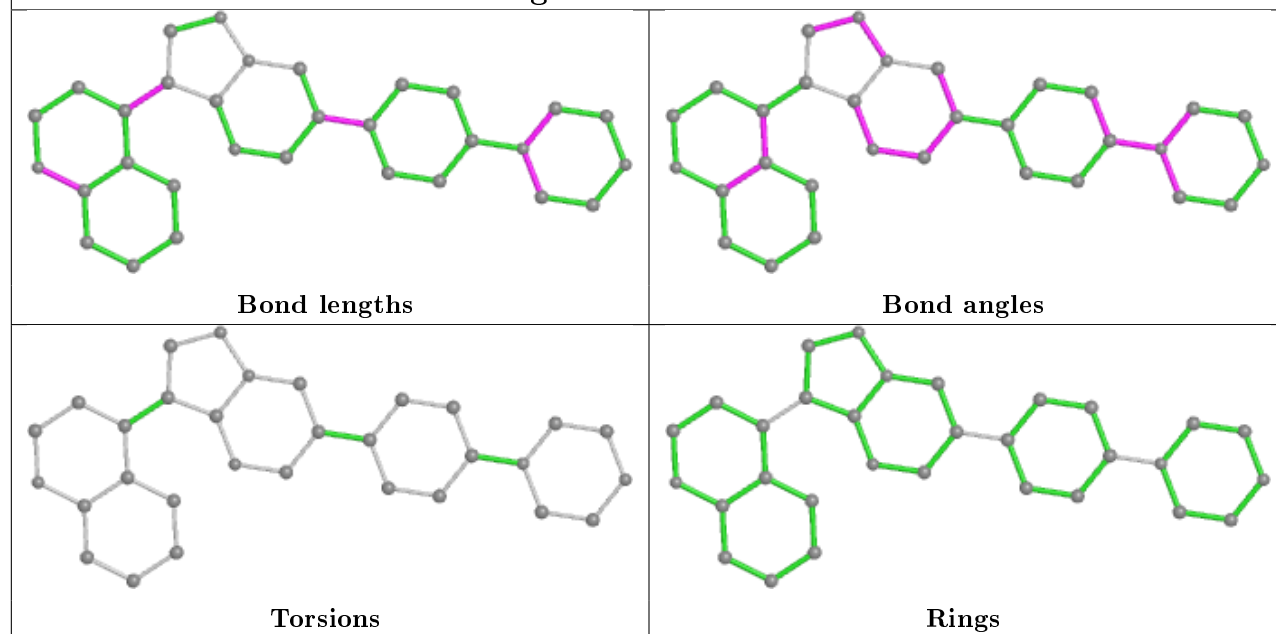




## Ligand LDN L 600

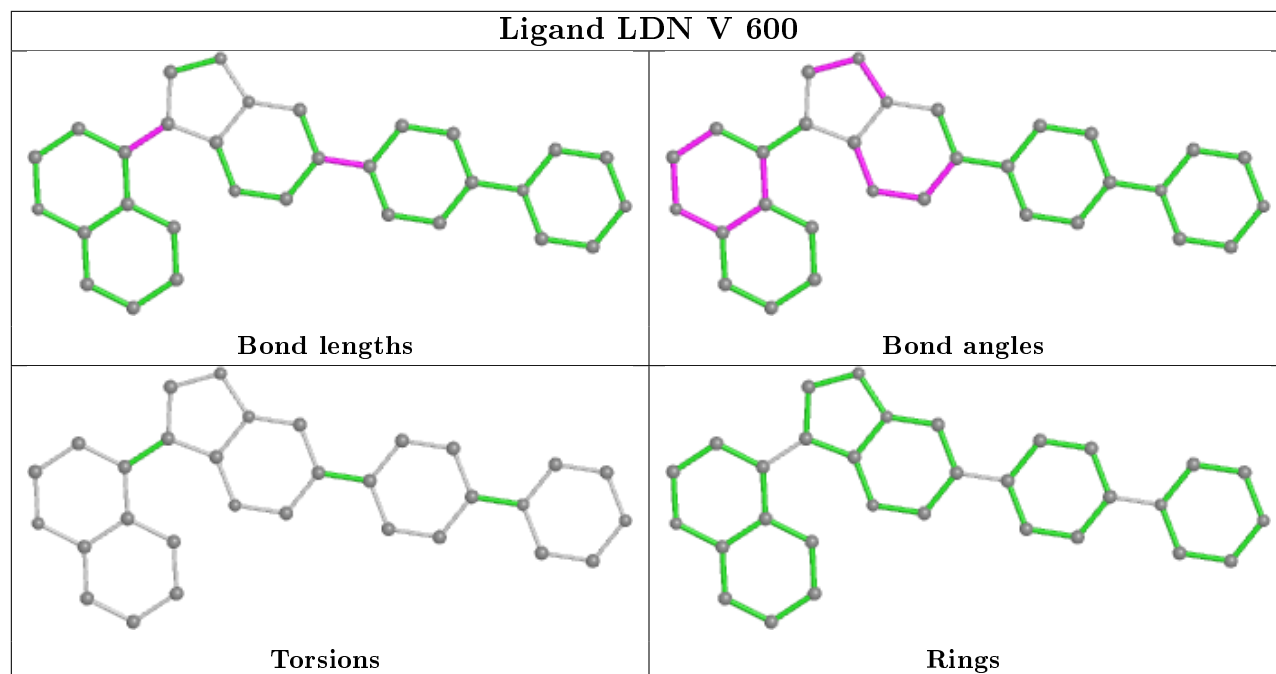


## Ligand LDN O 600

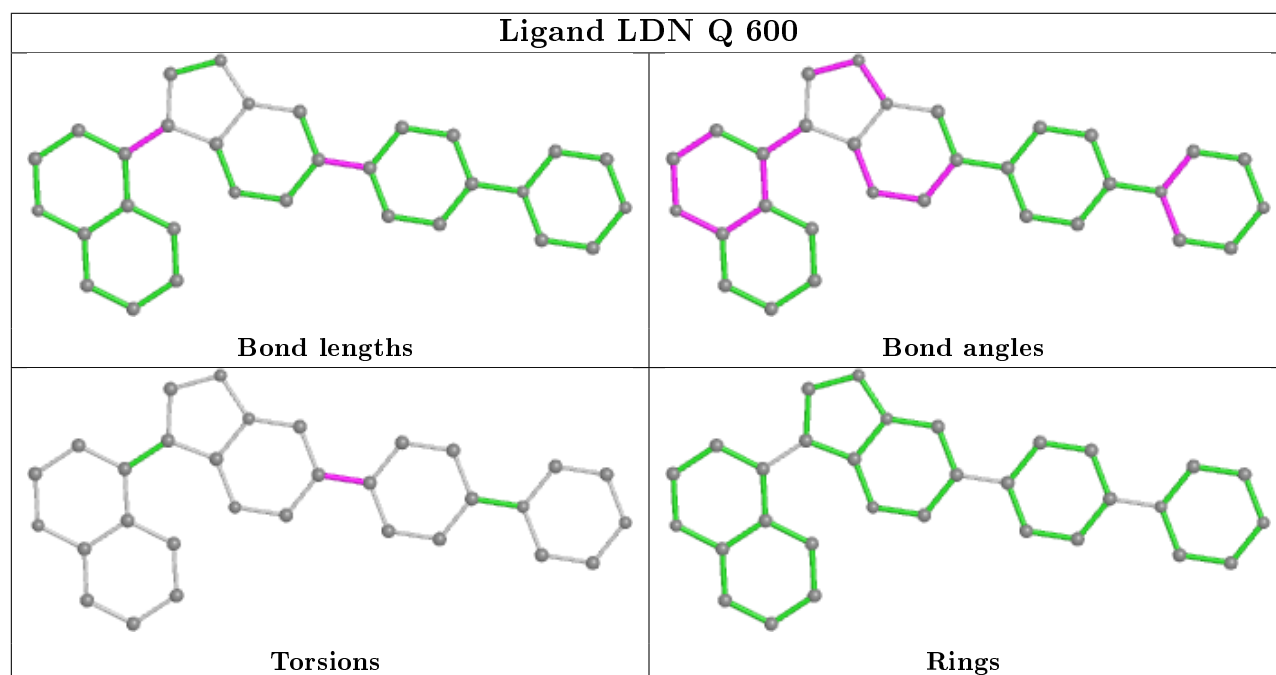




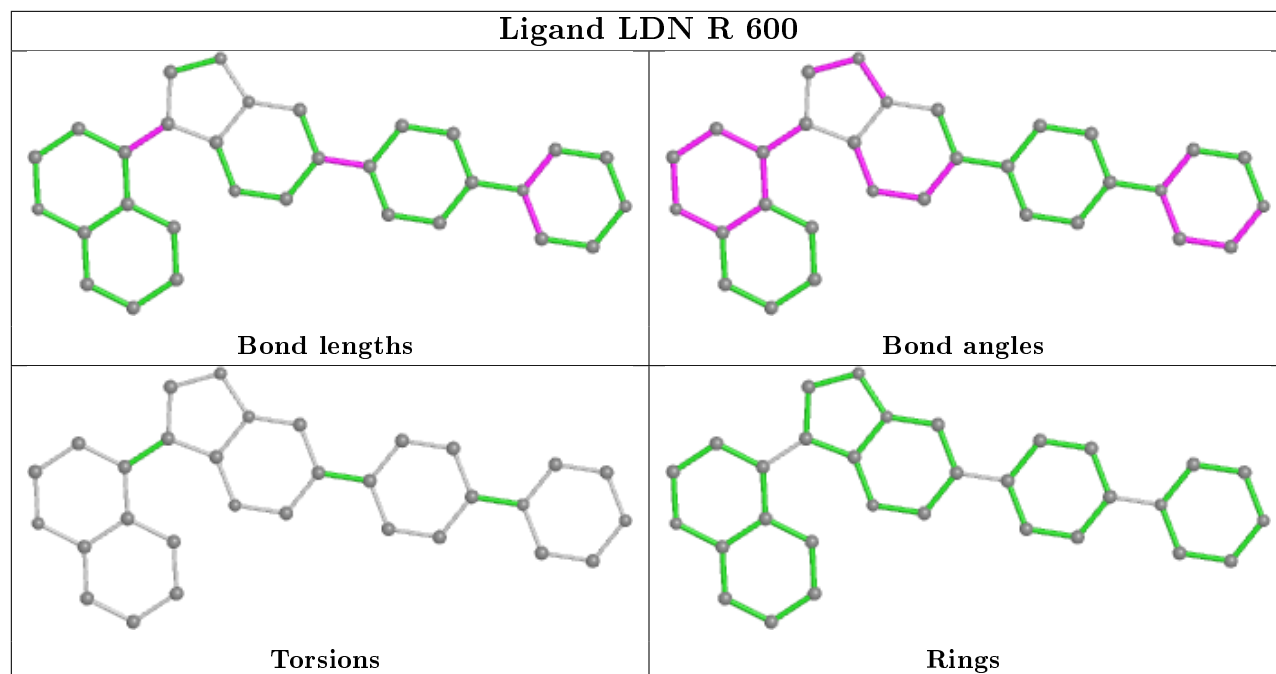
## Ligand LDN V 600



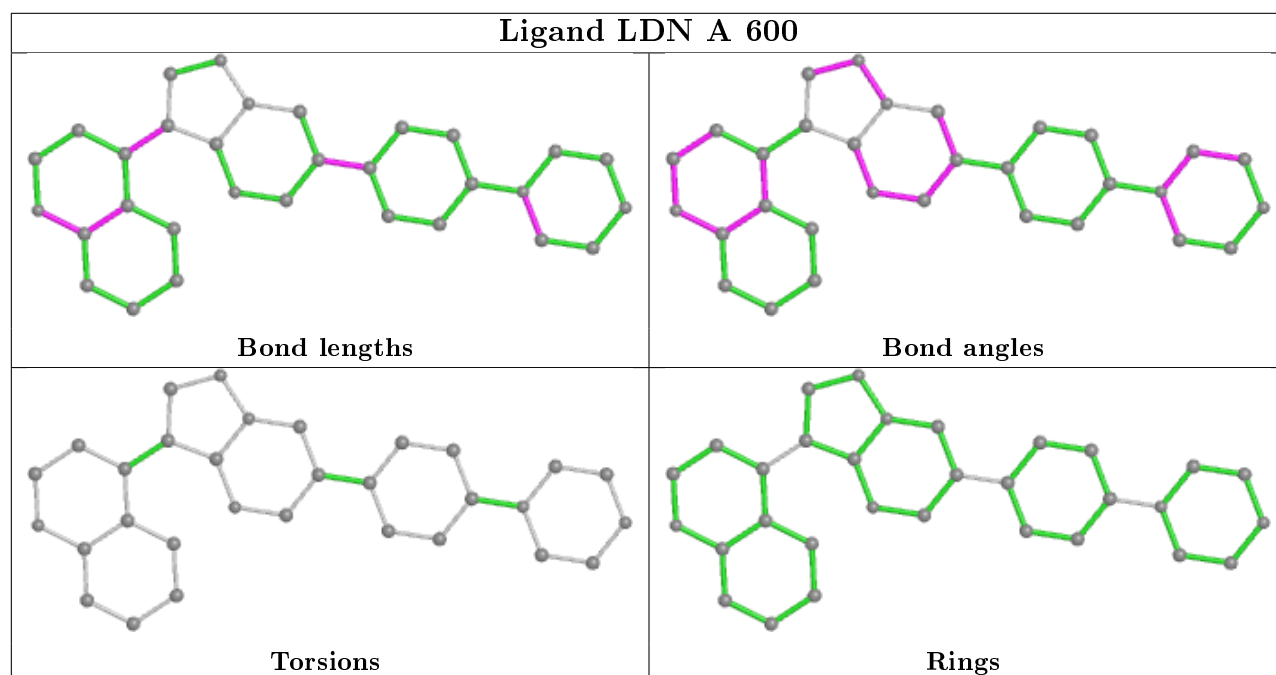
## Ligand LDN Q 600

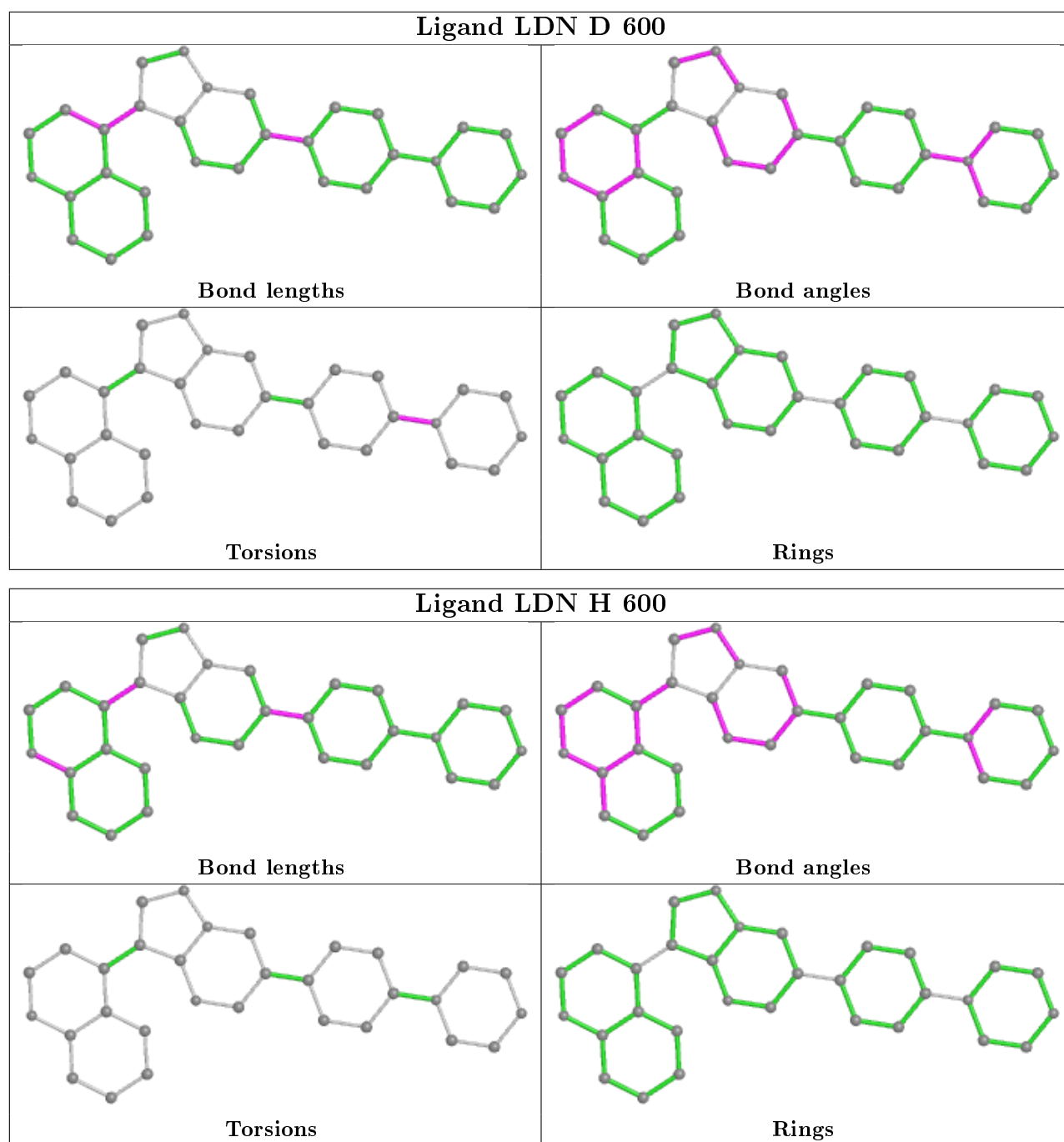


## Ligand LDN R 600



## Ligand LDN A 600





## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	296/305 (97%)	-0.13	1 (0%) 94 95	24, 39, 54, 64	0
1	B	295/305 (96%)	0.08	6 (2%) 65 60	31, 43, 58, 70	0
1	C	299/305 (98%)	-0.01	3 (1%) 82 81	24, 40, 58, 70	0
1	D	298/305 (97%)	-0.14	1 (0%) 94 95	25, 37, 51, 64	0
1	E	294/305 (96%)	-0.11	4 (1%) 75 73	26, 36, 51, 69	0
1	F	294/305 (96%)	0.04	8 (2%) 54 50	28, 44, 68, 87	0
1	G	294/305 (96%)	-0.07	2 (0%) 87 87	15, 27, 43, 58	0
1	H	294/305 (96%)	-0.04	5 (1%) 70 67	27, 40, 57, 63	0
1	I	293/305 (96%)	-0.10	1 (0%) 94 95	16, 27, 45, 55	0
1	J	252/305 (82%)	2.82	140 (55%) 0 0	62, 82, 101, 113	0
1	K	261/305 (85%)	3.38	165 (63%) 0 0	29, 88, 105, 112	0
1	L	296/305 (97%)	-0.03	6 (2%) 65 60	26, 40, 53, 70	0
1	M	298/305 (97%)	-0.10	2 (0%) 87 87	25, 35, 58, 65	0
1	N	300/305 (98%)	-0.04	1 (0%) 94 95	17, 30, 50, 68	0
1	O	297/305 (97%)	0.18	4 (1%) 77 75	29, 44, 59, 79	0
1	P	290/305 (95%)	2.59	149 (51%) 0 0	35, 79, 99, 110	0
1	Q	294/305 (96%)	-0.12	1 (0%) 94 95	27, 39, 55, 68	0
1	R	294/305 (96%)	-0.02	2 (0%) 87 87	26, 41, 56, 71	0
1	S	294/305 (96%)	-0.07	0 100 100	15, 33, 53, 71	0
1	T	292/305 (95%)	-0.03	2 (0%) 87 87	32, 44, 57, 67	0
1	U	285/305 (93%)	-0.06	4 (1%) 75 73	28, 39, 53, 66	0
1	V	282/305 (92%)	-0.01	3 (1%) 80 79	26, 39, 55, 69	0
1	W	281/305 (92%)	0.10	5 (1%) 68 65	28, 39, 54, 68	0
1	X	257/305 (84%)	3.32	160 (62%) 0 0	44, 90, 111, 129	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	6930/7320 (94%)	0.43	675 (9%) <b>7</b> <b>6</b>	15, 40, 90, 129	0

All (675) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	309	GLY	17.7
1	X	405	LEU	15.0
1	K	223	GLY	13.5
1	P	472	TRP	13.5
1	K	310	LEU	12.7
1	P	471	CYS	12.4
1	J	387	THR	12.3
1	X	465	ALA	12.1
1	J	353	VAL	11.8
1	P	221	TRP	11.6
1	K	305	SER	11.5
1	X	251	LEU	11.3
1	K	471	CYS	11.1
1	K	337	LEU	11.1
1	P	401	PHE	11.1
1	P	352	ALA	11.0
1	X	261	ALA	10.9
1	K	306	ALA	10.9
1	K	307	ALA	10.8
1	J	444	VAL	10.3
1	J	223	GLY	10.3
1	X	213	TYR	10.2
1	X	331	PHE	10.2
1	X	245	ILE	10.0
1	J	205	VAL	9.9
1	J	285	LEU	9.9
1	J	325	ALA	9.8
1	K	366	ASN	9.8
1	J	351	LEU	9.7
1	K	304	VAL	9.6
1	P	377	ALA	9.5
1	J	203	ALA	9.5
1	P	474	PRO	9.4
1	K	243	THR	9.3
1	K	488	THR	9.1
1	K	447	GLN	9.0
1	X	242	GLU	9.0

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Mol	Chain	Res	Type	RSRZ
1	J	445	ASP	8.9
1	P	223	GLY	8.8
1	P	378	PRO	8.8
1	K	228	VAL	8.8
1	J	474	PRO	8.8
1	J	390	PHE	8.7
1	J	220	LEU	8.5
1	K	425	PHE	8.4
1	K	403	LEU	8.4
1	K	421	TYR	8.4
1	X	250	LEU	8.3
1	K	420	ASP	8.3
1	K	470	GLU	8.2
1	X	407	GLU	8.1
1	J	424	PRO	8.1
1	X	367	ASN	8.0
1	P	325	ALA	7.9
1	P	222	HIS	7.9
1	K	251	LEU	7.8
1	K	445	ASP	7.8
1	X	471	CYS	7.8
1	X	334	ARG	7.7
1	J	326	ILE	7.7
1	X	262	SER	7.7
1	X	337	LEU	7.7
1	P	483	LEU	7.6
1	J	202	VAL	7.6
1	J	328	HIS	7.4
1	J	331	PHE	7.4
1	X	314	HIS	7.4
1	X	480	LEU	7.4
1	P	249	VAL	7.4
1	X	315	VAL	7.3
1	X	404	VAL	7.3
1	K	204	LEU	7.3
1	X	285	LEU	7.3
1	P	448	THR	7.2
1	J	248	THR	7.2
1	K	222	HIS	7.2
1	X	468	MET	7.2
1	X	449	PRO	7.1
1	K	308	CYS	7.1

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Mol	Chain	Res	Type	RSRZ
1	X	297	HIS	7.1
1	K	239	TRP	7.1
1	P	424	PRO	7.1
1	P	224	GLU	7.0
1	P	386	ARG	7.0
1	X	374	ARG	7.0
1	X	428	VAL	7.0
1	P	390	PHE	7.0
1	K	398	ILE	6.9
1	P	365	GLY	6.9
1	K	229	LYS	6.9
1	P	476	PRO	6.9
1	P	375	TYR	6.8
1	K	368	PRO	6.8
1	X	408	ILE	6.8
1	X	366	ASN	6.8
1	P	473	TYR	6.7
1	P	400	ALA	6.7
1	P	351	LEU	6.6
1	X	342	LEU	6.6
1	K	296	PRO	6.6
1	J	352	ALA	6.6
1	J	425	PHE	6.5
1	X	486	LYS	6.4
1	X	253	HIS	6.4
1	K	287	ASP	6.4
1	X	406	TRP	6.3
1	J	340	SER	6.3
1	X	293	THR	6.3
1	X	394	LYS	6.2
1	X	260	ILE	6.2
1	J	449	PRO	6.2
1	K	244	GLU	6.2
1	J	393	TYR	6.2
1	X	279	TYR	6.2
1	K	224	GLU	6.2
1	K	468	MET	6.1
1	J	335	ASN	6.1
1	K	408	ILE	6.1
1	P	320	THR	6.1
1	K	299	ALA	6.1
1	P	398	ILE	6.1

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Mol	Chain	Res	Type	RSRZ
1	K	245	ILE	6.1
1	K	472	TRP	6.1
1	X	203	ALA	6.1
1	K	328	HIS	6.0
1	K	373	LYS	6.0
1	X	304	VAL	6.0
1	P	245	ILE	6.0
1	X	478	ALA	6.0
1	X	419	GLU	5.9
1	X	330	ASP	5.9
1	X	488	THR	5.9
1	P	395	TRP	5.9
1	P	347	ALA	5.9
1	P	205	VAL	5.9
1	P	257	LEU	5.9
1	K	211	GLY	5.9
1	K	275	LEU	5.8
1	K	474	PRO	5.8
1	J	414	VAL	5.8
1	K	246	TYR	5.8
1	P	403	LEU	5.8
1	X	313	LEU	5.8
1	K	448	THR	5.7
1	J	337	LEU	5.7
1	J	477	SER	5.7
1	P	484	ARG	5.7
1	J	421	TYR	5.7
1	J	200	ARG	5.7
1	P	279	TYR	5.7
1	K	294	LEU	5.7
1	X	296	PRO	5.7
1	K	449	PRO	5.6
1	P	306	ALA	5.6
1	X	453	ASN	5.6
1	K	385	ILE	5.6
1	P	423	PRO	5.6
1	J	261	ALA	5.6
1	X	281	GLU	5.6
1	P	276	ILE	5.5
1	K	395	TRP	5.5
1	X	456	ALA	5.5
1	J	400	ALA	5.5

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Mol	Chain	Res	Type	RSRZ
1	K	249	VAL	5.5
1	J	478	ALA	5.5
1	K	284	SER	5.5
1	J	473	TYR	5.5
1	K	312	HIS	5.4
1	J	231	PHE	5.4
1	K	297	HIS	5.4
1	X	308	CYS	5.4
1	J	324	PRO	5.3
1	X	336	VAL	5.3
1	X	306	ALA	5.3
1	X	343	GLN	5.3
1	X	368	PRO	5.3
1	X	470	GLU	5.3
1	P	481	THR	5.3
1	X	310	LEU	5.3
1	P	447	GLN	5.2
1	X	401	PHE	5.2
1	P	480	LEU	5.2
1	X	280	HIS	5.2
1	K	303	ALA	5.2
1	P	324	PRO	5.2
1	J	207	CYS	5.2
1	J	345	CYS	5.1
1	X	221	TRP	5.1
1	J	448	THR	5.1
1	X	254	ASP	5.1
1	P	421	TYR	5.1
1	K	313	LEU	5.1
1	P	281	GLU	5.0
1	K	288	PHE	5.0
1	P	475	ASN	5.0
1	P	246	TYR	5.0
1	X	339	LYS	5.0
1	X	398	ILE	4.9
1	X	395	TRP	4.9
1	K	199	ALA	4.9
1	P	204	LEU	4.9
1	J	281	GLU	4.9
1	X	249	VAL	4.9
1	J	312	HIS	4.9
1	K	325	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
1	X	375	TYR	4.9
1	K	393	TYR	4.8
1	X	228	VAL	4.8
1	K	311	ALA	4.8
1	P	364	ILE	4.8
1	X	284	SER	4.8
1	X	423	PRO	4.8
1	X	482	ALA	4.8
1	J	204	LEU	4.8
1	P	209	GLY	4.8
1	P	309	GLY	4.8
1	X	329	ARG	4.8
1	K	343	GLN	4.8
1	J	313	LEU	4.8
1	X	421	TYR	4.7
1	K	336	VAL	4.7
1	K	396	THR	4.7
1	J	300	LEU	4.7
1	K	342	LEU	4.7
1	X	476	PRO	4.7
1	K	231	PHE	4.7
1	X	215	GLU	4.7
1	J	307	ALA	4.7
1	P	359	SER	4.7
1	J	245	ILE	4.7
1	P	230	ILE	4.7
1	K	257	LEU	4.7
1	X	258	GLY	4.6
1	K	279	TYR	4.6
1	K	230	ILE	4.6
1	P	340	SER	4.6
1	P	470	GLU	4.5
1	J	420	ASP	4.5
1	P	326	ILE	4.5
1	J	310	LEU	4.5
1	P	303	ALA	4.5
1	J	276	ILE	4.5
1	X	243	THR	4.5
1	X	396	THR	4.5
1	K	473	TYR	4.5
1	P	219	GLY	4.5
1	P	381	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	W	195	GLN	4.4
1	K	365	GLY	4.4
1	P	478	ALA	4.4
1	P	380	VAL	4.4
1	X	377	ALA	4.4
1	P	321	GLN	4.4
1	X	286	TYR	4.4
1	K	338	VAL	4.4
1	J	423	PRO	4.4
1	J	349	LEU	4.4
1	P	331	PHE	4.4
1	J	230	ILE	4.3
1	J	389	CYS	4.3
1	P	488	THR	4.3
1	J	225	SER	4.3
1	K	430	PRO	4.3
1	P	346	ILE	4.3
1	K	281	GLU	4.3
1	X	252	ARG	4.2
1	P	466	GLN	4.2
1	X	211	GLY	4.2
1	X	246	TYR	4.2
1	J	246	TYR	4.2
1	X	239	TRP	4.2
1	J	469	ARG	4.2
1	P	310	LEU	4.2
1	K	198	VAL	4.2
1	J	247	ASN	4.1
1	K	276	ILE	4.1
1	K	418	VAL	4.1
1	X	376	MET	4.1
1	X	353	VAL	4.1
1	J	401	PHE	4.1
1	X	303	ALA	4.1
1	K	485	ILE	4.1
1	X	202	VAL	4.1
1	P	239	TRP	4.1
1	X	229	LYS	4.1
1	P	376	MET	4.1
1	X	475	ASN	4.1
1	J	426	TYR	4.0
1	K	248	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	J	235	ASP	4.0
1	X	425	PHE	4.0
1	K	399	TRP	4.0
1	J	475	ASN	4.0
1	K	367	ASN	4.0
1	X	298	LEU	4.0
1	K	220	LEU	4.0
1	O	387	THR	4.0
1	P	335	ASN	4.0
1	X	464	LEU	4.0
1	X	439	LYS	4.0
1	J	385	ILE	4.0
1	J	201	GLN	4.0
1	P	207	CYS	4.0
1	X	474	PRO	4.0
1	X	352	ALA	4.0
1	J	288	PHE	3.9
1	K	438	MET	3.9
1	X	393	TYR	3.9
1	K	333	SER	3.9
1	X	477	SER	3.9
1	X	378	PRO	3.9
1	J	334	ARG	3.9
1	J	316	GLU	3.9
1	K	492	ILE	3.9
1	P	311	ALA	3.9
1	P	232	SER	3.9
1	P	243	THR	3.9
1	P	468	MET	3.9
1	X	481	THR	3.9
1	X	440	LYS	3.9
1	X	311	ALA	3.9
1	J	287	ASP	3.9
1	K	346	ILE	3.9
1	B	197	THR	3.9
1	K	387	THR	3.9
1	X	487	LYS	3.9
1	P	263	ASP	3.9
1	K	300	LEU	3.8
1	P	396	THR	3.8
1	X	338	VAL	3.8
1	P	248	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	K	340	SER	3.8
1	J	286	TYR	3.8
1	X	230	ILE	3.8
1	X	469	ARG	3.8
1	K	406	TRP	3.8
1	K	212	ARG	3.8
1	J	436	GLU	3.8
1	J	472	TRP	3.8
1	X	399	TRP	3.8
1	K	466	GLN	3.7
1	P	250	LEU	3.7
1	P	391	GLU	3.7
1	X	341	ASN	3.7
1	P	238	SER	3.7
1	P	302	LEU	3.7
1	J	241	ARG	3.7
1	P	216	VAL	3.7
1	X	426	TYR	3.7
1	J	437	ASP	3.7
1	R	388	ASP	3.7
1	P	313	LEU	3.7
1	J	440	LYS	3.6
1	K	315	VAL	3.6
1	K	467	MET	3.6
1	K	203	ALA	3.6
1	J	336	VAL	3.6
1	X	467	MET	3.6
1	K	295	GLU	3.6
1	K	345	CYS	3.6
1	K	317	ILE	3.6
1	K	327	ALA	3.6
1	J	221	TRP	3.6
1	F	388	ASP	3.6
1	K	444	VAL	3.5
1	P	220	LEU	3.5
1	X	420	ASP	3.5
1	O	213	TYR	3.5
1	P	394	LYS	3.5
1	I	0	MET	3.5
1	K	208	VAL	3.5
1	X	448	THR	3.5
1	P	438	MET	3.5

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Mol	Chain	Res	Type	RSRZ
1	X	442	VAL	3.5
1	P	297	HIS	3.5
1	J	255	ASN	3.5
1	P	206	GLU	3.4
1	K	431	ASN	3.4
1	K	410	ARG	3.4
1	P	317	ILE	3.4
1	J	399	TRP	3.4
1	K	283	GLY	3.4
1	J	308	CYS	3.4
1	X	312	HIS	3.4
1	X	390	PHE	3.4
1	X	197	THR	3.4
1	X	317	ILE	3.4
1	J	249	VAL	3.4
1	K	464	LEU	3.4
1	K	278	HIS	3.4
1	J	344	CYS	3.4
1	B	198	VAL	3.3
1	X	305	SER	3.3
1	J	376	MET	3.3
1	J	378	PRO	3.3
1	J	438	MET	3.3
1	X	316	GLU	3.3
1	J	397	ASP	3.3
1	X	387	THR	3.3
1	P	323	LYS	3.3
1	K	237	GLN	3.3
1	X	432	ASP	3.3
1	K	205	VAL	3.3
1	X	216	VAL	3.3
1	J	350	GLY	3.3
1	P	353	VAL	3.3
1	J	430	PRO	3.3
1	P	440	LYS	3.2
1	K	347	ALA	3.2
1	J	236	GLU	3.2
1	P	385	ILE	3.2
1	K	200	ARG	3.2
1	P	382	ASP	3.2
1	P	225	SER	3.2
1	K	331	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	P	198	VAL	3.2
1	X	257	LEU	3.2
1	K	352	ALA	3.2
1	P	453	ASN	3.2
1	J	234	ARG	3.2
1	K	274	TRP	3.1
1	J	280	HIS	3.1
1	X	354	MET	3.1
1	X	256	ILE	3.1
1	K	209	GLY	3.1
1	C	221	TRP	3.1
1	J	439	LYS	3.1
1	L	483	LEU	3.1
1	P	392	SER	3.1
1	X	409	ALA	3.1
1	X	292	GLN	3.1
1	X	422	ARG	3.1
1	X	307	ALA	3.1
1	J	388	ASP	3.1
1	K	422	ARG	3.1
1	P	199	ALA	3.1
1	J	256	ILE	3.1
1	B	195	GLN	3.1
1	K	334	ARG	3.1
1	J	476	PRO	3.1
1	K	247	ASN	3.1
1	X	204	LEU	3.1
1	F	474	PRO	3.0
1	J	375	TYR	3.0
1	X	240	PHE	3.0
1	X	255	ASN	3.0
1	K	484	ARG	3.0
1	P	290	GLN	3.0
1	P	274	TRP	3.0
1	P	332	LYS	3.0
1	P	286	TYR	3.0
1	J	342	LEU	3.0
1	K	350	GLY	3.0
1	K	351	LEU	3.0
1	P	296	PRO	3.0
1	B	260	ILE	2.9
1	F	250	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	K	226	VAL	2.9
1	K	262	SER	2.9
1	K	479	ARG	2.9
1	L	387	THR	2.9
1	X	400	ALA	2.9
1	F	395	TRP	2.9
1	J	332	LYS	2.9
1	X	410	ARG	2.9
1	F	477	SER	2.9
1	M	213	TYR	2.9
1	J	460	VAL	2.9
1	K	201	GLN	2.8
1	P	233	SER	2.8
1	F	476	PRO	2.8
1	K	271	THR	2.8
1	P	450	THR	2.8
1	X	345	CYS	2.8
1	J	384	GLN	2.8
1	X	277	THR	2.8
1	K	428	VAL	2.8
1	H	473	TYR	2.8
1	J	422	ARG	2.8
1	P	280	HIS	2.8
1	K	323	LYS	2.8
1	P	322	GLY	2.8
1	J	394	LYS	2.8
1	K	437	ASP	2.8
1	K	389	CYS	2.8
1	P	213	TYR	2.7
1	X	212	ARG	2.7
1	P	348	ASP	2.7
1	J	251	LEU	2.7
1	X	231	PHE	2.7
1	N	267	ARG	2.7
1	K	341	ASN	2.7
1	K	286	TYR	2.7
1	K	316	GLU	2.7
1	K	446	GLN	2.7
1	X	326	ILE	2.7
1	J	327	ALA	2.7
1	F	447	GLN	2.7
1	X	349	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	P	215	GLU	2.7
1	J	348	ASP	2.7
1	K	280	HIS	2.6
1	P	314	HIS	2.6
1	P	231	PHE	2.6
1	X	346	ILE	2.6
1	K	282	HIS	2.6
1	E	483	LEU	2.6
1	K	481	THR	2.6
1	W	223	GLY	2.6
1	J	243	THR	2.6
1	K	261	ALA	2.6
1	P	278	HIS	2.6
1	J	333	SER	2.6
1	K	293	THR	2.6
1	H	370	VAL	2.6
1	J	480	LEU	2.6
1	P	363	ASP	2.6
1	X	223	GLY	2.6
1	P	293	THR	2.6
1	U	387	THR	2.6
1	K	252	ARG	2.6
1	X	328	HIS	2.6
1	K	202	VAL	2.6
1	P	467	MET	2.6
1	K	324	PRO	2.5
1	X	444	VAL	2.5
1	X	373	LYS	2.5
1	J	470	GLU	2.5
1	P	258	GLY	2.5
1	X	424	PRO	2.5
1	C	307	ALA	2.5
1	J	406	TRP	2.5
1	J	219	GLY	2.5
1	P	441	VAL	2.5
1	L	452	PRO	2.5
1	P	312	HIS	2.5
1	K	221	TRP	2.5
1	J	489	LEU	2.5
1	O	308	CYS	2.5
1	X	287	ASP	2.5
1	K	478	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	X	327	ALA	2.5
1	P	425	PHE	2.5
1	P	449	PRO	2.4
1	J	450	THR	2.4
1	J	464	LEU	2.4
1	P	349	LEU	2.4
1	K	353	VAL	2.4
1	K	277	THR	2.4
1	H	460	VAL	2.4
1	X	241	ARG	2.4
1	W	213	TYR	2.4
1	X	247	ASN	2.4
1	K	423	PRO	2.4
1	K	400	ALA	2.4
1	K	292	GLN	2.4
1	K	401	PHE	2.4
1	W	474	PRO	2.4
1	J	260	ILE	2.4
1	P	370	VAL	2.4
1	P	252	ARG	2.4
1	K	314	HIS	2.4
1	B	456	ALA	2.4
1	K	475	ASN	2.4
1	T	213	TYR	2.4
1	P	457	ALA	2.4
1	P	330	ASP	2.4
1	J	488	THR	2.3
1	K	348	ASP	2.3
1	K	377	ALA	2.3
1	K	256	ILE	2.3
1	P	218	ARG	2.3
1	J	380	VAL	2.3
1	J	429	VAL	2.3
1	X	226	VAL	2.3
1	X	259	PHE	2.3
1	J	443	CYS	2.3
1	P	308	CYS	2.3
1	P	388	ASP	2.3
1	T	0	MET	2.3
1	K	381	LEU	2.3
1	P	393	TYR	2.3
1	J	213	TYR	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	J	214	GLY	2.3
1	M	204	LEU	2.3
1	P	341	ASN	2.3
1	P	486	LYS	2.3
1	K	370	VAL	2.3
1	X	205	VAL	2.3
1	P	379	GLU	2.3
1	J	314	HIS	2.3
1	J	465	ALA	2.3
1	K	439	LYS	2.3
1	J	224	GLU	2.3
1	J	315	VAL	2.3
1	X	348	ASP	2.3
1	P	337	LEU	2.3
1	A	405	LEU	2.3
1	V	213	TYR	2.3
1	J	304	VAL	2.3
1	F	466	GLN	2.2
1	X	340	SER	2.2
1	J	306	ALA	2.2
1	P	482	ALA	2.2
1	L	393	TYR	2.2
1	K	443	CYS	2.2
1	V	418	VAL	2.2
1	P	227	ALA	2.2
1	G	197	THR	2.2
1	P	287	ASP	2.2
1	K	384	GLN	2.2
1	P	399	TRP	2.2
1	P	405	LEU	2.2
1	L	377	ALA	2.2
1	P	254	ASP	2.2
1	P	240	PHE	2.2
1	K	429	VAL	2.2
1	J	467	MET	2.2
1	K	432	ASP	2.2
1	P	436	GLU	2.2
1	J	274	TRP	2.2
1	X	299	ALA	2.2
1	E	448	THR	2.2
1	K	390	PHE	2.2
1	J	228	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	Q	474	PRO	2.2
1	P	389	CYS	2.2
1	P	465	ALA	2.2
1	R	493	SER	2.2
1	X	302	LEU	2.2
1	G	388	ASP	2.2
1	J	277	THR	2.2
1	U	370	VAL	2.1
1	X	220	LEU	2.1
1	K	207	CYS	2.1
1	K	255	ASN	2.1
1	X	201	GLN	2.1
1	J	442	VAL	2.1
1	K	397	ASP	2.1
1	L	401	PHE	2.1
1	J	226	VAL	2.1
1	O	388	ASP	2.1
1	V	251	LEU	2.1
1	X	332	LYS	2.1
1	E	378	PRO	2.1
1	X	466	GLN	2.1
1	P	304	VAL	2.1
1	U	205	VAL	2.1
1	K	378	PRO	2.1
1	C	456	ALA	2.1
1	J	212	ARG	2.1
1	J	284	SER	2.1
1	J	428	VAL	2.1
1	E	279	TYR	2.1
1	H	361	TYR	2.1
1	J	396	THR	2.1
1	J	262	SER	2.1
1	J	454	ARG	2.1
1	P	344	CYS	2.1
1	P	463	GLY	2.1
1	X	309	GLY	2.1
1	X	210	LYS	2.0
1	J	482	ALA	2.0
1	P	469	ARG	2.0
1	K	265	THR	2.0
1	W	197	THR	2.0
1	X	222	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	J	279	TYR	2.0
1	B	431	ASN	2.0
1	H	371	GLY	2.0
1	X	402	GLY	2.0
1	P	452	PRO	2.0
1	J	227	ALA	2.0
1	D	315	VAL	2.0
1	U	460	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

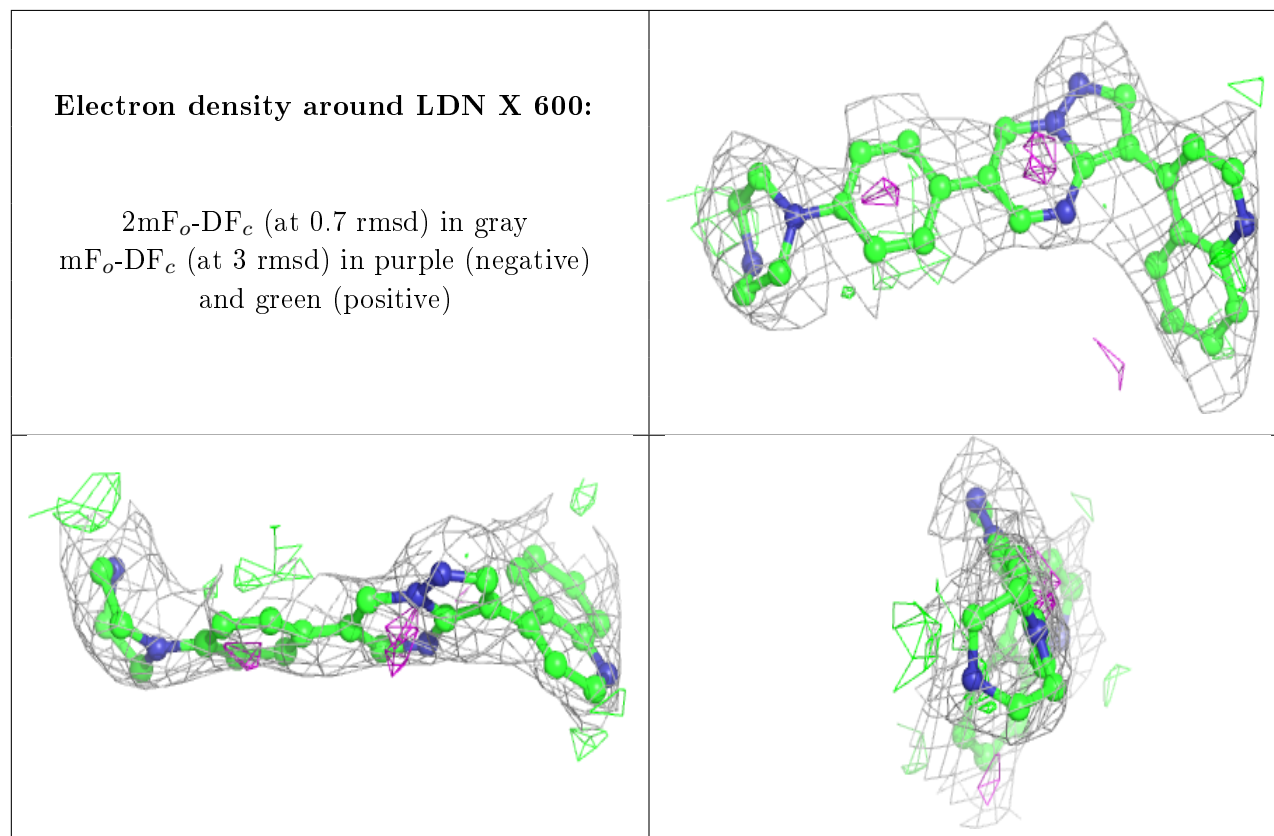
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	LDN	X	600	31/31	0.81	0.25	34,52,63,64	0
2	LDN	P	600	31/31	0.84	0.20	41,50,55,55	0
2	LDN	K	600	31/31	0.86	0.22	36,48,53,59	0
2	LDN	J	600	31/31	0.87	0.22	35,46,52,56	0
2	LDN	E	600	31/31	0.93	0.16	29,33,37,38	0
2	LDN	D	600	31/31	0.93	0.20	27,34,40,43	0
2	LDN	W	600	31/31	0.94	0.16	33,38,42,44	0
2	LDN	U	600	31/31	0.94	0.18	26,31,44,45	0
2	LDN	M	600	31/31	0.94	0.18	30,35,40,48	0
2	LDN	F	600	31/31	0.95	0.15	23,29,32,34	0
2	LDN	B	600	31/31	0.95	0.20	27,34,41,41	0
2	LDN	T	600	31/31	0.95	0.13	30,39,45,45	0
2	LDN	N	600	31/31	0.95	0.19	21,26,34,37	0
2	LDN	O	600	31/31	0.95	0.15	26,33,40,46	0
2	LDN	V	600	31/31	0.95	0.16	26,31,44,46	0

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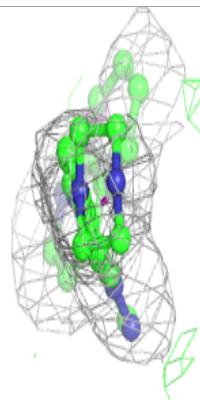
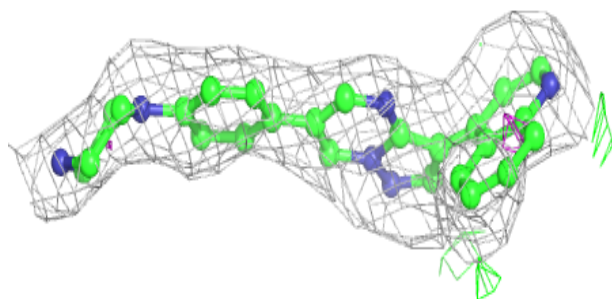
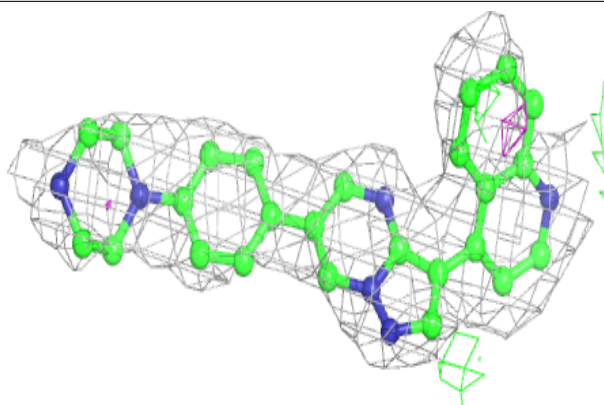
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	LDN	Q	600	31/31	0.95	0.15	25,31,39,45	0
2	LDN	R	600	31/31	0.95	0.14	25,31,36,38	0
2	LDN	A	600	31/31	0.95	0.16	24,36,47,50	0
2	LDN	C	600	31/31	0.95	0.16	27,33,42,45	0
2	LDN	I	600	31/31	0.97	0.14	24,27,39,40	0
2	LDN	L	600	31/31	0.97	0.14	27,32,36,37	0
2	LDN	S	600	31/31	0.97	0.15	20,27,45,50	0
2	LDN	G	600	31/31	0.97	0.16	21,26,36,36	0
2	LDN	H	600	31/31	0.97	0.14	24,27,39,42	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.

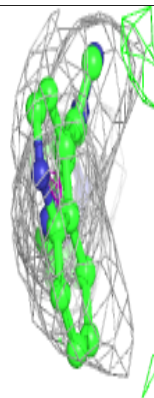
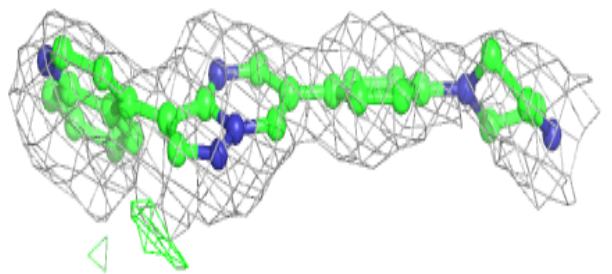
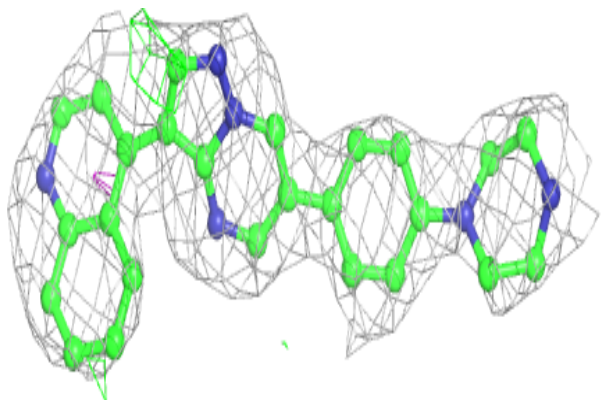


**Electron density around LDN P 600:**

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

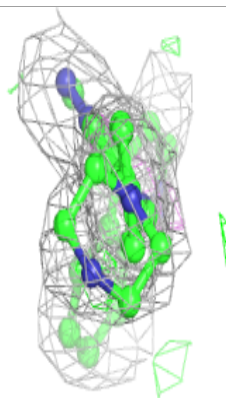
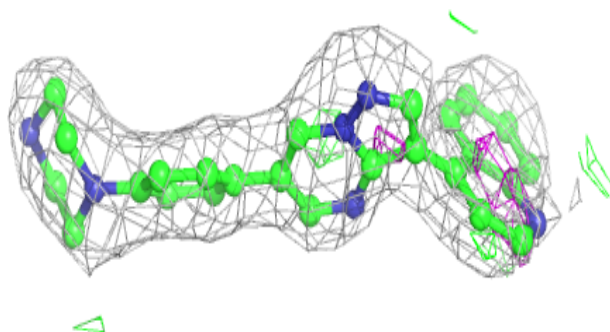
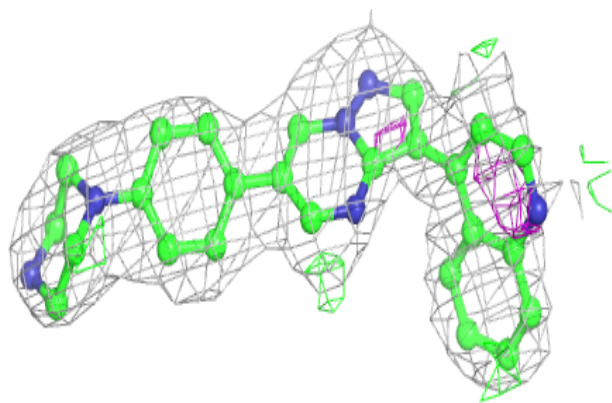
**Electron density around LDN K 600:**

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

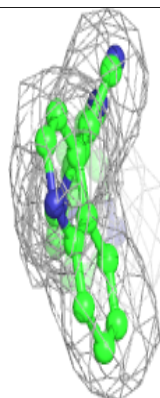
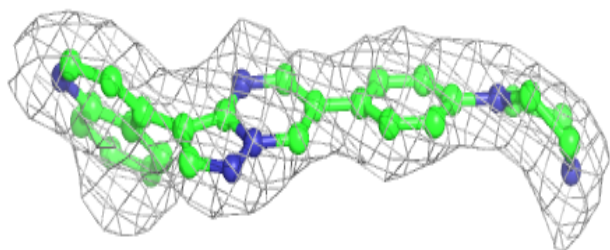
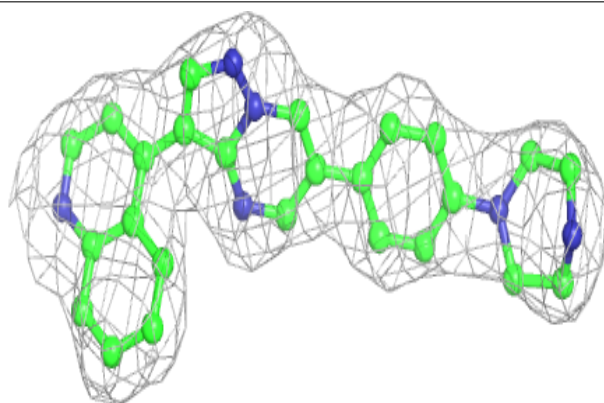


**Electron density around LDN J 600:**

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

**Electron density around LDN E 600:**

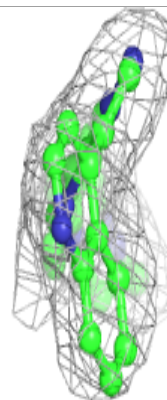
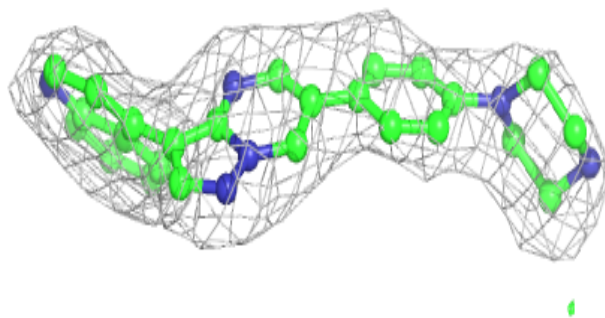
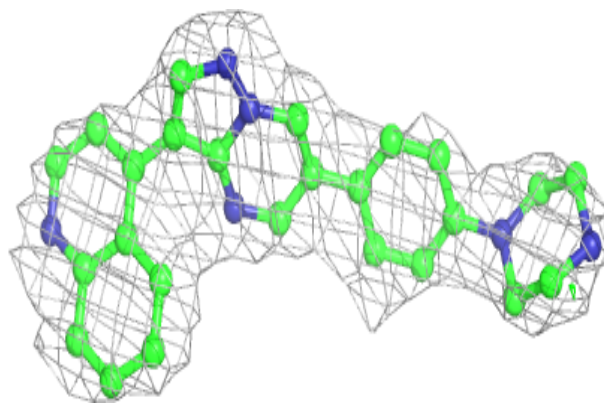
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



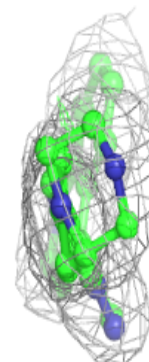
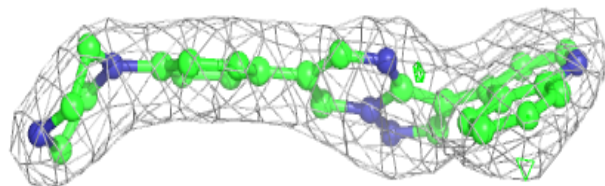
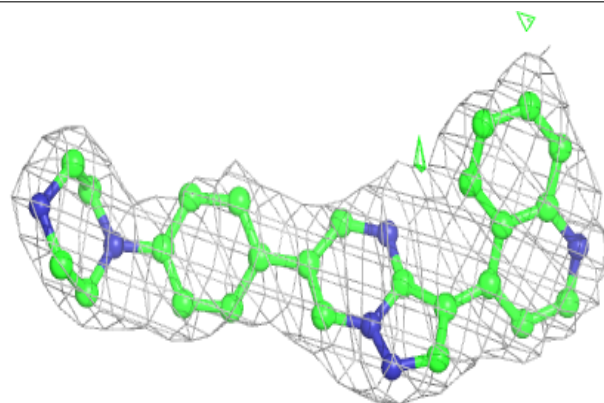


**Electron density around LDN D 600:**

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

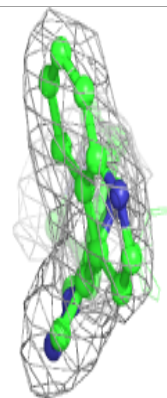
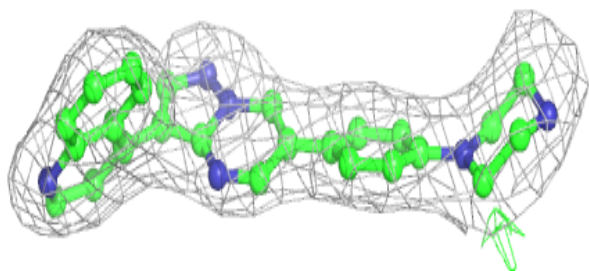
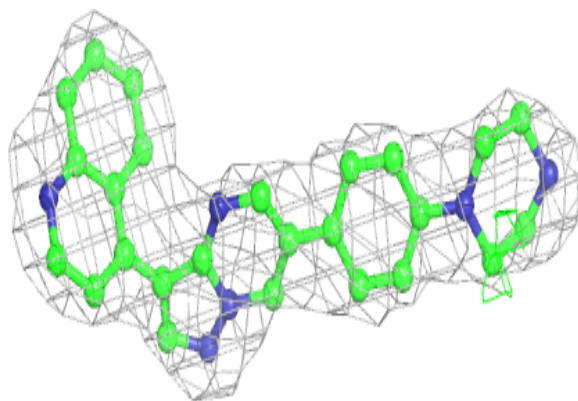
**Electron density around LDN W 600:**

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

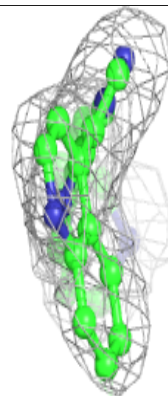
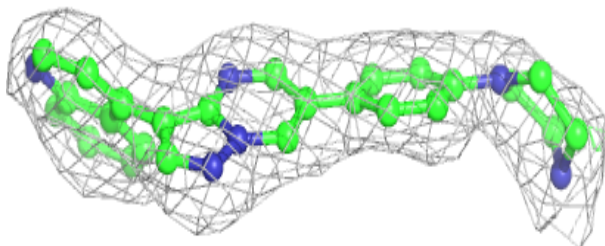
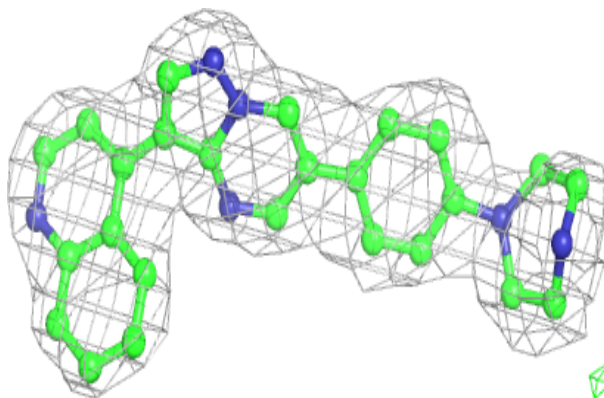


**Electron density around LDN U 600:**

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

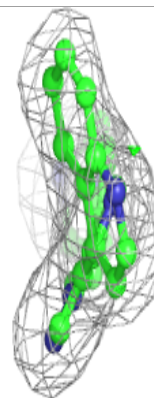
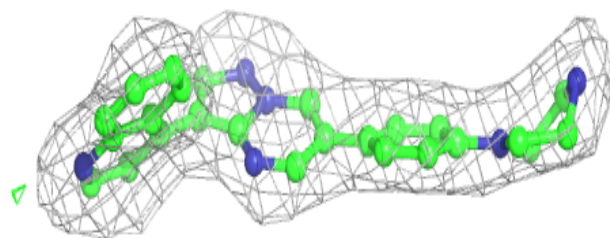
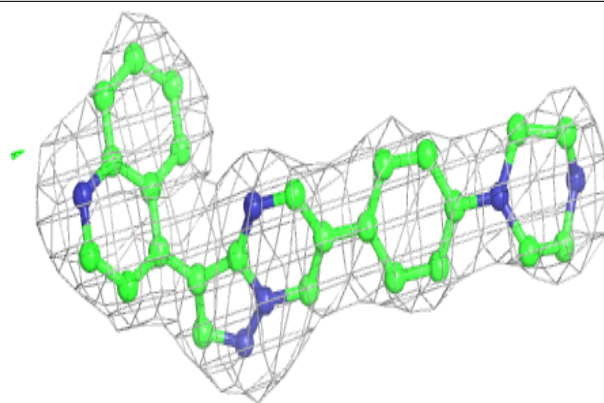
**Electron density around LDN M 600:**

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

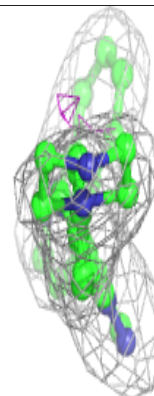
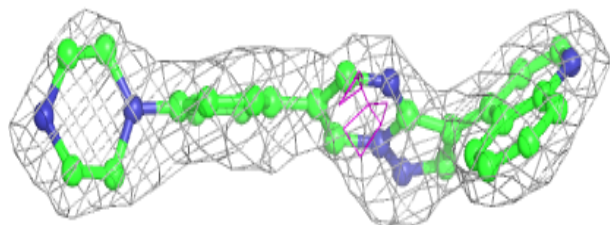
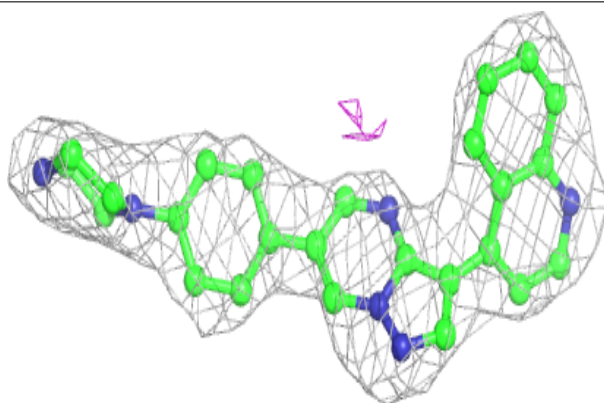


**Electron density around LDN F 600:**

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

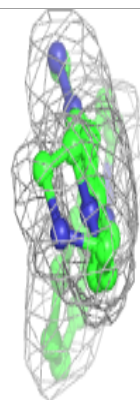
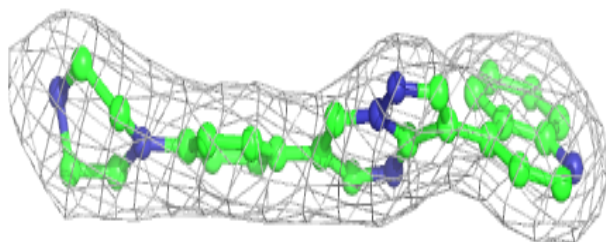
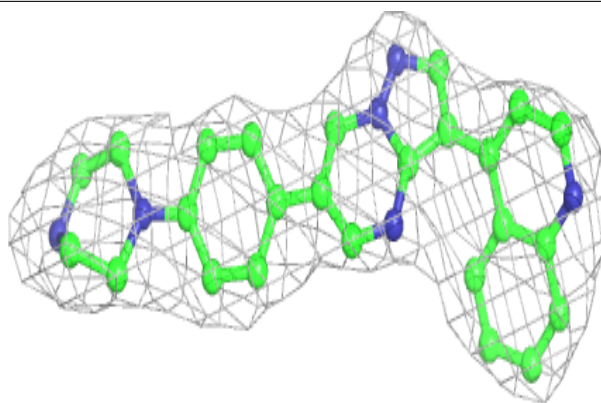
**Electron density around LDN B 600:**

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

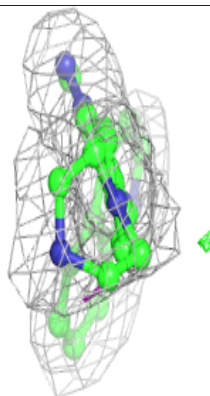
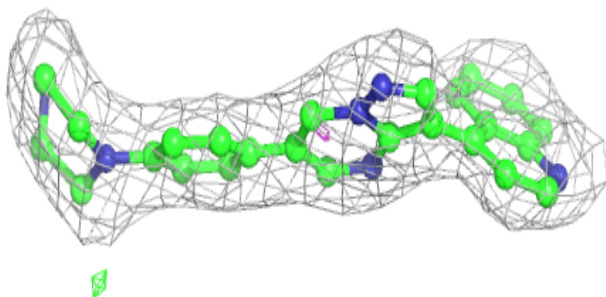
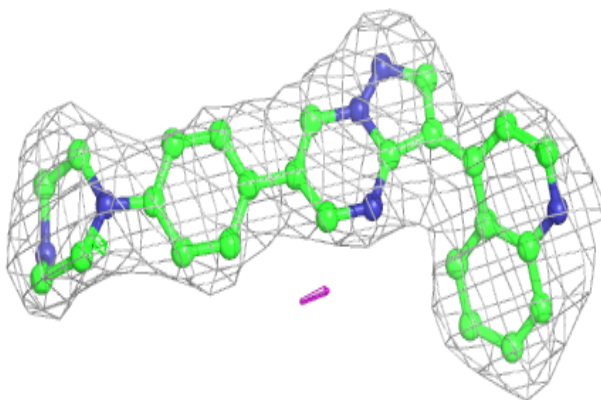


**Electron density around LDN T 600:**

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

**Electron density around LDN N 600:**

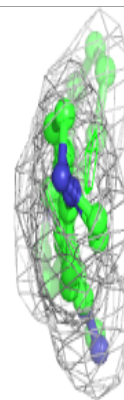
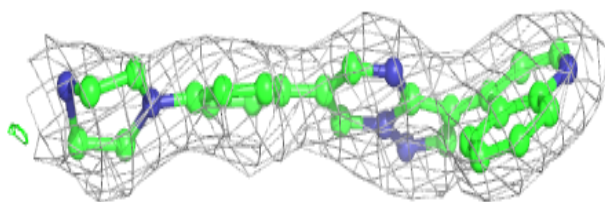
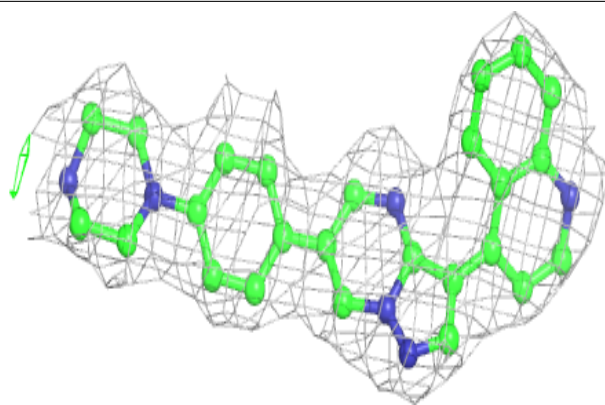
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



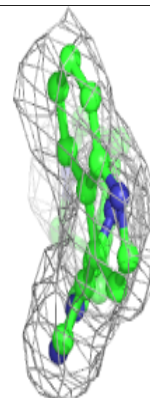
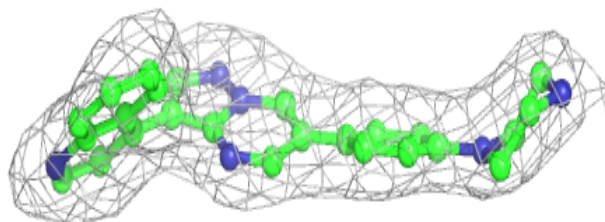
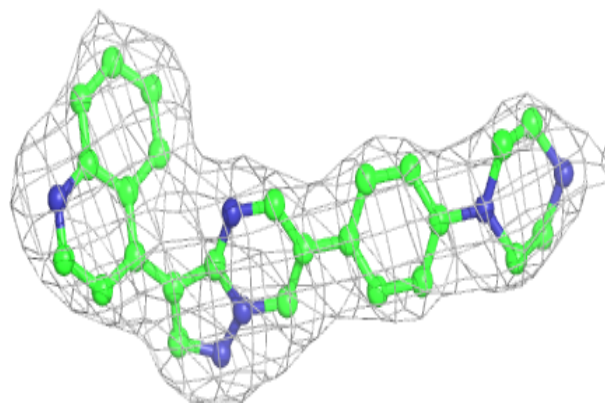


**Electron density around LDN O 600:**

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

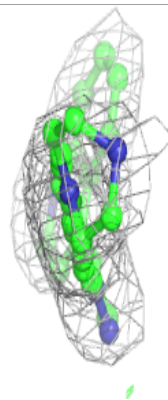
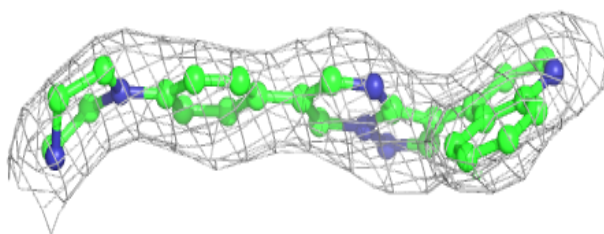
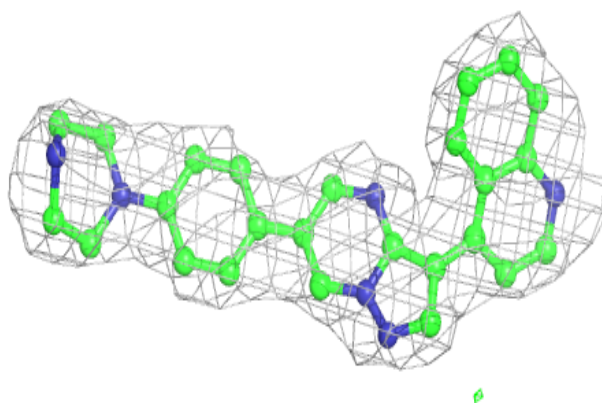
**Electron density around LDN V 600:**

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

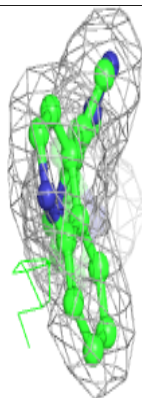
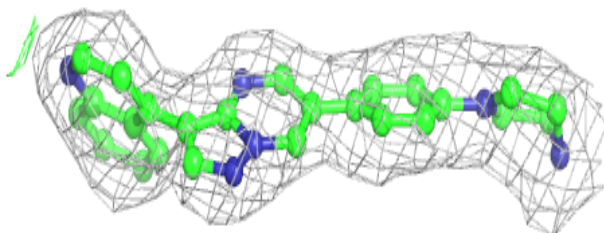
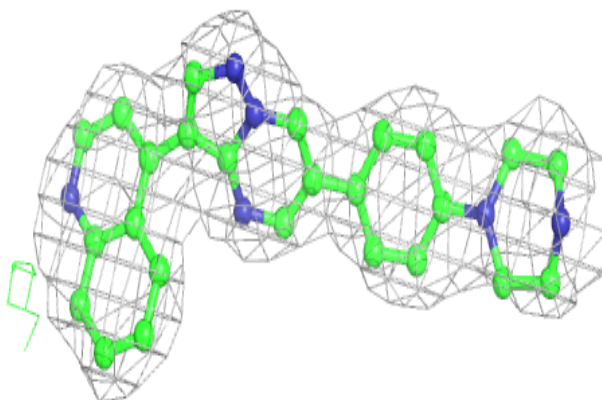


**Electron density around LDN Q 600:**

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

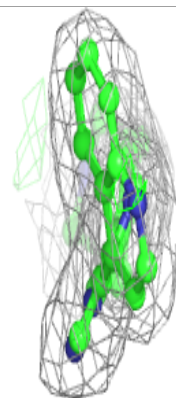
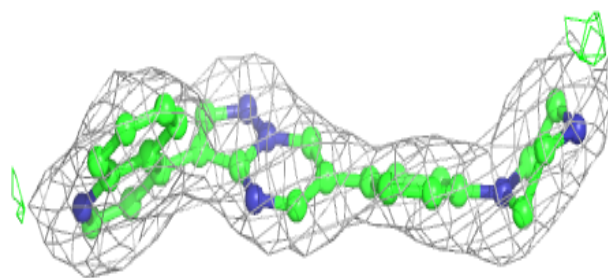
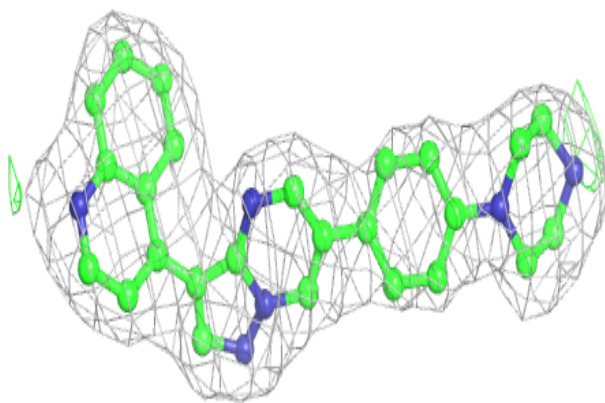
**Electron density around LDN R 600:**

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

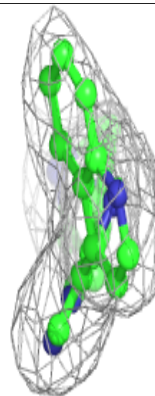
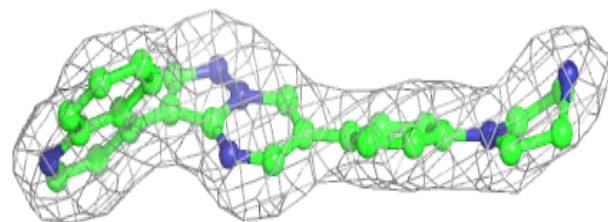
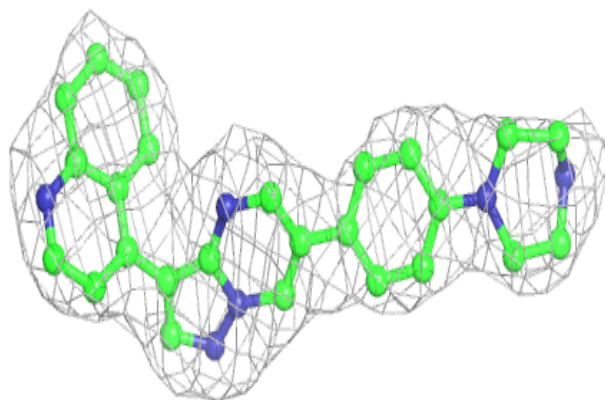


**Electron density around LDN A 600:**

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

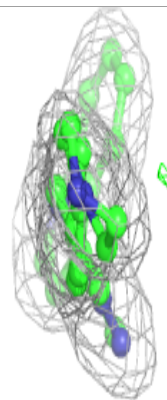
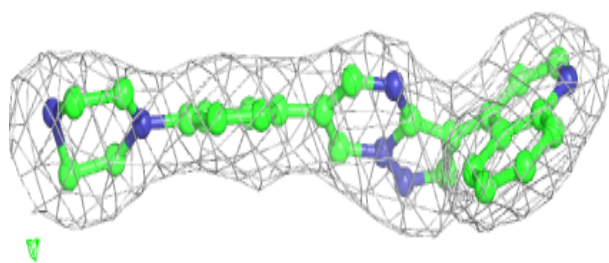
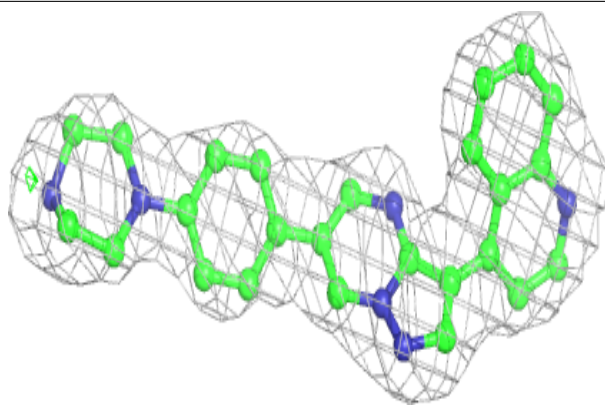
**Electron density around LDN C 600:**

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

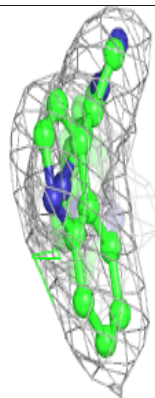
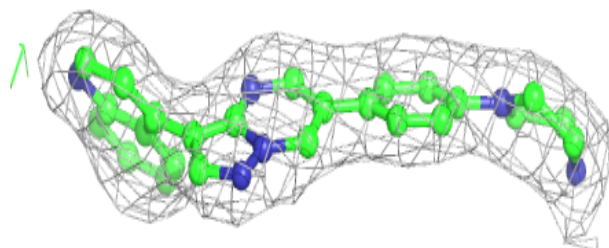
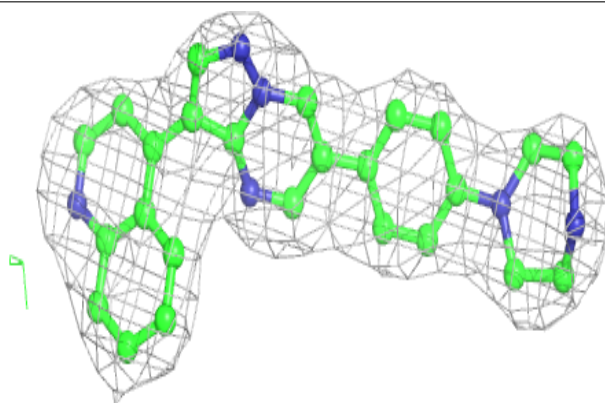


**Electron density around LDN I 600:**

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

**Electron density around LDN L 600:**

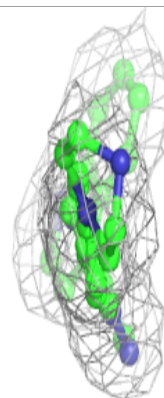
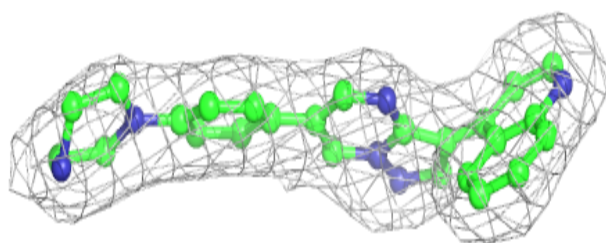
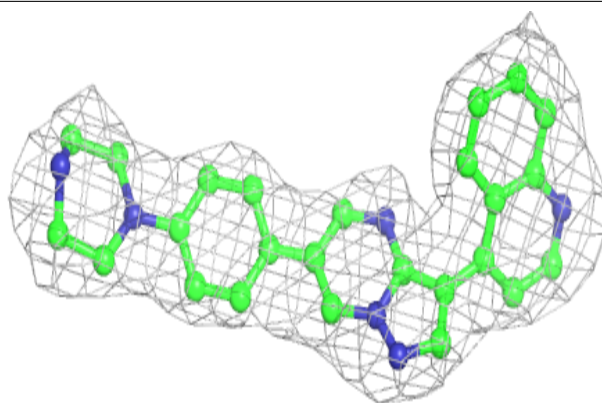
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



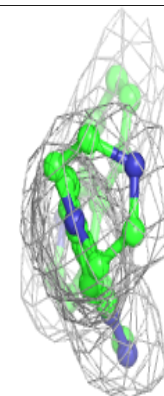
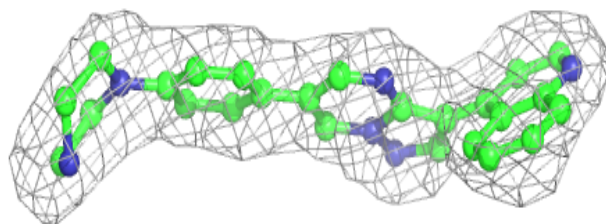
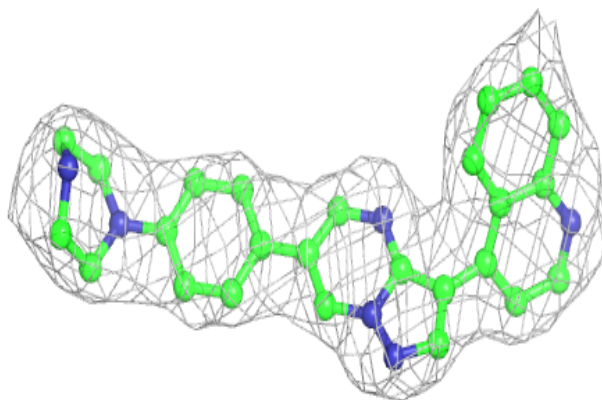


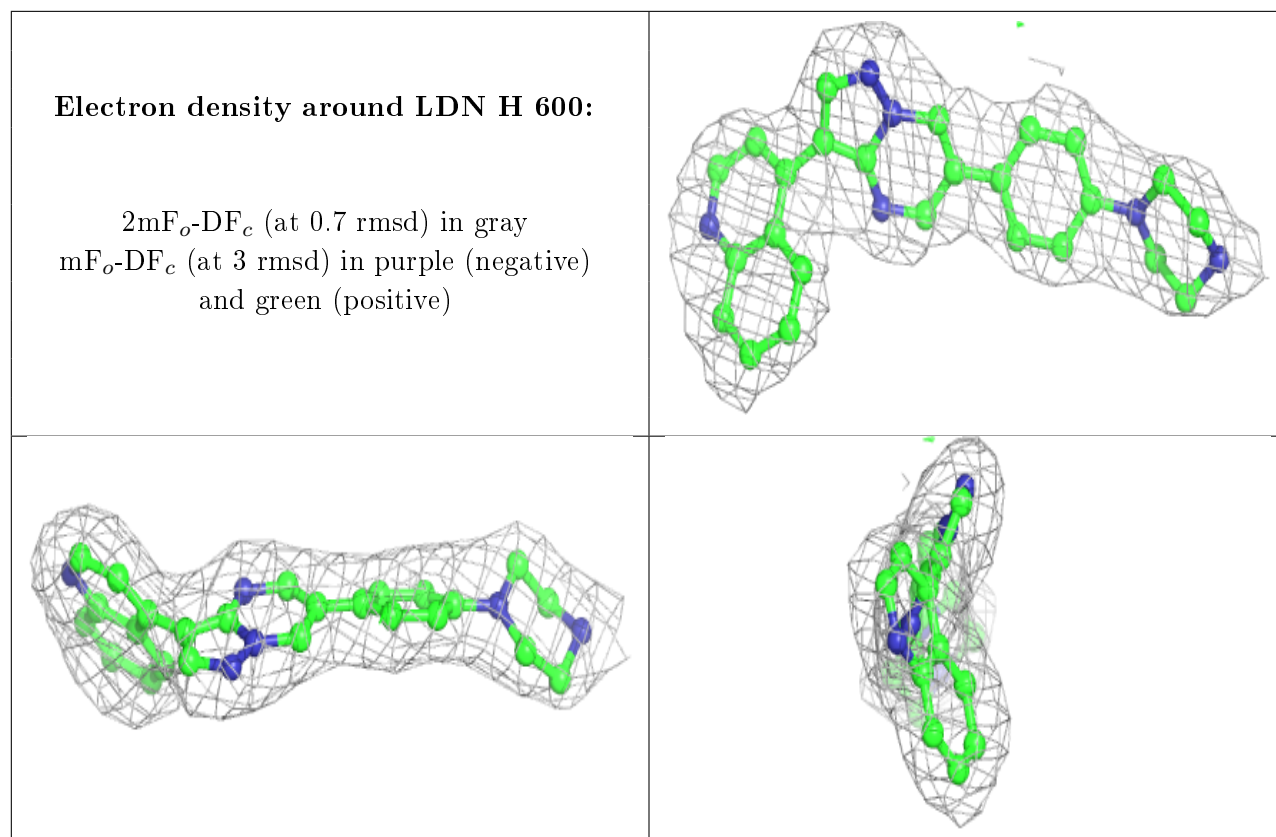
**Electron density around LDN S 600:**

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

**Electron density around LDN G 600:**

$2mF_o-DF_c$  (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.