



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:10 AM UTC

PDB ID : 4XYC / pdb_00004xyc
Title : NANOMOLAR INHIBITORS OF MYCOBACTERIUM TUBERCULOSIS
GLUTAMINE SYNTHETASE 1: SYNTHESIS, BIOLOGICAL EVALUA-
TION AND X-RAY CRYSTALLOGRAPHIC STUDIES
Authors : Couturier, C.; Silve, S.; Morales, R.; Ppessegue, B.; Llopart, S.; Nair, A.;
Bauer, A.; Scheiper, B.; poeverlein, c.; Ganzhorn, A.; Lagrange, S.; Bacque,
E.
Deposited on : 2015-02-02
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

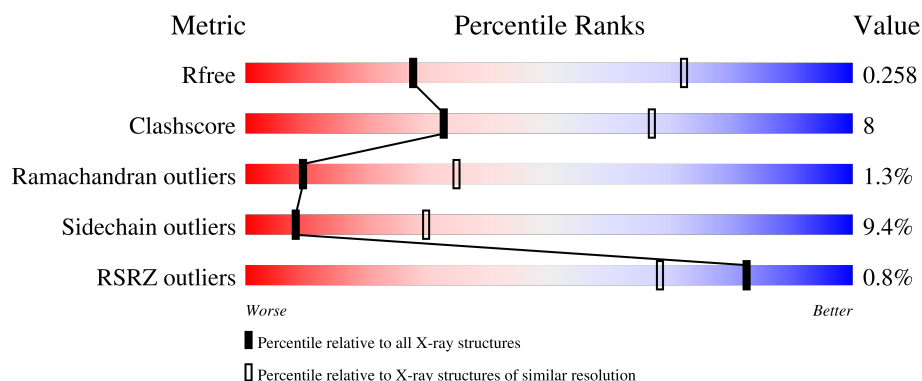
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

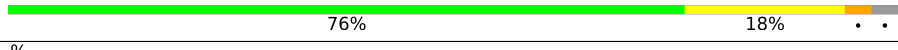
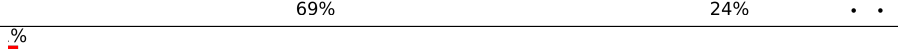
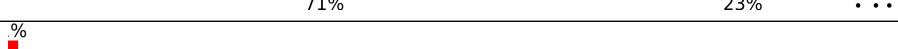
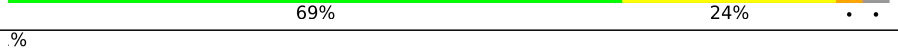
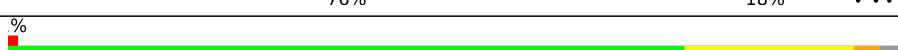
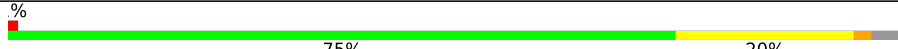
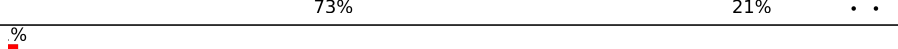
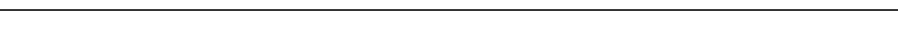
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Mol	Chain	Length	Quality of chain
1	A	478	% 76% 20% ..
1	B	478	% 66% 28% ..
1	C	478	% 71% 21% ..

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	D	478	%  74% 21% . .
1	E	478	 76% 18% . .
1	F	478	%  69% 24% . .
1	G	478	%  69% 26% . . .
1	H	478	%  71% 23% . .
1	I	478	%  75% 19% . .
1	J	478	%  76% 19% . .
1	K	478	%  76% 18% . .
1	L	478	%  71% 23% . . .
1	M	478	%  75% 19% . . .
1	N	478	%  72% 22% . .
1	O	478	%  71% 22% . .
1	P	478	%  74% 21% . .
1	Q	478	 69% 24% . .
1	R	478	%  76% 18% . . .
1	S	478	%  76% 19% . .
1	T	478	%  75% 20% . .
1	U	478	%  74% 19% . .
1	V	478	%  77% 18% . .
1	W	478	 73% 21% . .
1	X	478	%  74% 21% . .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 88848 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 Glutamine synthetase 1.

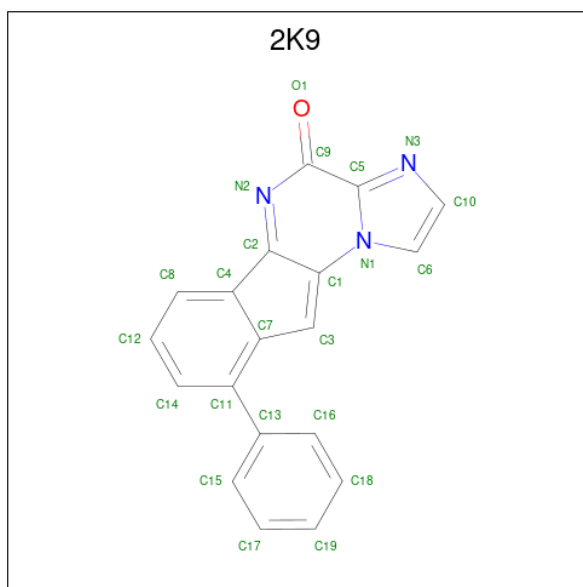
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	466	Total	C	N	O	S	0	0	0
			3693	2354	618	709	12			
1	B	464	Total	C	N	O	S	0	0	0
			3674	2342	613	707	12			
1	C	460	Total	C	N	O	S	0	0	0
			3645	2325	609	699	12			
1	D	466	Total	C	N	O	S	0	0	0
			3690	2352	616	710	12			
1	E	463	Total	C	N	O	S	0	0	0
			3670	2341	613	704	12			
1	F	467	Total	C	N	O	S	0	0	0
			3702	2359	619	712	12			
1	G	466	Total	C	N	O	S	0	0	0
			3693	2354	618	709	12			
1	H	464	Total	C	N	O	S	0	0	0
			3674	2342	613	707	12			
1	I	460	Total	C	N	O	S	0	0	0
			3645	2325	609	699	12			
1	J	466	Total	C	N	O	S	0	0	0
			3690	2352	616	710	12			
1	K	463	Total	C	N	O	S	0	0	0
			3670	2341	613	704	12			
1	L	467	Total	C	N	O	S	0	0	0
			3702	2359	619	712	12			
1	M	466	Total	C	N	O	S	0	0	0
			3693	2354	618	709	12			
1	N	464	Total	C	N	O	S	0	0	0
			3674	2342	613	707	12			
1	O	460	Total	C	N	O	S	0	0	0
			3645	2325	609	699	12			
1	P	466	Total	C	N	O	S	0	0	0
			3690	2352	616	710	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	463	Total	C	N	O	S	0	0	0
			3670	2341	613	704	12			
1	R	467	Total	C	N	O	S	0	0	0
			3702	2359	619	712	12			
1	S	466	Total	C	N	O	S	0	0	0
			3693	2354	618	709	12			
1	T	464	Total	C	N	O	S	0	0	0
			3674	2342	613	707	12			
1	U	460	Total	C	N	O	S	0	0	0
			3645	2325	609	699	12			
1	V	466	Total	C	N	O	S	0	0	0
			3690	2352	616	710	12			
1	W	463	Total	C	N	O	S	0	0	0
			3670	2341	613	704	12			
1	X	467	Total	C	N	O	S	0	0	0
			3702	2359	619	712	12			

- Molecule 2 is 9-phenyl-4H-imidazo[1,2-a]indeno[1,2-e]pyrazin-4-one (CCD ID: 2K9) (formula: C₁₉H₁₁N₃O).



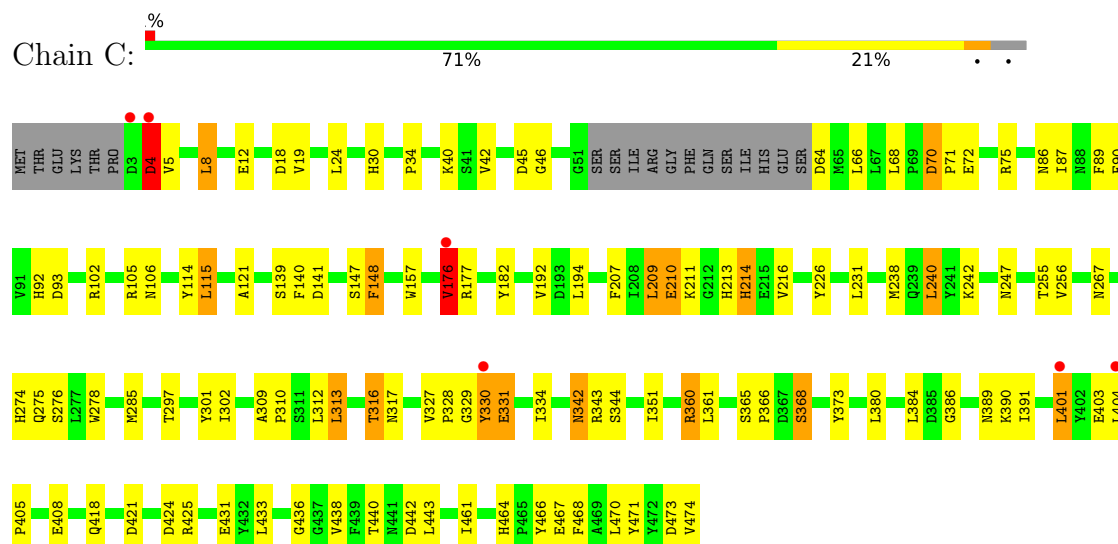
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			23	19	3	1		
2	B	1	Total	C	N	O	0	0
			23	19	3	1		
2	C	1	Total	C	N	O	0	0
			23	19	3	1		

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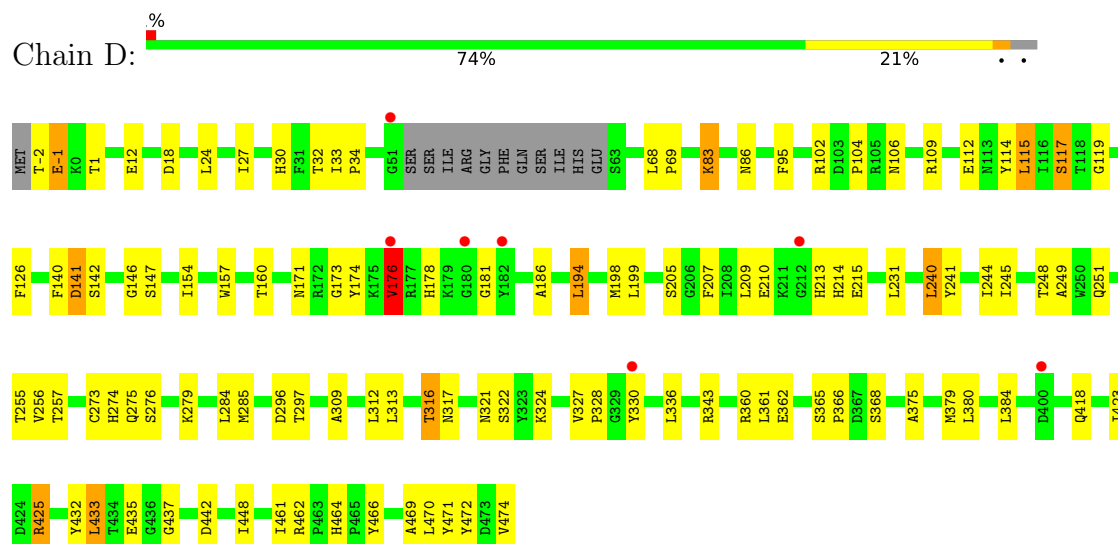
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total 23	C 19	N 3	O 1	0	0
2	E	1	Total 23	C 19	N 3	O 1	0	0
2	F	1	Total 23	C 19	N 3	O 1	0	0
2	G	1	Total 23	C 19	N 3	O 1	0	0
2	H	1	Total 23	C 19	N 3	O 1	0	0
2	I	1	Total 23	C 19	N 3	O 1	0	0
2	J	1	Total 23	C 19	N 3	O 1	0	0
2	K	1	Total 23	C 19	N 3	O 1	0	0
2	L	1	Total 23	C 19	N 3	O 1	0	0
2	M	1	Total 23	C 19	N 3	O 1	0	0
2	N	1	Total 23	C 19	N 3	O 1	0	0
2	O	1	Total 23	C 19	N 3	O 1	0	0
2	P	1	Total 23	C 19	N 3	O 1	0	0
2	Q	1	Total 23	C 19	N 3	O 1	0	0
2	R	1	Total 23	C 19	N 3	O 1	0	0
2	S	1	Total 23	C 19	N 3	O 1	0	0
2	T	1	Total 23	C 19	N 3	O 1	0	0
2	U	1	Total 23	C 19	N 3	O 1	0	0
2	V	1	Total 23	C 19	N 3	O 1	0	0
2	W	1	Total 23	C 19	N 3	O 1	0	0
2	X	1	Total 23	C 19	N 3	O 1	0	0

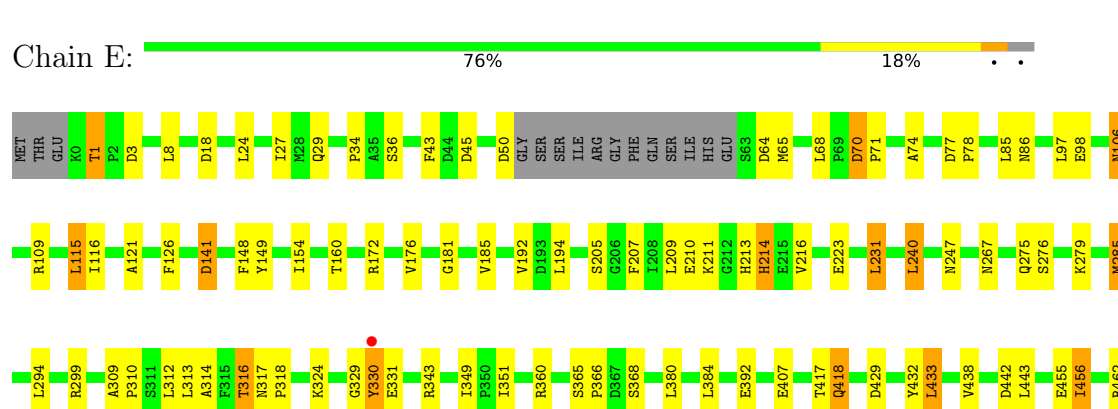
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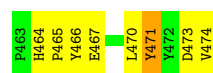


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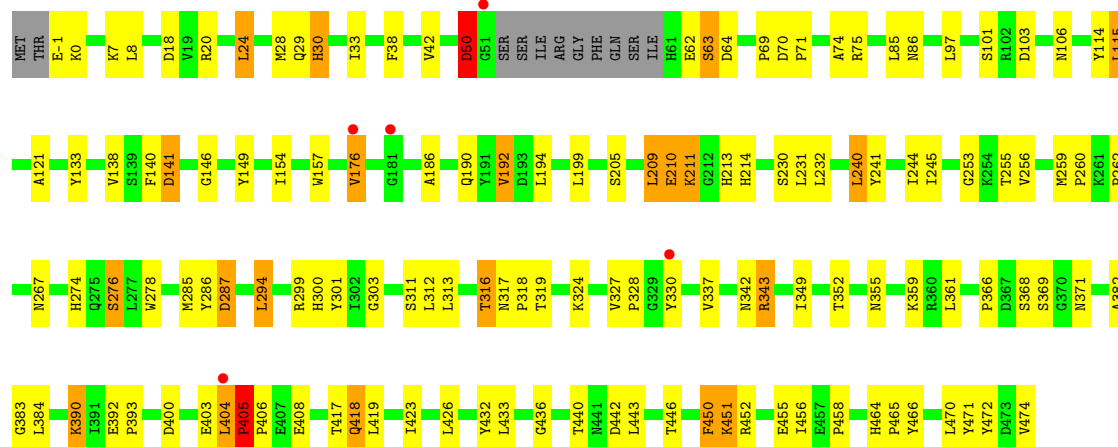


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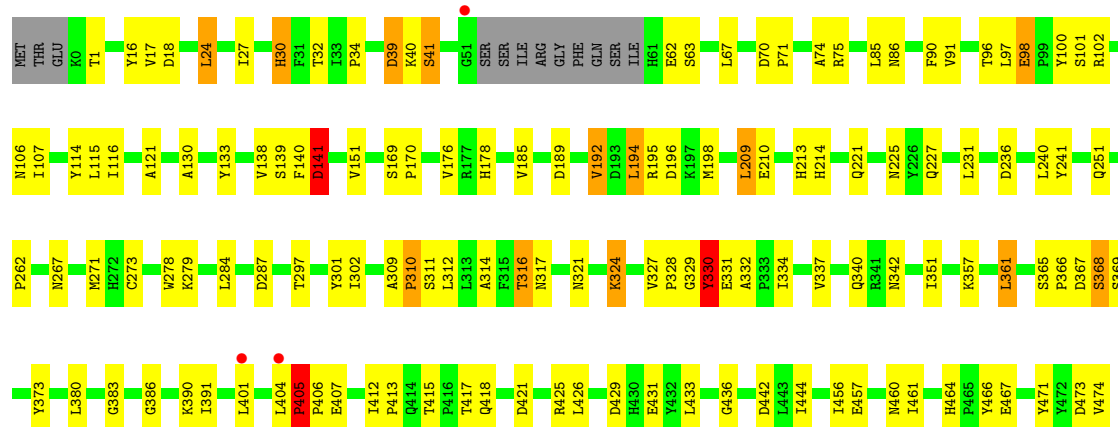




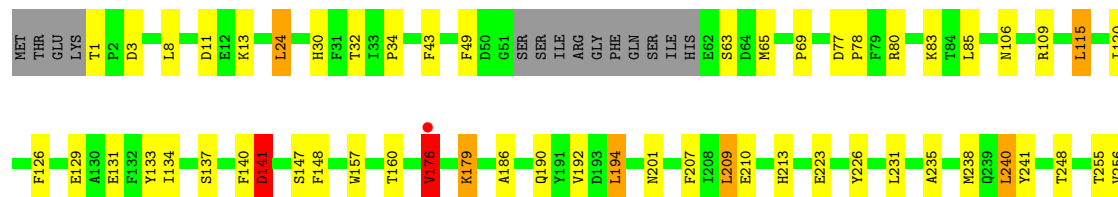
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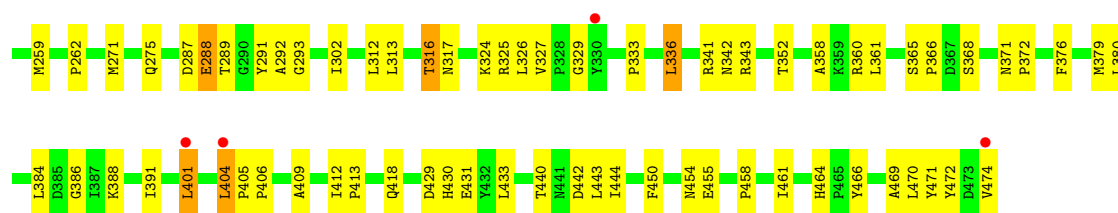


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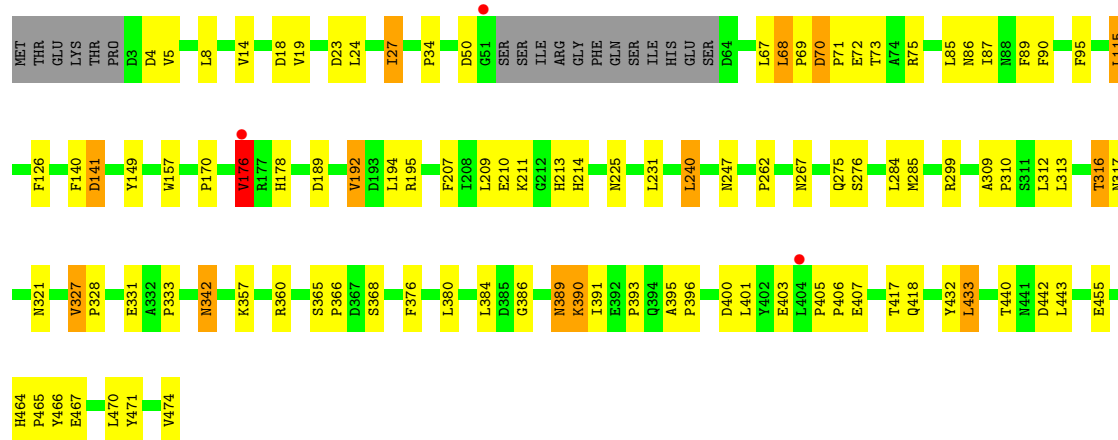
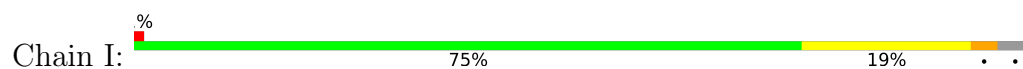


• Molecule 1: Glutamine synthetase 1

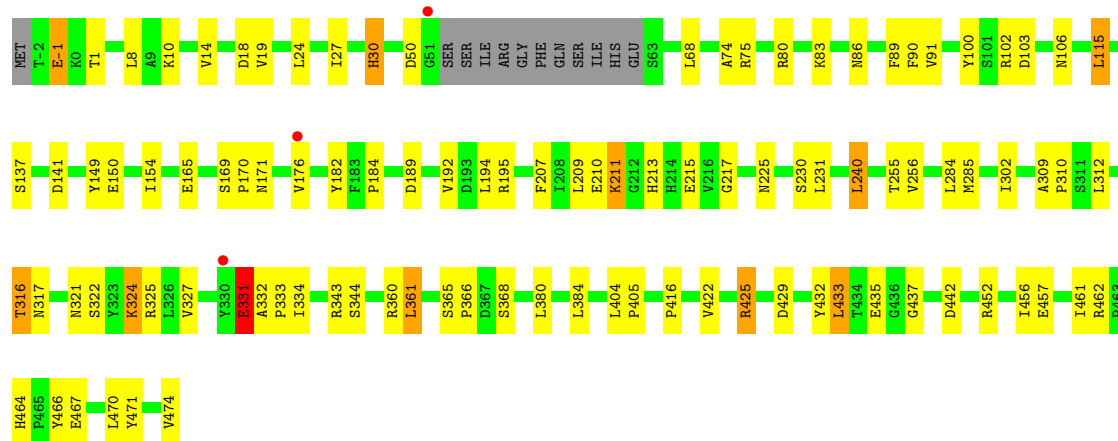
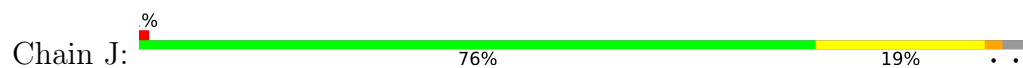




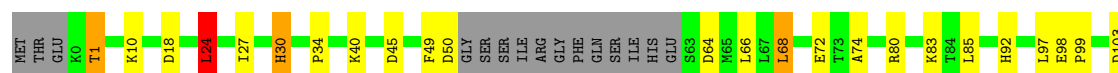
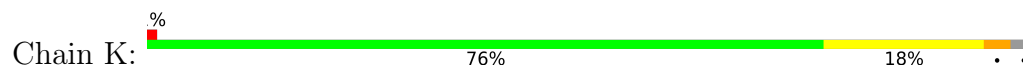
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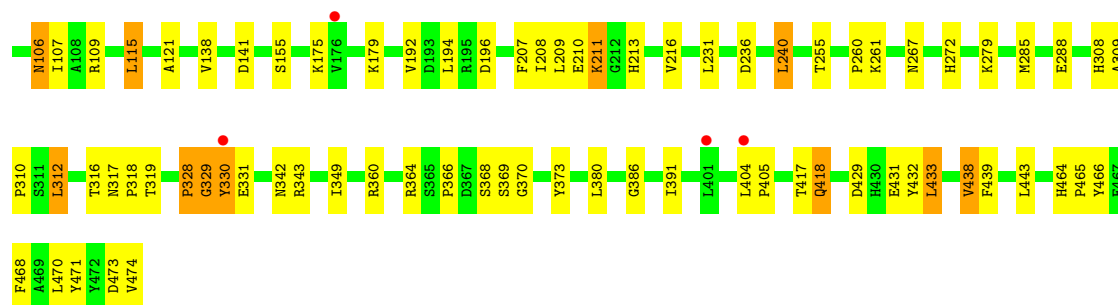


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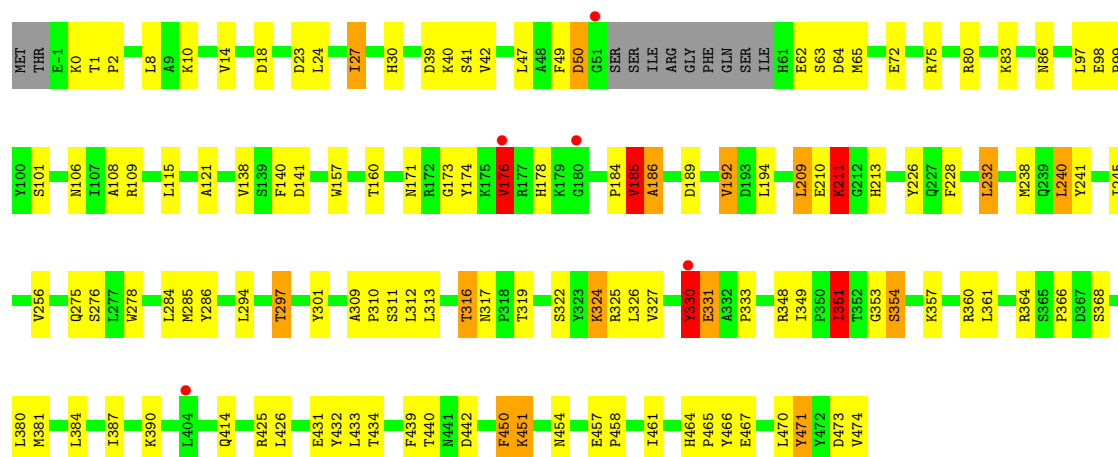


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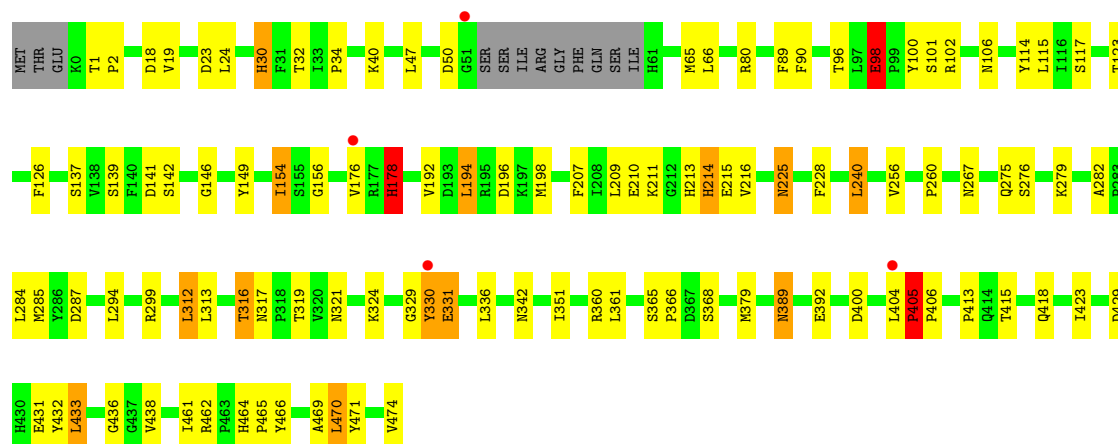
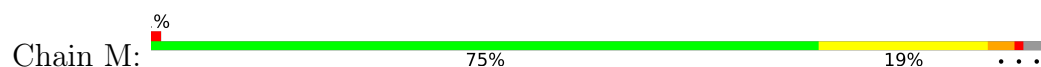




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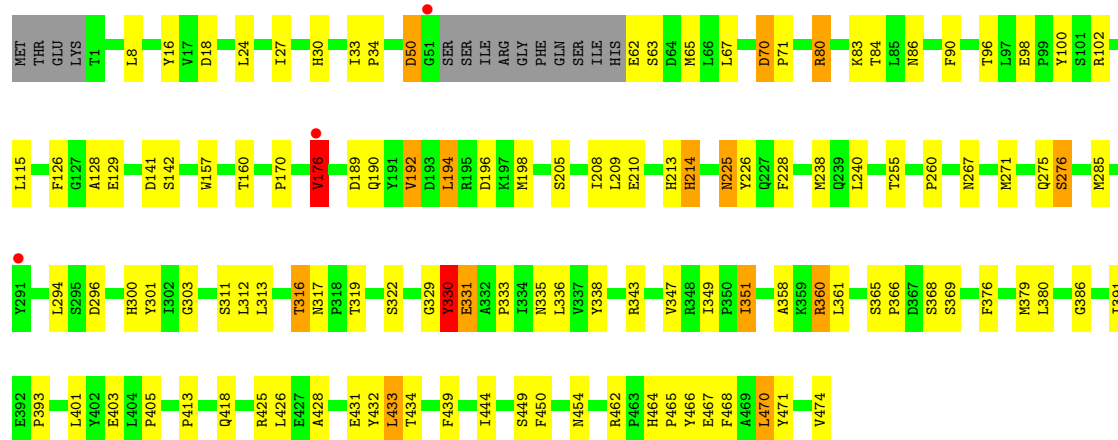


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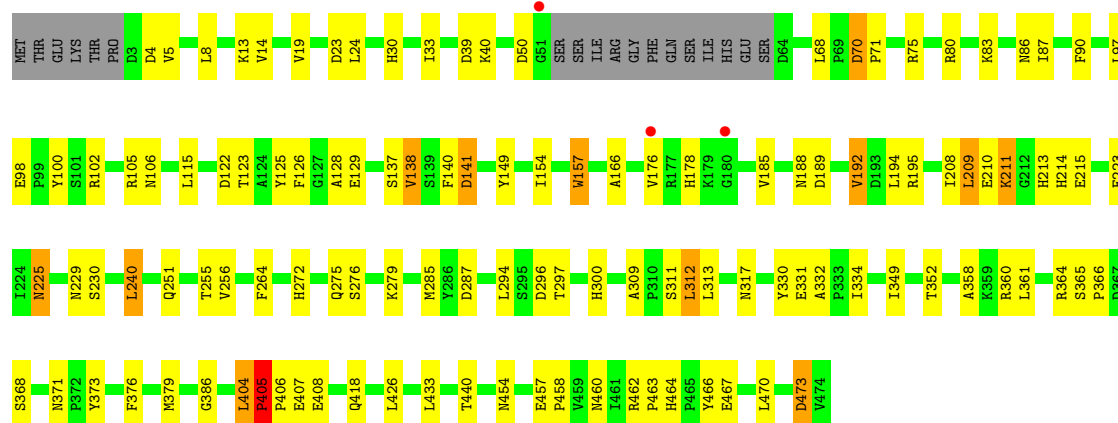


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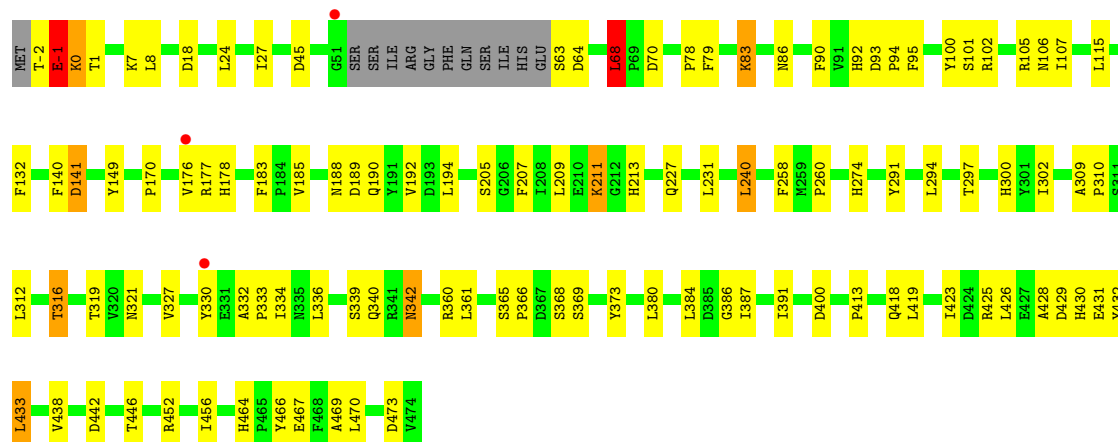
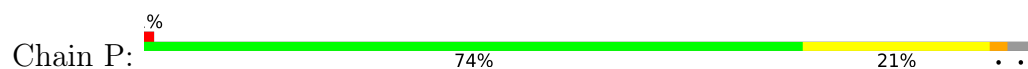




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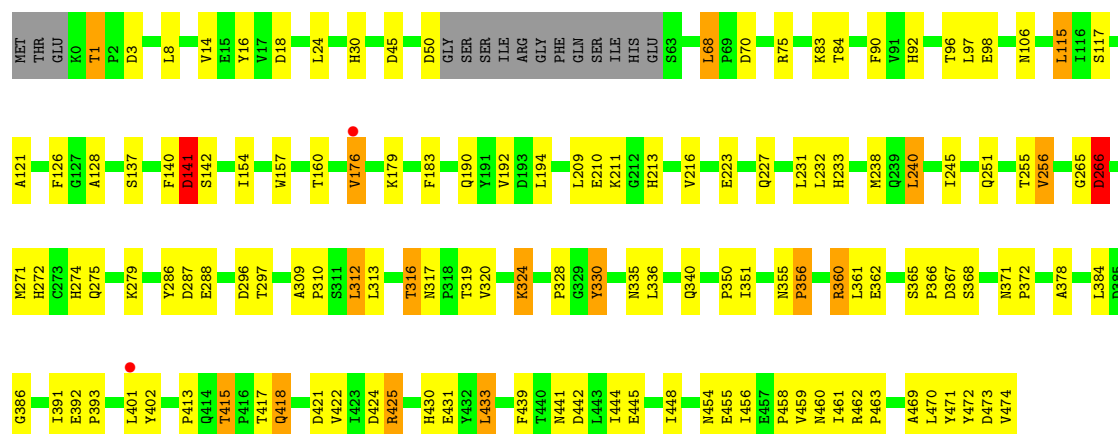


• Molecule 1: Glutamine synthetase 1



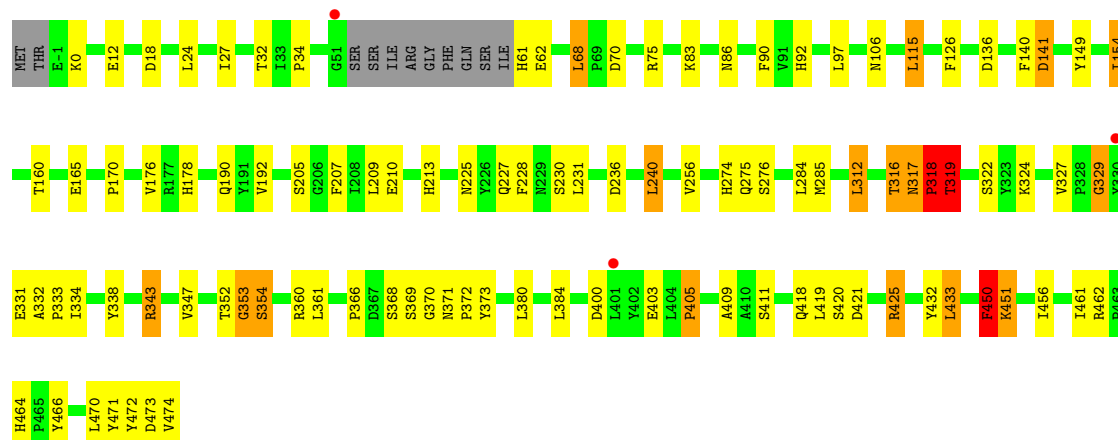
• Molecule 1: Glutamine synthetase 1

Chain Q:  69% 24% . .



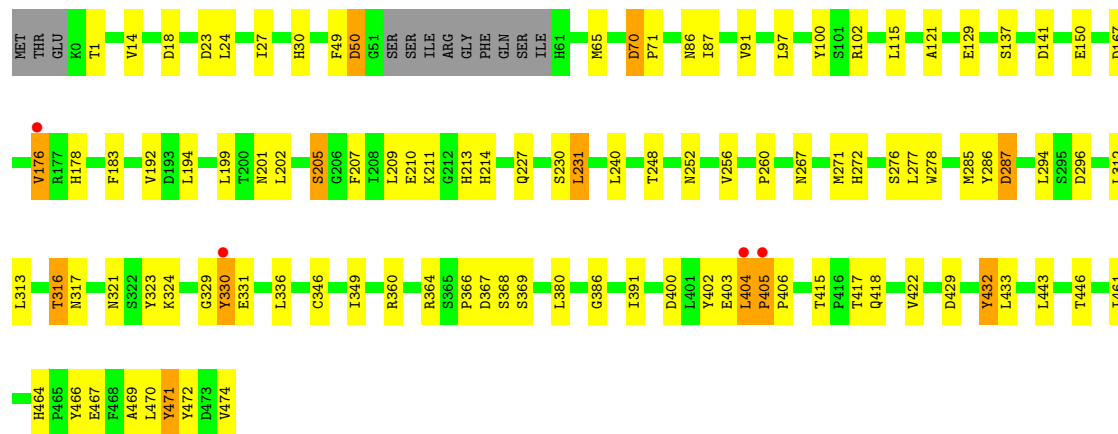
• Molecule 1: Glutamine synthetase 1

Chain R:  76% 18% . . .

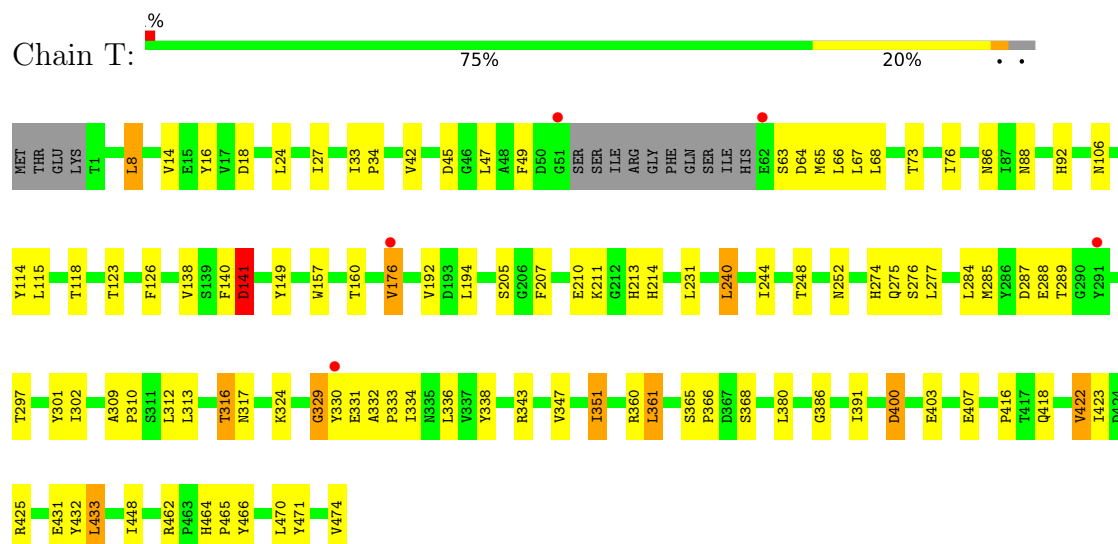


• Molecule 1: Glutamine synthetase 1

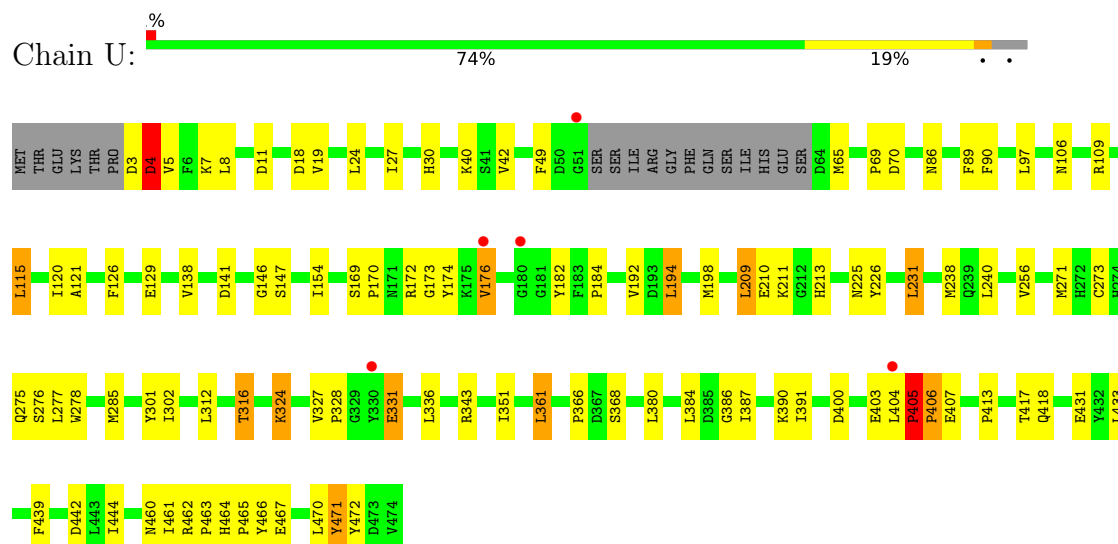
Chain S:  76% 19% . .



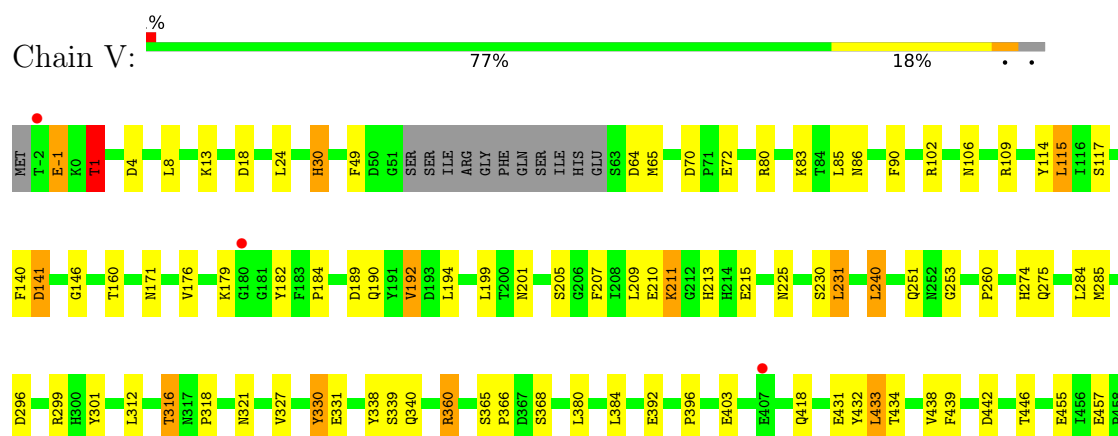
- Molecule 1: Glutamine synthetase 1



- Molecule 1: Glutamine synthetase 1



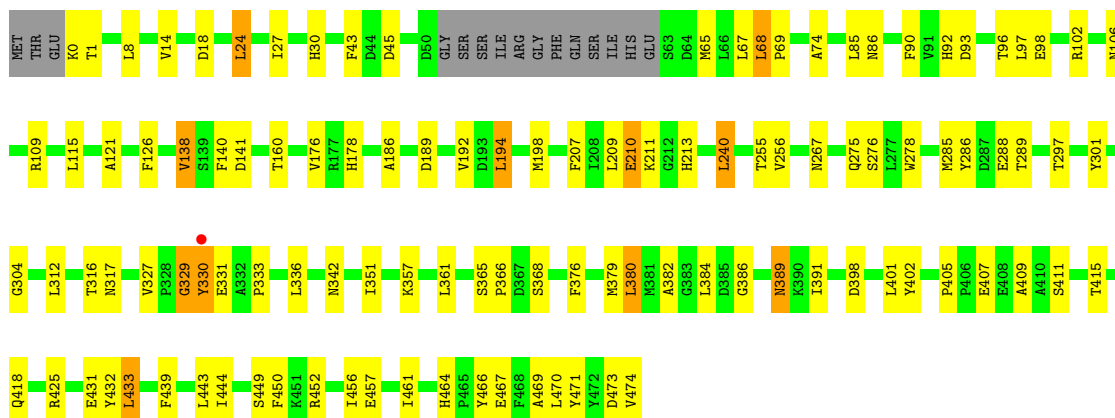
- Molecule 1: Glutamine synthetase 1





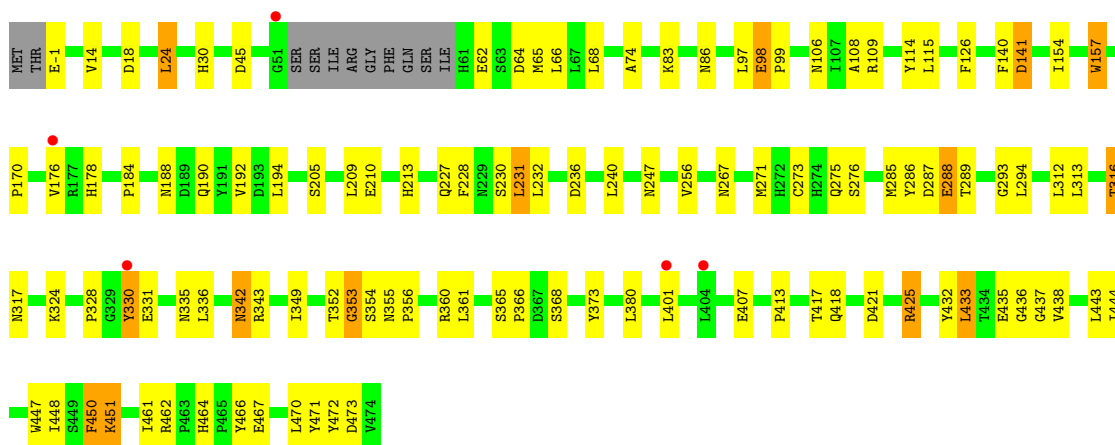
• Molecule 1: Glutamine synthetase 1

Chain W: 73% 21%



• Molecule 1: Glutamine synthetase 1

Chain X: 74% 21%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	260.11Å 273.50Å 207.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.30 50.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-3.30) 99.8 (50.00-3.30)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.200 , 0.265 0.197 , 0.258	Depositor DCC
R_{free} test set	11105 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	62.5	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 21.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	88848	wwPDB-VP
Average B, all atoms (Å ²)	57.0	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 34.86 % 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 6.3847e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 2K9

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	0.59	1/3797 (0.0%)	0.88	2/5161 (0.0%)
1	B	0.68	0/3777	0.95	6/5135 (0.1%)
1	C	0.62	1/3747 (0.0%)	0.94	6/5093 (0.1%)
1	D	0.60	1/3793 (0.0%)	0.89	1/5156 (0.0%)
1	E	0.60	0/3773	0.90	4/5129 (0.1%)
1	F	0.64	1/3806 (0.0%)	0.96	17/5173 (0.3%)
1	G	0.61	1/3797 (0.0%)	0.94	8/5161 (0.2%)
1	H	0.63	1/3777 (0.0%)	0.94	4/5135 (0.1%)
1	I	0.61	1/3747 (0.0%)	0.93	8/5093 (0.2%)
1	J	0.59	0/3793	0.90	4/5156 (0.1%)
1	K	0.59	0/3773	0.92	8/5129 (0.2%)
1	L	0.61	0/3806	0.93	7/5173 (0.1%)
1	M	0.63	0/3797	0.94	13/5161 (0.3%)
1	N	0.62	1/3777 (0.0%)	0.91	6/5135 (0.1%)
1	O	0.62	1/3747 (0.0%)	0.96	10/5093 (0.2%)
1	P	0.61	0/3793	0.92	2/5156 (0.0%)
1	Q	0.66	1/3773 (0.0%)	0.96	2/5129 (0.0%)
1	R	0.59	0/3806	0.99	12/5173 (0.2%)
1	S	0.60	1/3797 (0.0%)	0.93	9/5161 (0.2%)
1	T	0.61	0/3777	0.89	4/5135 (0.1%)
1	U	0.61	1/3747 (0.0%)	0.90	6/5093 (0.1%)
1	V	0.60	0/3793	0.91	4/5156 (0.1%)
1	W	0.60	1/3773 (0.0%)	0.90	2/5129 (0.0%)
1	X	0.57	0/3806	0.90	4/5173 (0.1%)
All	All	0.61	13/90772 (0.0%)	0.92	149/123388 (0.1%)

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	L	0	1
1	R	0	1
All	All	0	2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	176	VAL	CA-CB	7.37	1.61	1.54
1	G	62	GLU	CA-C	6.99	1.56	1.52
1	A	176	VAL	CA-CB	6.82	1.61	1.54
1	C	176	VAL	CA-CB	6.35	1.60	1.54
1	S	176	VAL	CA-CB	6.24	1.60	1.54
1	D	176	VAL	CA-CB	6.12	1.61	1.54
1	H	176	VAL	CA-CB	6.09	1.60	1.54
1	W	176	VAL	CA-CB	5.94	1.61	1.54
1	Q	176	VAL	CA-CB	5.74	1.60	1.54
1	U	176	VAL	CA-CB	5.56	1.59	1.54
1	F	176	VAL	CA-CB	5.29	1.59	1.54
1	I	176	VAL	CA-CB	5.15	1.61	1.54
1	O	154	ILE	CA-CB	5.10	1.60	1.54

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	318	PRO	CA-C-N	9.81	139.35	121.70
1	R	318	PRO	C-N-CA	9.81	139.35	121.70
1	R	317	ASN	CA-C-N	9.39	131.58	119.84
1	R	317	ASN	C-N-CA	9.39	131.58	119.84
1	R	318	PRO	N-CA-C	9.28	131.58	112.47
1	M	404	LEU	CA-C-N	8.97	129.62	120.38
1	M	404	LEU	C-N-CA	8.97	129.62	120.38
1	O	404	LEU	CA-C-N	8.63	129.27	120.38
1	O	404	LEU	C-N-CA	8.63	129.27	120.38
1	X	450	PHE	CA-C-N	7.66	135.49	121.70
1	X	450	PHE	C-N-CA	7.66	135.49	121.70
1	F	259	MET	CA-C-N	7.63	128.02	119.32
1	F	259	MET	C-N-CA	7.63	128.02	119.32
1	L	450	PHE	CA-C-N	7.54	135.28	121.70
1	L	450	PHE	C-N-CA	7.54	135.28	121.70
1	O	405	PRO	N-CA-C	7.33	119.65	110.70
1	R	450	PHE	CA-C-N	7.29	134.83	121.70
1	R	450	PHE	C-N-CA	7.29	134.83	121.70
1	L	324	LYS	N-CA-C	-7.08	104.28	114.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	450	PHE	CA-C-N	7.00	134.31	121.70
1	F	450	PHE	C-N-CA	7.00	134.31	121.70
1	G	404	LEU	CA-C-N	6.83	127.41	120.38
1	G	404	LEU	C-N-CA	6.83	127.41	120.38
1	I	70	ASP	CA-C-N	6.68	127.22	119.47
1	I	70	ASP	C-N-CA	6.68	127.22	119.47
1	H	259	MET	CA-C-N	6.57	126.51	119.28
1	H	259	MET	C-N-CA	6.57	126.51	119.28
1	F	214	HIS	N-CA-C	6.49	118.94	109.07
1	H	324	LYS	N-CA-C	-6.46	105.70	113.97
1	J	50	ASP	N-CA-C	6.40	119.04	108.99
1	G	407	GLU	N-CA-C	-6.33	107.40	114.62
1	V	1	THR	CA-C-N	6.29	127.70	119.84
1	V	1	THR	C-N-CA	6.29	127.70	119.84
1	I	68	LEU	CA-C-N	6.23	126.19	119.78
1	I	68	LEU	C-N-CA	6.23	126.19	119.78
1	K	261	LYS	CA-C-N	6.20	125.61	118.85
1	K	261	LYS	C-N-CA	6.20	125.61	118.85
1	K	30	HIS	N-CA-C	6.20	118.50	109.07
1	O	70	ASP	CA-C-N	6.20	127.59	119.84
1	O	70	ASP	C-N-CA	6.20	127.59	119.84
1	L	471	TYR	N-CA-C	6.18	122.28	114.31
1	G	169	SER	CA-C-N	6.16	127.55	119.84
1	G	169	SER	C-N-CA	6.16	127.55	119.84
1	F	324	LYS	N-CA-C	-6.16	105.56	114.12
1	O	68	LEU	CA-C-N	6.11	126.08	119.78
1	O	68	LEU	C-N-CA	6.11	126.08	119.78
1	K	24	LEU	CA-C-N	-6.10	113.68	120.45
1	K	24	LEU	C-N-CA	-6.10	113.68	120.45
1	S	70	ASP	CA-C-N	6.01	126.44	119.47
1	S	70	ASP	C-N-CA	6.01	126.44	119.47
1	F	50	ASP	N-CA-C	5.98	118.19	108.26
1	I	5	VAL	N-CA-C	5.98	116.04	110.42
1	M	324	LYS	N-CA-C	-5.95	106.02	113.28
1	C	70	ASP	CA-C-N	5.95	126.37	119.47
1	C	70	ASP	C-N-CA	5.95	126.37	119.47
1	G	324	LYS	N-CA-C	-5.95	106.06	113.38
1	M	342	ASN	N-CA-C	5.93	118.85	109.96
1	E	214	HIS	N-CA-C	5.90	117.75	108.96
1	B	259	MET	CA-C-N	5.90	125.60	119.05
1	B	259	MET	C-N-CA	5.90	125.60	119.05
1	S	471	TYR	N-CA-C	5.89	121.34	114.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	178	HIS	N-CA-C	5.88	119.30	109.95
1	F	371	ASN	CA-C-N	5.86	126.27	119.47
1	F	371	ASN	C-N-CA	5.86	126.27	119.47
1	K	342	ASN	N-CA-C	5.86	119.09	110.30
1	C	4	ASP	CA-C-N	5.85	128.01	120.70
1	C	4	ASP	C-N-CA	5.85	128.01	120.70
1	F	342	ASN	N-CA-C	5.83	117.70	108.67
1	U	405	PRO	CA-C-N	5.83	127.12	119.84
1	U	405	PRO	C-N-CA	5.83	127.12	119.84
1	B	214	HIS	N-CA-C	5.79	117.59	108.96
1	V	327	VAL	CA-C-N	5.78	127.07	119.84
1	V	327	VAL	C-N-CA	5.78	127.07	119.84
1	Q	141	ASP	N-CA-C	5.78	117.26	108.07
1	F	405	PRO	CA-C-N	5.77	125.44	119.56
1	F	405	PRO	C-N-CA	5.77	125.44	119.56
1	O	371	ASN	CA-C-N	5.74	126.13	119.47
1	O	371	ASN	C-N-CA	5.74	126.13	119.47
1	M	405	PRO	CA-C-N	5.72	127.00	119.84
1	M	405	PRO	C-N-CA	5.72	127.00	119.84
1	T	64	ASP	N-CA-C	5.64	117.88	109.59
1	T	214	HIS	N-CA-C	5.63	117.62	109.07
1	S	50	ASP	N-CA-C	5.62	117.89	108.73
1	B	438	VAL	N-CA-C	-5.62	105.63	110.74
1	T	324	LYS	N-CA-C	-5.57	106.47	113.72
1	P	68	LEU	CA-C-N	5.57	125.33	119.76
1	P	68	LEU	C-N-CA	5.57	125.33	119.76
1	N	405	PRO	CA-C-N	5.57	125.93	119.47
1	N	405	PRO	C-N-CA	5.57	125.93	119.47
1	I	214	HIS	N-CA-C	5.57	117.65	109.24
1	F	30	HIS	N-CA-C	5.55	117.83	109.23
1	I	178	HIS	N-CA-C	5.55	117.84	109.41
1	M	405	PRO	N-CA-C	5.54	117.46	110.70
1	G	405	PRO	N-CA-C	5.53	117.45	110.70
1	J	324	LYS	N-CA-C	-5.53	106.43	114.12
1	F	319	THR	N-CA-C	5.50	117.64	110.43
1	A	324	LYS	N-CA-C	-5.47	106.65	113.38
1	M	98	GLU	CA-C-N	5.45	125.46	119.90
1	M	98	GLU	C-N-CA	5.45	125.46	119.90
1	G	141	ASP	N-CA-C	5.44	116.41	108.14
1	R	0	LYS	N-CA-C	5.44	118.31	109.06
1	R	70	ASP	CA-C-N	5.38	125.02	119.05
1	R	70	ASP	C-N-CA	5.38	125.02	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	183	PHE	CA-C-N	-5.38	115.20	120.52
1	S	183	PHE	C-N-CA	-5.38	115.20	120.52
1	D	214	HIS	N-CA-C	5.34	116.96	108.79
1	M	214	HIS	N-CA-C	5.33	117.09	109.14
1	N	214	HIS	N-CA-C	5.33	117.19	108.76
1	R	319	THR	N-CA-CB	5.32	120.54	111.50
1	C	214	HIS	N-CA-C	5.30	116.89	108.79
1	T	400	ASP	N-CA-C	5.29	118.14	110.42
1	L	185	VAL	CA-C-N	5.28	131.21	121.70
1	L	185	VAL	C-N-CA	5.28	131.21	121.70
1	K	349	ILE	CA-C-N	5.28	125.53	119.83
1	K	349	ILE	C-N-CA	5.28	125.53	119.83
1	N	63	SER	N-CA-C	5.27	117.47	108.67
1	B	50	ASP	N-CA-C	5.25	117.24	108.99
1	X	342	ASN	N-CA-C	5.21	117.87	110.10
1	M	282	ALA	CA-C-N	5.21	125.15	119.78
1	M	282	ALA	C-N-CA	5.21	125.15	119.78
1	S	324	LYS	N-CA-C	-5.19	106.99	113.38
1	U	324	LYS	N-CA-C	-5.18	106.80	113.23
1	W	1	THR	CA-C-N	5.17	125.47	119.47
1	W	1	THR	C-N-CA	5.17	125.47	119.47
1	I	342	ASN	N-CA-C	5.17	117.96	110.42
1	Q	324	LYS	N-CA-C	-5.16	107.03	113.38
1	J	-1	GLU	N-CA-C	5.14	121.76	110.80
1	X	450	PHE	N-CA-C	5.14	121.75	110.80
1	L	176	VAL	N-CA-C	5.13	116.03	109.30
1	F	192	VAL	N-CA-C	5.13	115.36	110.53
1	R	405	PRO	N-CA-C	5.13	116.96	110.70
1	U	471	TYR	N-CA-C	5.13	121.83	114.39
1	B	470	LEU	N-CA-C	5.13	116.55	111.07
1	A	214	HIS	N-CA-C	5.12	116.63	108.79
1	U	4	ASP	CA-C-N	5.12	127.12	120.56
1	U	4	ASP	C-N-CA	5.12	127.12	120.56
1	O	214	HIS	N-CA-C	5.08	116.54	108.96
1	E	70	ASP	CA-C-N	5.08	125.36	119.47
1	E	70	ASP	C-N-CA	5.08	125.36	119.47
1	E	471	TYR	N-CA-C	5.07	120.84	114.31
1	J	325	ARG	N-CA-C	-5.06	105.95	112.68
1	S	404	LEU	CA-C-N	5.06	125.59	120.38
1	S	404	LEU	C-N-CA	5.06	125.59	120.38
1	H	30	HIS	N-CA-C	5.04	116.72	108.76
1	F	404	LEU	CA-C-N	5.03	125.56	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	404	LEU	C-N-CA	5.03	125.56	120.38
1	N	70	ASP	CA-C-N	5.02	125.05	119.32
1	N	70	ASP	C-N-CA	5.02	125.05	119.32
1	C	5	VAL	N-CA-C	5.02	115.17	110.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	185	VAL	Peptide
1	R	318	PRO	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3693	0	3523	56	0
1	B	3674	0	3503	86	0
1	C	3645	0	3475	65	0
1	D	3690	0	3523	64	0
1	E	3670	0	3507	61	0
1	F	3702	0	3529	82	0
1	G	3693	0	3523	78	0
1	H	3674	0	3503	66	0
1	I	3645	0	3475	58	0
1	J	3690	0	3523	53	0
1	K	3670	0	3507	47	0
1	L	3702	0	3529	70	0
1	M	3693	0	3523	64	0
1	N	3674	0	3503	68	0
1	O	3645	0	3475	62	0
1	P	3690	0	3523	55	0
1	Q	3670	0	3507	71	0
1	R	3702	0	3529	65	0
1	S	3693	0	3523	52	0
1	T	3674	0	3503	61	0
1	U	3645	0	3475	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	V	3690	0	3523	54	0
1	W	3670	0	3507	60	0
1	X	3702	0	3529	62	0
2	A	23	0	11	0	0
2	B	23	0	11	1	0
2	C	23	0	11	0	0
2	D	23	0	11	0	0
2	E	23	0	11	0	0
2	F	23	0	11	2	0
2	G	23	0	11	0	0
2	H	23	0	11	0	0
2	I	23	0	11	0	0
2	J	23	0	11	0	0
2	K	23	0	11	0	0
2	L	23	0	11	0	0
2	M	23	0	11	2	0
2	N	23	0	11	1	0
2	O	23	0	11	0	0
2	P	23	0	11	1	0
2	Q	23	0	11	0	0
2	R	23	0	11	1	0
2	S	23	0	11	0	0
2	T	23	0	11	0	0
2	U	23	0	11	0	0
2	V	23	0	11	0	0
2	W	23	0	11	0	0
2	X	23	0	11	0	0
All	All	88848	0	84504	1370	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (1370) 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:H:313:LEU:HG	1:H:317:ASN:HD22	1.29	0.98
1:P:68:LEU:HD23	1:P:92:HIS:CD2	1.99	0.96
1:R:318:PRO:HG2	1:R:370:GLY:HA2	1.48	0.96
1:J:464:HIS:HD2	1:J:466:TYR:H	1.14	0.95
1:I:210:GLU:H	1:I:213:HIS:HD2	1.12	0.95
1:U:464:HIS:HD2	1:U:466:TYR:H	1.13	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:464:HIS:HD2	1:K:466:TYR:H	1.12	0.95
1:F:450:PHE:HB3	1:F:451:LYS:HB2	1.46	0.94
1:K:210:GLU:H	1:K:213:HIS:HD2	1.00	0.93
1:E:343:ARG:HH12	1:F:63:SER:HA	1.33	0.93
1:R:464:HIS:HD2	1:R:466:TYR:H	1.17	0.92
1:K:210:GLU:H	1:K:213:HIS:CD2	1.88	0.90
1:T:464:HIS:HD2	1:T:466:TYR:H	1.20	0.90
1:R:450:PHE:HB3	1:R:451:LYS:HB2	1.51	0.90
1:R:209:LEU:HD13	1:R:213:HIS:HB3	1.54	0.88
1:S:464:HIS:HD2	1:S:466:TYR:H	1.19	0.87
1:I:313:LEU:HG	1:I:317:ASN:HD22	1.38	0.87
1:S:18:ASP:HB3	1:S:86:ASN:HD22	1.38	0.86
1:O:313:LEU:HG	1:O:317:ASN:HD22	1.38	0.86
1:I:210:GLU:H	1:I:213:HIS:CD2	1.95	0.85
1:G:178:HIS:HE1	1:W:473:ASP:HB2	1.41	0.85
1:A:50:ASP:HB2	1:F:343:ARG:HH22	1.41	0.84
1:F:418:GLN:HE21	1:F:418:GLN:HA	1.40	0.84
1:H:464:HIS:HD2	1:H:466:TYR:H	1.25	0.83
1:W:276:SER:HA	1:W:285:MET:HE2	1.61	0.82
1:M:210:GLU:H	1:M:213:HIS:HD2	1.28	0.82
1:Q:386:GLY:HA2	1:Q:391:ILE:HD12	1.61	0.81
1:M:50:ASP:HB2	1:R:343:ARG:HH12	1.46	0.81
1:S:317:ASN:OD1	1:S:366:PRO:HA	1.79	0.81
1:X:450:PHE:HB3	1:X:451:LYS:HB2	1.60	0.81
1:G:213:HIS:HA	1:G:225:ASN:HD21	1.46	0.80
1:A:464:HIS:HD2	1:A:466:TYR:H	1.27	0.80
1:Q:209:LEU:HD13	1:Q:213:HIS:HB3	1.64	0.79
1:D:471:TYR:O	1:D:474:VAL:HG22	1.80	0.79
1:G:317:ASN:OD1	1:G:366:PRO:HA	1.82	0.79
1:B:425:ARG:HB3	1:B:425:ARG:HH21	1.45	0.79
1:F:121:ALA:HB1	1:F:278:TRP:O	1.81	0.79
1:Q:336:LEU:HD21	1:Q:415:THR:HG23	1.66	0.78
1:I:464:HIS:HD2	1:I:466:TYR:H	1.29	0.78
1:V:464:HIS:HD2	1:V:466:TYR:H	1.30	0.78
1:L:185:VAL:HB	1:L:186:ALA:HB3	1.66	0.78
1:J:18:ASP:HB3	1:J:86:ASN:HD22	1.50	0.77
1:M:464:HIS:HD2	1:M:466:TYR:H	1.33	0.76
1:Q:90:PHE:HD2	1:Q:106:ASN:ND2	1.84	0.76
1:A:317:ASN:OD1	1:A:366:PRO:HA	1.86	0.76
1:S:209:LEU:HD13	1:S:213:HIS:HB3	1.68	0.76
1:J:471:TYR:O	1:J:474:VAL:HG22	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:328:PRO:HD3	1:Q:417:THR:HG21	1.65	0.75
1:E:317:ASN:OD1	1:E:366:PRO:HA	1.86	0.75
1:E:464:HIS:HD2	1:E:466:TYR:H	1.35	0.75
1:L:209:LEU:HD13	1:L:213:HIS:HB3	1.69	0.75
1:L:473:ASP:HB2	1:X:178:HIS:HE1	1.50	0.74
1:B:467:GLU:OE1	1:Q:324:LYS:HE3	1.87	0.74
1:M:210:GLU:H	1:M:213:HIS:CD2	2.06	0.74
1:N:343:ARG:HH11	1:O:50:ASP:HB2	1.53	0.74
1:N:157:TRP:HB3	1:N:176:VAL:HA	1.70	0.74
1:B:313:LEU:HG	1:B:317:ASN:HD22	1.52	0.74
1:P:386:GLY:HA2	1:P:391:ILE:HD12	1.70	0.74
1:A:18:ASP:HB3	1:A:86:ASN:HD22	1.53	0.73
1:I:18:ASP:HB3	1:I:86:ASN:HD22	1.53	0.73
1:L:186:ALA:H	1:L:189:ASP:H	1.35	0.73
1:M:209:LEU:HD13	1:M:213:HIS:HB3	1.68	0.73
1:S:464:HIS:CD2	1:S:466:TYR:H	2.05	0.73
1:U:18:ASP:HB3	1:U:86:ASN:HD22	1.53	0.73
1:O:464:HIS:HD2	1:O:466:TYR:H	1.36	0.72
1:O:75:ARG:HG3	1:O:240:LEU:HD11	1.72	0.72
1:R:464:HIS:CD2	1:R:466:TYR:H	2.04	0.72
1:F:455:GLU:O	1:F:458:PRO:HD2	1.90	0.72
1:W:18:ASP:HB3	1:W:86:ASN:HD22	1.54	0.72
1:H:313:LEU:HG	1:H:317:ASN:ND2	2.04	0.71
1:F:450:PHE:CB	1:F:451:LYS:HB2	2.21	0.71
1:S:18:ASP:OD2	1:S:30:HIS:HD2	1.74	0.71
1:E:343:ARG:HH22	1:F:63:SER:HB2	1.56	0.71
1:B:317:ASN:OD1	1:B:366:PRO:HA	1.90	0.71
1:H:341:ARG:HH11	1:I:95:PHE:HE1	1.39	0.71
1:X:316:THR:HG23	1:X:366:PRO:HA	1.73	0.71
1:W:464:HIS:HD2	1:W:466:TYR:H	1.37	0.71
1:C:210:GLU:H	1:C:213:HIS:HD2	1.38	0.71
1:D:115:LEU:HD23	1:D:384:LEU:HD11	1.71	0.71
1:L:330:TYR:O	1:L:331:GLU:HB2	1.91	0.71
1:E:210:GLU:H	1:E:213:HIS:CD2	2.09	0.70
1:C:18:ASP:HB3	1:C:86:ASN:HD22	1.55	0.70
1:N:464:HIS:HD2	1:N:466:TYR:H	1.37	0.70
1:S:18:ASP:HB3	1:S:86:ASN:ND2	2.06	0.70
1:A:471:TYR:O	1:A:474:VAL:HG22	1.90	0.70
1:E:210:GLU:H	1:E:213:HIS:HD2	1.37	0.70
1:M:213:HIS:HA	1:M:225:ASN:HD21	1.57	0.70
1:E:126:PHE:CE2	1:E:275:GLN:HG2	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:39:ASP:OD1	1:L:41:SER:HB3	1.91	0.70
1:S:464:HIS:HD2	1:S:466:TYR:N	1.90	0.69
1:X:464:HIS:HD2	1:X:466:TYR:H	1.37	0.69
1:T:274:HIS:HB3	1:T:360:ARG:HD2	1.73	0.69
1:C:207:PHE:HE1	1:C:240:LEU:HD13	1.57	0.69
1:F:464:HIS:HD2	1:F:466:TYR:H	1.39	0.68
1:G:271:MET:HE3	1:G:273:CYS:SG	2.34	0.68
1:K:272:HIS:HD2	1:K:364:ARG:HG2	1.58	0.68
1:X:432:TYR:CE1	1:X:433:LEU:HD13	2.29	0.68
1:G:39:ASP:OD1	1:G:41:SER:HB3	1.94	0.67
1:S:214:HIS:HB3	1:T:33:ILE:HG22	1.75	0.67
1:E:464:HIS:HB3	1:E:467:GLU:HG3	1.77	0.67
1:L:464:HIS:HD2	1:L:466:TYR:H	1.41	0.67
1:Q:90:PHE:CD2	1:Q:106:ASN:ND2	2.61	0.67
1:O:210:GLU:H	1:O:213:HIS:CD2	2.13	0.67
1:H:201:ASN:ND2	1:H:248:THR:OG1	2.27	0.67
1:I:400:ASP:HB3	1:I:403:GLU:HG3	1.74	0.67
1:O:209:LEU:HD13	1:O:213:HIS:HB3	1.77	0.67
1:S:49:PHE:HD1	1:S:65:MET:HE3	1.60	0.67
1:K:317:ASN:OD1	1:K:366:PRO:HA	1.94	0.67
1:S:313:LEU:HA	1:S:316:THR:HB	1.76	0.67
1:O:210:GLU:H	1:O:213:HIS:HD2	1.41	0.67
1:G:464:HIS:HD2	1:G:466:TYR:H	1.43	0.66
1:R:126:PHE:CE2	1:R:275:GLN:HG2	2.31	0.66
1:T:432:TYR:CE1	1:T:433:LEU:HD13	2.30	0.66
1:T:313:LEU:HG	1:T:317:ASN:HD22	1.59	0.66
1:O:90:PHE:HB3	1:O:106:ASN:HD21	1.60	0.66
1:U:172:ARG:NH2	1:V:253:GLY:HA2	2.10	0.66
1:F:209:LEU:HD13	1:F:213:HIS:HB3	1.78	0.66
1:G:213:HIS:HA	1:G:225:ASN:ND2	2.10	0.66
1:G:457:GLU:O	1:G:461:ILE:HG12	1.95	0.66
1:O:19:VAL:O	1:O:30:HIS:HA	1.96	0.66
1:B:115:LEU:HD23	1:B:384:LEU:HD11	1.78	0.66
1:J:210:GLU:H	1:J:213:HIS:HD2	1.44	0.66
1:M:100:TYR:HD2	1:M:102:ARG:H	1.44	0.66
1:U:226:TYR:OH	1:U:238:MET:HE2	1.96	0.66
1:G:178:HIS:CE1	1:W:473:ASP:HB2	2.29	0.65
1:L:471:TYR:O	1:L:474:VAL:HG22	1.96	0.65
1:U:18:ASP:HB3	1:U:86:ASN:ND2	2.10	0.65
1:C:329:GLY:O	1:C:331:GLU:N	2.27	0.65
1:L:286:TYR:OH	1:L:354:SER:HA	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:327:VAL:HG21	1:X:461:ILE:HG22	1.77	0.65
1:H:342:ASN:HD21	1:H:401:LEU:HB2	1.62	0.65
1:R:276:SER:HB2	1:R:285:MET:HG3	1.79	0.65
1:D:313:LEU:HG	1:D:317:ASN:HD22	1.61	0.64
1:W:464:HIS:CD2	1:W:466:TYR:H	2.14	0.64
1:U:275:GLN:NE2	1:U:301:TYR:OH	2.29	0.64
1:A:343:ARG:HH12	1:B:50:ASP:HB2	1.63	0.64
1:F:276:SER:HB3	2:F:900:2K9:H11	1.78	0.64
1:N:351:ILE:HD12	1:N:351:ILE:H	1.61	0.64
1:E:471:TYR:O	1:E:474:VAL:HG22	1.98	0.64
1:U:464:HIS:CD2	1:U:466:TYR:H	2.05	0.64
1:A:34:PRO:HG3	1:F:209:LEU:HB3	1.79	0.64
1:C:210:GLU:H	1:C:213:HIS:CD2	2.14	0.64
1:L:324:LYS:HE3	1:S:467:GLU:OE1	1.98	0.64
1:M:100:TYR:CE2	1:M:102:ARG:HB2	2.32	0.64
1:B:209:LEU:HD13	1:B:213:HIS:CB	2.27	0.64
1:C:473:ASP:HB2	1:O:178:HIS:HE1	1.61	0.64
1:L:178:HIS:HE1	1:X:473:ASP:HB2	1.61	0.64
1:M:432:TYR:CE1	1:M:433:LEU:HD13	2.33	0.64
1:Q:418:GLN:HE21	1:Q:418:GLN:HA	1.63	0.64
1:B:464:HIS:HD2	1:B:466:TYR:H	1.46	0.63
1:F:313:LEU:HA	1:F:316:THR:HG22	1.80	0.63
1:F:18:ASP:HB2	1:F:86:ASN:HD22	1.63	0.63
1:I:207:PHE:HE1	1:I:240:LEU:HD13	1.62	0.63
1:L:473:ASP:HB2	1:X:178:HIS:CE1	2.32	0.63
1:M:471:TYR:O	1:M:474:VAL:HG22	1.99	0.63
1:V:210:GLU:H	1:V:213:HIS:HD2	1.47	0.63
1:A:309:ALA:HB3	1:A:310:PRO:HD3	1.81	0.63
1:T:386:GLY:HA2	1:T:391:ILE:HD12	1.80	0.63
1:F:313:LEU:HG	1:F:317:ASN:HD22	1.63	0.63
1:I:149:TYR:CE1	1:V:146:GLY:HA2	2.33	0.63
1:P:302:ILE:CG1	1:P:361:LEU:HD22	2.29	0.63
1:R:210:GLU:H	1:R:213:HIS:CD2	2.17	0.63
1:S:336:LEU:HD21	1:S:415:THR:HG22	1.80	0.63
1:X:313:LEU:HG	1:X:317:ASN:HD22	1.64	0.63
1:G:210:GLU:H	1:G:213:HIS:CD2	2.17	0.62
1:I:316:THR:HG22	1:I:317:ASN:ND2	2.14	0.62
1:M:317:ASN:OD1	1:M:366:PRO:HA	2.00	0.62
1:R:210:GLU:H	1:R:213:HIS:HD2	1.46	0.62
1:T:18:ASP:HB3	1:T:86:ASN:HD22	1.64	0.62
1:E:209:LEU:HD13	1:E:213:HIS:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:330:TYR:HD1	1:N:330:TYR:H	1.48	0.62
1:E:121:ALA:HA	1:E:279:LYS:HB2	1.79	0.62
1:L:450:PHE:HB3	1:L:451:LYS:HB2	1.81	0.62
1:P:68:LEU:HD23	1:P:92:HIS:HD2	1.63	0.62
1:Q:115:LEU:HD23	1:Q:384:LEU:HD11	1.80	0.62
1:X:126:PHE:CE2	1:X:275:GLN:HG2	2.35	0.62
1:K:473:ASP:HB2	1:S:178:HIS:HE1	1.65	0.62
1:T:49:PHE:O	1:T:65:MET:HG2	2.00	0.62
1:E:18:ASP:HB3	1:E:86:ASN:HD22	1.65	0.61
1:P:70:ASP:HB2	1:P:90:PHE:CE1	2.35	0.61
1:T:302:ILE:HG13	1:T:361:LEU:HD22	1.82	0.61
1:N:471:TYR:O	1:N:474:VAL:HG22	1.99	0.61
1:Q:286:TYR:CE2	1:Q:288:GLU:HG3	2.35	0.61
1:Q:317:ASN:OD1	1:Q:366:PRO:HA	2.01	0.61
1:A:461:ILE:HG22	1:R:327:VAL:HG21	1.80	0.61
1:F:115:LEU:HD23	1:F:384:LEU:HD11	1.81	0.61
1:Q:140:PHE:O	1:Q:141:ASP:HB3	2.00	0.61
1:D:343:ARG:NH1	1:E:50:ASP:HB2	2.15	0.61
1:F:328:PRO:HD3	1:F:417:THR:HG21	1.81	0.61
1:F:405:PRO:HB2	1:F:408:GLU:HB3	1.82	0.61
1:I:405:PRO:C	1:I:407:GLU:H	2.07	0.61
1:J:207:PHE:HE1	1:J:240:LEU:HD13	1.66	0.61
1:T:329:GLY:O	1:T:331:GLU:N	2.34	0.61
1:D:140:PHE:O	1:D:141:ASP:HB3	2.00	0.61
1:K:18:ASP:OD2	1:K:30:HIS:HD2	1.84	0.61
1:N:276:SER:HB2	1:N:285:MET:HG3	1.82	0.61
1:A:330:TYR:O	1:A:331:GLU:HB2	1.99	0.61
1:F:18:ASP:CB	1:F:86:ASN:HD22	2.13	0.61
1:B:425:ARG:HB3	1:B:425:ARG:NH2	2.16	0.60
1:I:170:PRO:HB2	1:J:137:SER:HB3	1.83	0.60
1:W:464:HIS:HD2	1:W:466:TYR:N	1.99	0.60
1:B:469:ALA:HA	1:Q:140:PHE:CE1	2.36	0.60
1:C:461:ILE:HG22	1:P:327:VAL:HG21	1.84	0.60
1:J:404:LEU:HG	1:J:405:PRO:HD2	1.82	0.60
1:Q:68:LEU:HD23	1:Q:92:HIS:CD2	2.36	0.60
1:M:330:TYR:O	1:M:331:GLU:HG3	2.01	0.60
1:E:18:ASP:HB3	1:E:86:ASN:ND2	2.15	0.60
1:F:317:ASN:OD1	1:F:366:PRO:HA	2.01	0.60
1:Q:128:ALA:HA	1:Q:272:HIS:O	2.00	0.60
1:T:309:ALA:HB3	1:T:310:PRO:HD3	1.81	0.60
1:L:101:SER:HB2	1:L:440:THR:HG21	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:210:GLU:H	1:N:213:HIS:CD2	2.20	0.60
1:J:321:ASN:ND2	1:U:467:GLU:OE2	2.28	0.60
1:C:351:ILE:HG21	1:D:95:PHE:HZ	1.66	0.60
1:E:172:ARG:NH2	1:F:253:GLY:HA2	2.17	0.60
1:J:210:GLU:H	1:J:213:HIS:CD2	2.19	0.60
1:K:74:ALA:HB1	1:K:85:LEU:HD11	1.84	0.60
1:B:209:LEU:HD13	1:B:213:HIS:HB3	1.84	0.59
1:C:309:ALA:HB3	1:C:310:PRO:HD3	1.82	0.59
1:C:317:ASN:OD1	1:C:366:PRO:HA	2.02	0.59
1:C:351:ILE:HG21	1:D:95:PHE:CZ	2.37	0.59
1:H:316:THR:HG22	1:H:317:ASN:ND2	2.16	0.59
1:I:386:GLY:HA2	1:I:391:ILE:HD12	1.84	0.59
1:P:207:PHE:HE1	1:P:240:LEU:HD13	1.68	0.59
1:S:201:ASN:O	1:S:205:SER:HB2	2.02	0.59
1:E:473:ASP:HB2	1:M:178:HIS:HE1	1.67	0.59
1:H:157:TRP:HB3	1:H:176:VAL:HA	1.84	0.59
1:L:18:ASP:OD2	1:L:30:HIS:HD2	1.84	0.59
1:V:316:THR:HG23	1:V:366:PRO:HA	1.84	0.59
1:G:456:ILE:O	1:G:460:ASN:HB2	2.03	0.59
1:H:209:LEU:HD13	1:H:213:HIS:HB3	1.84	0.59
1:Q:121:ALA:HA	1:Q:279:LYS:HB2	1.84	0.59
1:T:207:PHE:HE1	1:T:240:LEU:HD13	1.67	0.59
1:A:464:HIS:HE1	1:R:462:ARG:O	1.86	0.59
1:O:464:HIS:CD2	1:O:466:TYR:H	2.20	0.59
1:P:207:PHE:CE1	1:P:240:LEU:HD13	2.38	0.59
1:C:115:LEU:HD23	1:C:384:LEU:HD11	1.83	0.59
1:W:386:GLY:HA2	1:W:391:ILE:HD12	1.84	0.59
1:A:464:HIS:CD2	1:A:466:TYR:H	2.16	0.59
1:D:375:ALA:O	1:D:379:MET:HE3	2.01	0.59
1:Q:455:GLU:O	1:Q:458:PRO:HD2	2.03	0.58
1:B:276:SER:HB3	2:B:900:2K9:H11	1.85	0.58
1:F:471:TYR:CZ	1:M:319:THR:HB	2.38	0.58
1:I:471:TYR:O	1:I:474:VAL:HG22	2.03	0.58
1:L:327:VAL:HG21	1:S:461:ILE:HG22	1.85	0.58
1:R:319:THR:O	1:R:322:SER:HB2	2.04	0.58
1:I:126:PHE:CE2	1:I:275:GLN:HG2	2.39	0.58
1:K:464:HIS:CD2	1:K:466:TYR:H	2.05	0.58
1:D:313:LEU:HG	1:D:317:ASN:ND2	2.18	0.58
1:M:299:ARG:NH2	1:M:392:GLU:OE2	2.36	0.58
1:D:276:SER:HB2	1:D:285:MET:HG3	1.84	0.58
1:J:461:ILE:HG22	1:U:327:VAL:HG21	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:74:ALA:HB1	1:E:85:LEU:HD11	1.84	0.58
1:J:207:PHE:CE1	1:J:240:LEU:HD13	2.39	0.58
1:I:157:TRP:HB3	1:I:176:VAL:HA	1.84	0.58
1:R:421:ASP:O	1:R:425:ARG:HG2	2.04	0.58
1:C:471:TYR:O	1:C:474:VAL:HG22	2.03	0.58
1:O:365:SER:N	1:O:366:PRO:HD3	2.18	0.58
1:W:409:ALA:C	1:W:411:SER:H	2.11	0.58
1:A:39:ASP:OD1	1:A:41:SER:HB3	2.04	0.57
1:I:328:PRO:HD3	1:I:417:THR:HG21	1.85	0.57
1:J:317:ASN:OD1	1:J:366:PRO:HA	2.03	0.57
1:E:43:PHE:HE2	1:E:71:PRO:HD3	1.69	0.57
1:R:471:TYR:O	1:R:474:VAL:HG22	2.04	0.57
1:W:106:ASN:ND2	1:W:109:ARG:HH11	2.01	0.57
1:W:317:ASN:OD1	1:W:366:PRO:HA	2.04	0.57
1:B:178:HIS:HE1	1:P:473:ASP:HB2	1.69	0.57
1:B:240:LEU:HD22	1:B:244:ILE:HD11	1.87	0.57
1:B:327:VAL:HG21	1:Q:461:ILE:HG22	1.86	0.57
1:B:464:HIS:CD2	1:B:466:TYR:H	2.22	0.57
1:H:302:ILE:HG13	1:H:361:LEU:HD22	1.86	0.57
1:J:302:ILE:HG13	1:J:361:LEU:HD22	1.86	0.57
1:O:189:ASP:O	1:O:192:VAL:HG22	2.04	0.57
1:E:106:ASN:HD21	1:E:109:ARG:HH11	1.52	0.57
1:G:324:LYS:HE3	1:X:467:GLU:OE1	2.05	0.57
1:A:386:GLY:HA2	1:A:391:ILE:HD12	1.87	0.57
1:I:432:TYR:CE1	1:I:433:LEU:HD13	2.40	0.57
1:N:432:TYR:CE1	1:N:433:LEU:HD13	2.40	0.57
1:G:97:LEU:O	1:G:97:LEU:HD23	2.05	0.57
1:V:260:PRO:HD2	1:V:321:ASN:OD1	2.03	0.57
1:R:68:LEU:HD23	1:R:92:HIS:CD2	2.40	0.57
1:B:291:TYR:C	1:B:293:GLY:H	2.13	0.57
1:D:327:VAL:HG23	1:D:328:PRO:HD2	1.87	0.57
1:R:425:ARG:HH21	1:R:425:ARG:HB3	1.69	0.57
1:B:126:PHE:CZ	1:B:275:GLN:HG2	2.40	0.56
1:R:213:HIS:HA	1:R:225:ASN:ND2	2.20	0.56
1:O:157:TRP:CD1	1:O:157:TRP:H	2.23	0.56
1:A:96:THR:OG1	1:A:98:GLU:HB2	2.04	0.56
1:B:157:TRP:HB3	1:B:176:VAL:HA	1.87	0.56
1:H:106:ASN:ND2	1:H:109:ARG:HH11	2.03	0.56
1:L:157:TRP:HB3	1:L:176:VAL:HA	1.88	0.56
1:O:454:ASN:O	1:O:458:PRO:HG2	2.04	0.56
1:P:365:SER:N	1:P:366:PRO:CD	2.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:316:THR:HG23	1:U:366:PRO:HA	1.88	0.56
1:D:18:ASP:HB3	1:D:86:ASN:HD22	1.70	0.56
1:N:194:LEU:HD22	1:N:198:MET:HE3	1.88	0.56
1:R:464:HIS:HD2	1:R:466:TYR:N	1.97	0.56
1:C:276:SER:HB2	1:C:285:MET:HG3	1.87	0.56
1:E:1:THR:HG22	1:E:3:ASP:H	1.71	0.56
1:E:309:ALA:HB3	1:E:310:PRO:HD3	1.87	0.56
1:H:210:GLU:H	1:H:213:HIS:HD2	1.54	0.56
1:D:324:LYS:HE3	1:O:467:GLU:OE1	2.06	0.56
1:N:313:LEU:HA	1:N:316:THR:OG1	2.04	0.56
1:X:184:PRO:HB2	1:X:188:ASN:HB2	1.87	0.56
1:L:325:ARG:HG2	1:L:326:LEU:HD12	1.86	0.56
1:U:18:ASP:OD2	1:U:30:HIS:HD2	1.87	0.56
1:X:464:HIS:HD2	1:X:466:TYR:N	2.04	0.56
1:D:324:LYS:HD3	1:O:460:ASN:O	2.05	0.56
1:H:325:ARG:HG2	1:H:326:LEU:HD12	1.88	0.56
1:W:186:ALA:HB1	1:X:247:ASN:HD21	1.70	0.56
1:N:209:LEU:HD13	1:N:213:HIS:HB3	1.87	0.56
1:W:102:ARG:HG2	1:W:443:LEU:HD13	1.88	0.56
1:G:301:TYR:CE1	1:G:383:GLY:HA3	2.41	0.55
1:N:434:THR:HA	1:N:439:PHE:O	2.05	0.55
1:U:169:SER:HB2	1:U:170:PRO:HD2	1.88	0.55
1:C:214:HIS:HB3	1:D:33:ILE:HG22	1.89	0.55
1:K:464:HIS:HE1	1:T:462:ARG:O	1.88	0.55
1:I:327:VAL:HG21	1:V:461:ILE:HG22	1.88	0.55
1:R:236:ASP:OD1	1:R:373:TYR:OH	2.18	0.55
1:H:49:PHE:HB3	1:H:65:MET:HE3	1.88	0.55
1:L:121:ALA:HB1	1:L:278:TRP:O	2.07	0.55
1:M:287:ASP:HB3	1:M:294:LEU:O	2.06	0.55
1:P:360:ARG:HH11	2:P:900:2K9:H5	1.71	0.55
1:S:137:SER:HB3	1:X:170:PRO:HB2	1.88	0.55
1:T:365:SER:N	1:T:366:PRO:CD	2.69	0.55
1:U:404:LEU:HD12	1:U:405:PRO:HD2	1.87	0.55
1:A:16:TYR:CE2	1:F:199:LEU:HD23	2.41	0.55
1:B:309:ALA:HB3	1:B:310:PRO:HD3	1.88	0.55
1:C:316:THR:HG23	1:C:366:PRO:HA	1.89	0.55
1:D:126:PHE:CE2	1:D:275:GLN:HG2	2.41	0.55
1:G:138:VAL:HG23	1:G:151:VAL:HG12	1.88	0.55
1:I:464:HIS:HD2	1:I:466:TYR:N	2.03	0.55
1:T:313:LEU:HG	1:T:317:ASN:ND2	2.21	0.55
1:W:90:PHE:HB3	1:W:106:ASN:HD21	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:329:GLY:C	1:T:331:GLU:H	2.14	0.55
1:D:472:TYR:CZ	1:O:138:VAL:HG11	2.42	0.55
1:H:461:ILE:HG22	1:W:327:VAL:HG21	1.89	0.55
1:O:185:VAL:O	1:O:188:ASN:HB2	2.06	0.55
1:K:386:GLY:HA2	1:K:391:ILE:HD12	1.88	0.55
1:K:473:ASP:HB2	1:S:178:HIS:CE1	2.41	0.55
1:R:432:TYR:CE1	1:R:433:LEU:HD13	2.42	0.55
1:V:432:TYR:CE1	1:V:433:LEU:HD13	2.42	0.55
1:G:34:PRO:HG3	1:L:209:LEU:HB3	1.89	0.55
1:J:462:ARG:O	1:U:464:HIS:HE1	1.89	0.55
1:Q:126:PHE:CE2	1:Q:275:GLN:HG2	2.41	0.55
1:S:272:HIS:HD2	1:S:364:ARG:HG2	1.71	0.55
1:M:114:TYR:CD2	1:M:436:GLY:HA3	2.42	0.55
1:R:209:LEU:HD13	1:R:213:HIS:CB	2.31	0.55
1:W:376:PHE:HA	1:W:379:MET:HE3	1.88	0.55
1:B:126:PHE:CE1	1:B:231:LEU:HD12	2.42	0.54
1:C:274:HIS:CD2	1:C:360:ARG:HH21	2.25	0.54
1:F:294:LEU:HD21	1:F:349:ILE:HG12	1.87	0.54
1:R:18:ASP:HB3	1:R:86:ASN:ND2	2.23	0.54
1:I:207:PHE:CE1	1:I:240:LEU:HD13	2.41	0.54
1:J:464:HIS:CD2	1:J:466:TYR:H	2.06	0.54
1:L:450:PHE:CA	1:L:451:LYS:HB2	2.37	0.54
1:V:106:ASN:HD21	1:V:109:ARG:HH11	1.55	0.54
1:L:311:SER:HB2	1:L:426:LEU:HA	1.90	0.54
1:B:209:LEU:HD13	1:B:213:HIS:HB2	1.90	0.54
1:I:464:HIS:CD2	1:I:466:TYR:H	2.19	0.54
1:A:365:SER:N	1:A:366:PRO:HD3	2.21	0.54
1:I:299:ARG:HG2	1:I:393:PRO:HG3	1.90	0.54
1:N:275:GLN:NE2	1:N:301:TYR:OH	2.41	0.54
1:P:274:HIS:ND1	1:P:360:ARG:HD2	2.23	0.54
1:U:194:LEU:HD22	1:U:198:MET:HE3	1.88	0.54
1:B:464:HIS:O	1:B:467:GLU:HB2	2.07	0.54
1:U:276:SER:HB2	1:U:285:MET:HG3	1.89	0.54
1:B:456:ILE:O	1:B:460:ASN:HB2	2.08	0.54
1:D:343:ARG:HH12	1:E:50:ASP:HB2	1.72	0.54
1:L:50:ASP:N	1:L:50:ASP:OD2	2.40	0.54
1:P:132:PHE:HB3	1:P:258:PHE:CE1	2.42	0.54
1:C:331:GLU:HG2	1:C:344:SER:HB3	1.90	0.54
1:G:140:PHE:O	1:G:141:ASP:HB3	2.08	0.54
1:H:133:TYR:CD1	1:H:262:PRO:HG2	2.42	0.54
1:T:464:HIS:CD2	1:T:465:PRO:HD2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:321:ASN:ND2	1:O:467:GLU:OE2	2.37	0.54
1:G:464:HIS:HE1	1:X:462:ARG:O	1.90	0.54
1:X:157:TRP:H	1:X:157:TRP:CD1	2.26	0.54
1:X:464:HIS:CD2	1:X:466:TYR:H	2.23	0.54
1:A:70:ASP:HB2	1:A:90:PHE:CE1	2.43	0.53
1:J:316:THR:HG22	1:J:317:ASN:OD1	2.07	0.53
1:N:464:HIS:CD2	1:N:465:PRO:HD2	2.43	0.53
1:Q:421:ASP:O	1:Q:425:ARG:HG2	2.07	0.53
1:S:102:ARG:HA	1:S:443:LEU:HD12	1.90	0.53
1:S:386:GLY:HA2	1:S:391:ILE:HD12	1.90	0.53
1:B:209:LEU:HB3	1:C:34:PRO:HG3	1.90	0.53
1:P:332:ALA:O	1:P:334:ILE:N	2.41	0.53
1:S:100:TYR:CZ	1:S:102:ARG:HB2	2.44	0.53
1:T:317:ASN:OD1	1:T:366:PRO:HA	2.08	0.53
1:C:72:GLU:O	1:C:75:ARG:NH2	2.41	0.53
1:C:365:SER:N	1:C:366:PRO:CD	2.71	0.53
1:F:316:THR:OG1	1:F:366:PRO:HB3	2.07	0.53
1:I:405:PRO:C	1:I:407:GLU:N	2.65	0.53
1:J:18:ASP:HB3	1:J:86:ASN:ND2	2.21	0.53
1:O:100:TYR:CE2	1:O:102:ARG:HB2	2.44	0.53
1:P:115:LEU:HD23	1:P:384:LEU:HD11	1.91	0.53
1:K:318:PRO:HG2	1:K:370:GLY:HA2	1.89	0.53
1:K:471:TYR:O	1:K:474:VAL:HG22	2.09	0.53
1:Q:340:GLN:HB3	1:Q:351:ILE:HD11	1.90	0.53
1:R:213:HIS:CE1	1:R:227:GLN:HA	2.44	0.53
1:A:170:PRO:HB2	1:B:137:SER:HB3	1.90	0.53
1:G:121:ALA:HB1	1:G:278:TRP:O	2.08	0.53
1:P:464:HIS:O	1:P:467:GLU:HB2	2.09	0.53
1:O:189:ASP:CG	1:O:195:ARG:HH12	2.16	0.53
1:P:336:LEU:HB2	1:P:413:PRO:HG2	1.90	0.53
1:Q:471:TYR:HA	1:Q:474:VAL:HG13	1.90	0.53
1:B:49:PHE:HD1	1:B:65:MET:HE3	1.73	0.53
1:S:121:ALA:HB1	1:S:278:TRP:O	2.08	0.53
1:U:120:ILE:HG21	1:U:387:ILE:HG21	1.91	0.53
1:W:209:LEU:HD13	1:W:213:HIS:HB3	1.90	0.53
1:K:236:ASP:OD1	1:K:373:TYR:OH	2.15	0.53
1:X:18:ASP:HB3	1:X:86:ASN:HD22	1.74	0.53
1:G:100:TYR:CE2	1:G:102:ARG:HB2	2.43	0.53
1:M:279:LYS:HB2	1:M:284:LEU:HD11	1.91	0.53
1:T:207:PHE:CE1	1:T:240:LEU:HD13	2.44	0.53
1:T:210:GLU:HB3	1:T:211:LYS:HD2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:24:LEU:HD21	1:W:443:LEU:HD11	1.90	0.53
1:M:194:LEU:HD13	1:M:198:MET:HE3	1.91	0.53
1:W:464:HIS:HB3	1:W:467:GLU:HG3	1.90	0.53
1:B:210:GLU:H	1:B:213:HIS:HD2	1.56	0.52
1:H:106:ASN:HD21	1:H:109:ARG:HH11	1.56	0.52
1:L:381:MET:HE3	1:L:432:TYR:O	2.10	0.52
1:T:210:GLU:H	1:T:213:HIS:HD2	1.57	0.52
1:V:18:ASP:OD2	1:V:30:HIS:HD2	1.93	0.52
1:E:324:LYS:HE3	1:N:467:GLU:OE1	2.09	0.52
1:E:365:SER:N	1:E:366:PRO:CD	2.72	0.52
1:X:353:GLY:O	1:X:355:ASN:N	2.40	0.52
1:O:332:ALA:O	1:O:334:ILE:HG12	2.09	0.52
1:W:329:GLY:O	1:W:331:GLU:N	2.42	0.52
1:U:70:ASP:HB2	1:U:90:PHE:CE1	2.44	0.52
1:C:386:GLY:HA2	1:C:391:ILE:HD12	1.89	0.52
1:L:313:LEU:HG	1:L:317:ASN:HD22	1.73	0.52
1:L:319:THR:O	1:L:322:SER:HB2	2.10	0.52
1:Q:157:TRP:HB3	1:Q:176:VAL:HA	1.92	0.52
1:W:126:PHE:CE2	1:W:275:GLN:HG2	2.44	0.52
1:W:304:GLY:HA3	1:W:382:ALA:O	2.10	0.52
1:A:126:PHE:CE1	1:A:231:LEU:HD12	2.45	0.52
1:F:20:ARG:HB3	1:F:28:MET:HE3	1.91	0.52
1:F:301:TYR:CE1	1:F:383:GLY:HA3	2.45	0.52
1:L:316:THR:HG23	1:L:366:PRO:HA	1.90	0.52
1:P:432:TYR:CE1	1:P:433:LEU:HD13	2.45	0.52
1:Q:320:VAL:HG11	1:Q:459:VAL:HG11	1.92	0.52
1:T:365:SER:N	1:T:366:PRO:HD3	2.24	0.52
1:U:328:PRO:HD3	1:U:417:THR:HG21	1.90	0.52
1:V:210:GLU:H	1:V:213:HIS:CD2	2.27	0.52
1:B:323:TYR:HB3	1:B:417:THR:O	2.09	0.52
1:I:313:LEU:HA	1:I:316:THR:HB	1.91	0.52
1:K:329:GLY:C	1:K:331:GLU:H	2.17	0.52
1:Q:286:TYR:HE2	1:Q:288:GLU:HG3	1.74	0.52
1:W:275:GLN:NE2	1:W:301:TYR:OH	2.43	0.52
1:A:316:THR:HG23	1:A:366:PRO:HB3	1.90	0.52
1:G:139:SER:HB3	1:L:171:ASN:HD22	1.74	0.52
1:L:309:ALA:HB3	1:L:310:PRO:HD3	1.92	0.52
1:B:100:TYR:CE2	1:B:102:ARG:HB2	2.45	0.52
1:B:342:ASN:HD21	1:B:401:LEU:H	1.57	0.52
1:K:329:GLY:O	1:K:331:GLU:N	2.42	0.52
1:M:1:THR:HB	1:M:2:PRO:CD	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:115:LEU:HD23	1:R:384:LEU:HD11	1.91	0.52
1:D:432:TYR:CE1	1:D:433:LEU:HD13	2.45	0.51
1:H:336:LEU:HD12	1:H:413:PRO:HB2	1.91	0.51
1:W:207:PHE:CE1	1:W:240:LEU:HD13	2.45	0.51
1:X:336:LEU:HD12	1:X:413:PRO:HB2	1.92	0.51
1:E:18:ASP:CB	1:E:86:ASN:ND2	2.73	0.51
1:E:418:GLN:HE21	1:E:418:GLN:HA	1.75	0.51
1:J:425:ARG:HB3	1:J:425:ARG:HH21	1.76	0.51
1:M:213:HIS:HA	1:M:225:ASN:ND2	2.24	0.51
1:O:376:PHE:HA	1:O:379:MET:HE3	1.92	0.51
1:A:18:ASP:CB	1:A:86:ASN:HD22	2.21	0.51
1:S:210:GLU:H	1:S:213:HIS:CD2	2.28	0.51
1:V:275:GLN:NE2	1:V:301:TYR:OH	2.43	0.51
1:C:207:PHE:HE1	1:C:240:LEU:CD1	2.23	0.51
1:G:236:ASP:OD1	1:G:373:TYR:OH	2.24	0.51
1:I:210:GLU:N	1:I:213:HIS:HD2	1.94	0.51
1:R:425:ARG:HB3	1:R:425:ARG:NH2	2.25	0.51
1:C:18:ASP:OD2	1:C:30:HIS:HD2	1.93	0.51
1:F:418:GLN:HA	1:F:418:GLN:NE2	2.16	0.51
1:L:42:VAL:HG22	1:L:47:LEU:HD21	1.91	0.51
1:R:319:THR:HG21	1:R:369:SER:HB2	1.93	0.51
1:S:199:LEU:HD23	1:T:16:TYR:CE2	2.46	0.51
1:V:199:LEU:HD22	1:V:215:GLU:HB2	1.93	0.51
1:D:157:TRP:HB3	1:D:176:VAL:HA	1.93	0.51
1:D:207:PHE:CE1	1:D:240:LEU:HD13	2.45	0.51
1:K:309:ALA:HB3	1:K:310:PRO:HD3	1.92	0.51
1:V:213:HIS:HA	1:V:225:ASN:ND2	2.25	0.51
1:V:455:GLU:O	1:V:459:VAL:HG23	2.11	0.51
1:H:129:GLU:O	1:H:271:MET:HA	2.11	0.51
1:T:211:LYS:HD2	1:T:211:LYS:N	2.26	0.51
1:X:276:SER:HB2	1:X:285:MET:HG3	1.93	0.51
1:A:365:SER:N	1:A:366:PRO:CD	2.73	0.51
1:S:23:ASP:OD1	1:S:27:ILE:N	2.42	0.51
1:C:467:GLU:OE2	1:P:321:ASN:ND2	2.36	0.51
1:D:464:HIS:CD2	1:D:466:TYR:H	2.29	0.51
1:A:0:LYS:HG2	1:A:72:GLU:OE1	2.10	0.51
1:B:195:ARG:CZ	1:B:217:GLY:HA3	2.41	0.51
1:G:365:SER:N	1:G:366:PRO:HD3	2.26	0.51
1:L:351:ILE:HG22	1:L:351:ILE:O	2.11	0.51
1:L:380:LEU:HD13	1:L:384:LEU:HD12	1.93	0.51
1:M:313:LEU:HA	1:M:316:THR:HB	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:ALA:HB1	1:C:278:TRP:O	2.11	0.50
1:L:189:ASP:OD2	1:L:192:VAL:HG23	2.11	0.50
1:A:316:THR:HG23	1:A:366:PRO:CB	2.42	0.50
1:P:342:ASN:HD21	1:P:400:ASP:HA	1.77	0.50
1:A:432:TYR:CE1	1:A:433:LEU:HD13	2.47	0.50
1:B:314:ALA:O	1:B:318:PRO:HB3	2.11	0.50
1:F:240:LEU:HD22	1:F:244:ILE:HD11	1.93	0.50
1:G:329:GLY:O	1:G:331:GLU:N	2.44	0.50
1:M:329:GLY:C	1:M:331:GLU:H	2.19	0.50
1:V:365:SER:N	1:V:366:PRO:CD	2.75	0.50
1:W:432:TYR:CE1	1:W:433:LEU:HD13	2.46	0.50
1:D:181:GLY:HA3	1:E:29:GLN:NE2	2.25	0.50
1:D:425:ARG:HB3	1:D:425:ARG:HH21	1.76	0.50
1:D:461:ILE:HD12	1:O:264:PHE:HE1	1.76	0.50
1:J:309:ALA:HB3	1:J:310:PRO:HD3	1.93	0.50
1:K:260:PRO:HD3	1:K:369:SER:HB3	1.94	0.50
1:K:432:TYR:CE1	1:K:433:LEU:HD13	2.46	0.50
1:L:464:HIS:CD2	1:L:465:PRO:HD2	2.46	0.50
1:W:96:THR:OG1	1:W:98:GLU:HB2	2.12	0.50
1:D:160:THR:HG21	1:D:176:VAL:HG13	1.93	0.50
1:G:96:THR:OG1	1:G:98:GLU:HB2	2.11	0.50
1:N:329:GLY:C	1:N:331:GLU:H	2.20	0.50
1:Q:309:ALA:HB3	1:Q:310:PRO:HD3	1.94	0.50
1:S:471:TYR:O	1:S:474:VAL:HG22	2.11	0.50
1:V:-1:GLU:HA	1:V:72:GLU:OE1	2.12	0.50
1:V:179:LYS:HB2	1:W:450:PHE:HZ	1.77	0.50
1:W:452:ARG:HA	1:W:456:ILE:HD12	1.94	0.50
1:A:247:ASN:HD21	1:F:186:ALA:HB1	1.77	0.50
1:F:318:PRO:O	1:F:419:LEU:HD13	2.12	0.50
1:G:70:ASP:HB2	1:G:90:PHE:CE1	2.47	0.50
1:H:207:PHE:CE1	1:H:240:LEU:HD13	2.47	0.50
1:J:149:TYR:CE1	1:U:146:GLY:HA2	2.47	0.50
1:J:327:VAL:HG21	1:U:461:ILE:HG22	1.93	0.50
1:K:438:VAL:HG12	1:K:439:PHE:CD2	2.47	0.50
1:P:316:THR:HG23	1:P:366:PRO:HA	1.94	0.50
1:P:452:ARG:HA	1:P:456:ILE:HD12	1.94	0.50
1:Q:209:LEU:HB3	1:R:34:PRO:HG3	1.94	0.50
1:B:466:TYR:O	1:B:469:ALA:HB3	2.12	0.50
1:E:473:ASP:HB2	1:M:178:HIS:CE1	2.46	0.50
1:I:321:ASN:ND2	1:V:467:GLU:OE2	2.41	0.50
1:W:389:ASN:N	1:W:389:ASN:HD22	2.08	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:PHE:HE1	1:A:240:LEU:HD13	1.76	0.50
1:C:86:ASN:C	1:C:87:ILE:HG13	2.37	0.50
1:C:148:PHE:CD1	1:C:148:PHE:C	2.90	0.50
1:E:18:ASP:CB	1:E:86:ASN:HD22	2.23	0.50
1:F:50:ASP:OD2	1:F:50:ASP:N	2.45	0.50
1:H:469:ALA:HA	1:W:140:PHE:CE1	2.47	0.50
1:N:189:ASP:OD1	1:N:192:VAL:HG13	2.12	0.50
1:N:376:PHE:HA	1:N:379:MET:HE3	1.94	0.50
1:O:276:SER:HB2	1:O:285:MET:HG3	1.93	0.50
1:V:102:ARG:HH21	1:V:446:THR:HG21	1.76	0.50
1:A:276:SER:HB2	1:A:285:MET:HG3	1.93	0.50
1:P:302:ILE:HG13	1:P:361:LEU:HD22	1.93	0.50
1:R:154:ILE:HG12	1:R:165:GLU:OE2	2.12	0.50
1:T:287:ASP:O	1:T:289:THR:N	2.45	0.50
1:M:464:HIS:CD2	1:M:465:PRO:HD2	2.47	0.49
1:O:140:PHE:O	1:O:141:ASP:HB3	2.12	0.49
1:X:365:SER:N	1:X:366:PRO:CD	2.75	0.49
1:C:405:PRO:O	1:C:408:GLU:HG2	2.12	0.49
1:G:133:TYR:CE2	1:G:221:GLN:HB2	2.47	0.49
1:O:40:LYS:HD2	1:O:40:LYS:H	1.77	0.49
1:O:365:SER:N	1:O:366:PRO:CD	2.75	0.49
1:B:313:LEU:HG	1:B:317:ASN:ND2	2.22	0.49
1:C:313:LEU:HA	1:C:316:THR:HB	1.93	0.49
1:F:42:VAL:HG12	1:F:69:PRO:HG3	1.94	0.49
1:J:432:TYR:CE1	1:J:433:LEU:HD13	2.47	0.49
1:N:18:ASP:CB	1:N:86:ASN:HD22	2.25	0.49
1:N:126:PHE:CE2	1:N:275:GLN:HG2	2.47	0.49
1:T:18:ASP:HB3	1:T:86:ASN:ND2	2.26	0.49
1:T:313:LEU:HA	1:T:316:THR:HB	1.94	0.49
1:G:213:HIS:CE1	1:G:227:GLN:HA	2.47	0.49
1:G:365:SER:N	1:G:366:PRO:CD	2.75	0.49
1:N:18:ASP:HB3	1:N:86:ASN:HD22	1.76	0.49
1:N:210:GLU:H	1:N:213:HIS:HD2	1.59	0.49
1:R:136:ASP:OD2	1:R:154:ILE:HD12	2.12	0.49
1:T:332:ALA:O	1:T:334:ILE:HG12	2.12	0.49
1:W:18:ASP:CB	1:W:86:ASN:HD22	2.22	0.49
1:H:126:PHE:CE2	1:H:275:GLN:HG2	2.47	0.49
1:K:319:THR:HB	1:T:471:TYR:CZ	2.48	0.49
1:N:170:PRO:HB2	1:O:137:SER:HB3	1.95	0.49
1:Q:160:THR:HG23	1:R:141:ASP:HB2	1.95	0.49
1:R:317:ASN:N	1:R:318:PRO:HD3	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:189:ASP:OD1	1:V:192:VAL:HG13	2.12	0.49
1:H:287:ASP:OD2	1:H:288:GLU:N	2.39	0.49
1:L:457:GLU:O	1:L:461:ILE:HG12	2.12	0.49
1:V:339:SER:OG	1:V:340:GLN:N	2.45	0.49
1:K:404:LEU:HG	1:K:405:PRO:HD2	1.95	0.49
1:L:18:ASP:HB3	1:L:86:ASN:HD22	1.78	0.49
1:B:186:ALA:HB1	1:C:247:ASN:HD21	1.77	0.49
1:B:299:ARG:NH2	1:B:392:GLU:OE2	2.46	0.49
1:L:464:HIS:HB3	1:L:467:GLU:HG3	1.95	0.49
1:M:287:ASP:C	1:M:287:ASP:OD1	2.55	0.49
1:N:303:GLY:HA2	1:N:393:PRO:HB3	1.93	0.49
1:N:343:ARG:NH1	1:O:50:ASP:HB2	2.24	0.49
1:U:386:GLY:HA2	1:U:391:ILE:HD12	1.95	0.49
1:D:317:ASN:HB3	1:D:322:SER:HB3	1.93	0.49
1:H:291:TYR:C	1:H:293:GLY:H	2.21	0.49
1:A:467:GLU:OE1	1:R:324:LYS:HE3	2.13	0.49
1:E:141:ASP:HB3	1:E:148:PHE:CE2	2.48	0.49
1:E:455:GLU:O	1:E:456:ILE:C	2.56	0.49
1:F:404:LEU:HD12	1:F:405:PRO:HD2	1.95	0.49
1:G:17:VAL:HG22	1:G:85:LEU:HB3	1.95	0.49
1:G:330:TYR:O	1:G:331:GLU:HB2	2.13	0.49
1:L:450:PHE:CB	1:L:451:LYS:HB2	2.43	0.49
1:S:129:GLU:O	1:S:271:MET:HA	2.13	0.49
1:U:277:LEU:HB2	1:U:285:MET:HE3	1.95	0.49
1:W:106:ASN:ND2	1:W:109:ARG:NH1	2.60	0.49
1:F:450:PHE:CA	1:F:451:LYS:HB2	2.43	0.48
1:K:115:LEU:O	1:K:115:LEU:HD22	2.13	0.48
1:T:332:ALA:O	1:T:334:ILE:N	2.45	0.48
1:W:329:GLY:C	1:W:331:GLU:H	2.21	0.48
1:A:49:PHE:HD1	1:A:65:MET:HE3	1.76	0.48
1:E:214:HIS:HB3	1:F:33:ILE:HG22	1.94	0.48
1:G:421:ASP:O	1:G:425:ARG:HG2	2.13	0.48
1:I:67:LEU:HB3	1:I:89:PHE:CD2	2.47	0.48
1:R:316:THR:HG22	1:R:317:ASN:OD1	2.13	0.48
1:W:210:GLU:H	1:W:213:HIS:HD2	1.61	0.48
1:E:106:ASN:ND2	1:E:109:ARG:HH11	2.11	0.48
1:E:207:PHE:CE1	1:E:240:LEU:HD13	2.49	0.48
1:P:100:TYR:CE2	1:P:102:ARG:HB2	2.48	0.48
1:Q:265:GLY:HA2	1:Q:330:TYR:OH	2.12	0.48
1:V:274:HIS:HB3	1:V:360:ARG:HD2	1.95	0.48
1:W:471:TYR:HA	1:W:474:VAL:HG13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:181:GLY:HA3	1:E:29:GLN:HE22	1.78	0.48
1:D:199:LEU:HD22	1:D:215:GLU:HB2	1.94	0.48
1:F:303:GLY:HA2	1:F:393:PRO:HB3	1.96	0.48
1:P:426:LEU:O	1:P:430:HIS:HB3	2.13	0.48
1:U:106:ASN:HD21	1:U:109:ARG:NH1	2.11	0.48
1:C:274:HIS:CD2	1:C:360:ARG:NH2	2.82	0.48
1:G:74:ALA:HA	1:G:86:ASN:O	2.13	0.48
1:G:417:THR:O	1:G:418:GLN:NE2	2.47	0.48
1:G:473:ASP:HB2	1:W:178:HIS:HE1	1.78	0.48
1:H:43:PHE:CD2	1:H:69:PRO:HG2	2.48	0.48
1:P:140:PHE:O	1:P:141:ASP:HB3	2.13	0.48
1:S:248:THR:O	1:S:252:ASN:ND2	2.45	0.48
1:A:299:ARG:NH2	1:A:392:GLU:OE2	2.47	0.48
1:C:157:TRP:HB3	1:C:176:VAL:HA	1.94	0.48
1:C:351:ILE:HD12	1:C:351:ILE:H	1.79	0.48
1:I:18:ASP:CB	1:I:86:ASN:HD22	2.26	0.48
1:J:209:LEU:HD13	1:J:213:HIS:HB3	1.96	0.48
1:N:365:SER:N	1:N:366:PRO:CD	2.76	0.48
1:T:45:ASP:O	1:T:66:LEU:HD11	2.13	0.48
1:T:275:GLN:NE2	1:T:301:TYR:OH	2.47	0.48
1:A:327:VAL:HG21	1:R:461:ILE:HG22	1.96	0.48
1:E:160:THR:HG23	1:F:141:ASP:HB2	1.95	0.48
1:F:241:TYR:O	1:F:245:ILE:HG12	2.13	0.48
1:F:464:HIS:CD2	1:F:465:PRO:HD2	2.49	0.48
1:H:120:ILE:HD11	1:H:388:LYS:HE3	1.95	0.48
1:K:24:LEU:HD21	1:K:443:LEU:HD11	1.96	0.48
1:K:417:THR:O	1:K:418:GLN:NE2	2.46	0.48
1:L:275:GLN:NE2	1:L:301:TYR:OH	2.47	0.48
1:L:294:LEU:HD11	1:L:349:ILE:HG12	1.95	0.48
1:M:196:ASP:OD1	1:N:80:ARG:NH2	2.47	0.48
1:S:432:TYR:H	1:S:432:TYR:HD2	1.62	0.48
1:W:18:ASP:HB3	1:W:86:ASN:ND2	2.26	0.48
1:A:178:HIS:HE1	1:Q:473:ASP:HB2	1.79	0.48
1:J:324:LYS:HD3	1:U:460:ASN:O	2.14	0.48
1:R:213:HIS:HA	1:R:225:ASN:HD21	1.78	0.48
1:V:49:PHE:HB3	1:V:65:MET:HE3	1.95	0.48
1:D:273:CYS:O	1:D:362:GLU:HA	2.14	0.48
1:J:317:ASN:HB3	1:J:322:SER:HB3	1.96	0.48
1:Q:1:THR:HG22	1:Q:3:ASP:H	1.79	0.48
1:T:210:GLU:H	1:T:213:HIS:CD2	2.32	0.48
1:T:240:LEU:HD22	1:T:244:ILE:CD1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:464:HIS:CD2	1:V:465:PRO:HD2	2.49	0.48
1:A:146:GLY:HA2	1:R:149:TYR:CE1	2.49	0.47
1:I:464:HIS:HE1	1:V:462:ARG:O	1.96	0.47
1:K:121:ALA:HA	1:K:279:LYS:HB2	1.96	0.47
1:K:210:GLU:N	1:K:213:HIS:HD2	1.85	0.47
1:N:464:HIS:O	1:N:467:GLU:HB2	2.14	0.47
1:O:352:THR:HG21	1:O:358:ALA:O	2.14	0.47
1:P:260:PRO:HD3	1:P:369:SER:HB3	1.94	0.47
1:V:106:ASN:ND2	1:V:109:ARG:HH11	2.11	0.47
1:D:106:ASN:ND2	1:D:109:ARG:HH11	2.12	0.47
1:J:18:ASP:OD1	1:J:30:HIS:HD2	1.97	0.47
1:M:137:SER:HB3	1:R:170:PRO:HB2	1.96	0.47
1:U:3:ASP:C	1:U:5:VAL:H	2.22	0.47
1:U:49:PHE:HD1	1:U:65:MET:HE3	1.79	0.47
1:U:209:LEU:HD13	1:U:213:HIS:HB3	1.96	0.47
1:B:240:LEU:O	1:B:244:ILE:HG13	2.14	0.47
1:F:471:TYR:O	1:F:474:VAL:HG22	2.14	0.47
1:G:471:TYR:O	1:G:474:VAL:HG22	2.14	0.47
1:I:189:ASP:OD1	1:I:192:VAL:HG13	2.14	0.47
1:M:1:THR:HB	1:M:2:PRO:HD2	1.95	0.47
1:P:213:HIS:NE2	1:P:227:GLN:HA	2.30	0.47
1:W:194:LEU:HD22	1:W:198:MET:HE3	1.95	0.47
1:X:24:LEU:HD21	1:X:443:LEU:CD1	2.44	0.47
1:B:473:ASP:HB2	1:P:178:HIS:HE1	1.80	0.47
1:D:18:ASP:HB3	1:D:86:ASN:ND2	2.30	0.47
1:F:405:PRO:HA	1:F:406:PRO:HD3	1.77	0.47
1:F:240:LEU:HD22	1:F:244:ILE:CD1	2.43	0.47
1:G:67:LEU:HD23	1:G:91:VAL:HG22	1.96	0.47
1:I:189:ASP:CG	1:I:195:ARG:HH12	2.22	0.47
1:J:189:ASP:CG	1:J:195:ARG:HH12	2.22	0.47
1:S:210:GLU:H	1:S:213:HIS:HD2	1.62	0.47
1:S:336:LEU:HD23	1:S:346:CYS:SG	2.54	0.47
1:U:302:ILE:HG13	1:U:361:LEU:HD22	1.95	0.47
1:I:455:GLU:OE1	1:V:471:TYR:OH	2.30	0.47
1:L:108:ALA:HB3	1:L:232:LEU:HD12	1.97	0.47
1:L:278:TRP:CH2	1:L:357:LYS:HG2	2.50	0.47
1:N:300:HIS:HB3	1:N:386:GLY:O	2.14	0.47
1:X:45:ASP:O	1:X:66:LEU:HD11	2.14	0.47
1:A:126:PHE:CE2	1:A:275:GLN:HG2	2.50	0.47
1:B:291:TYR:O	1:B:293:GLY:N	2.47	0.47
1:C:468:PHE:CZ	1:P:149:TYR:CE1	3.02	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:244:ILE:O	1:D:248:THR:OG1	2.23	0.47
1:D:330:TYR:HD2	1:D:330:TYR:O	1.97	0.47
1:D:365:SER:N	1:D:366:PRO:CD	2.78	0.47
1:E:432:TYR:CE1	1:E:433:LEU:HD13	2.49	0.47
1:G:386:GLY:HA2	1:G:391:ILE:HD12	1.97	0.47
1:H:186:ALA:HB1	1:I:247:ASN:HD21	1.78	0.47
1:L:178:HIS:CE1	1:X:473:ASP:HB2	2.45	0.47
1:N:311:SER:HB2	1:N:426:LEU:HA	1.97	0.47
1:Q:157:TRP:HB2	1:Q:176:VAL:HG23	1.96	0.47
1:S:294:LEU:HD21	1:S:349:ILE:HG12	1.96	0.47
1:T:211:LYS:HD2	1:T:211:LYS:H	1.79	0.47
1:W:68:LEU:HD23	1:W:92:HIS:CD2	2.50	0.47
1:X:24:LEU:HD21	1:X:443:LEU:HD11	1.97	0.47
1:X:471:TYR:O	1:X:472:TYR:C	2.56	0.47
1:C:473:ASP:HB2	1:O:178:HIS:CE1	2.45	0.47
1:J:365:SER:N	1:J:366:PRO:CD	2.77	0.47
1:K:210:GLU:HB3	1:K:211:LYS:H	1.56	0.47
1:L:450:PHE:N	1:L:451:LYS:HB2	2.30	0.47
1:M:432:TYR:CD1	1:M:433:LEU:HD13	2.50	0.47
1:U:42:VAL:HG12	1:U:69:PRO:HG3	1.96	0.47
1:C:102:ARG:HG2	1:C:443:LEU:HD13	1.96	0.47
1:D:309:ALA:HB3	1:D:336:LEU:HD21	1.96	0.47
1:F:210:GLU:H	1:F:213:HIS:CD2	2.33	0.47
1:H:131:GLU:HG2	1:H:223:GLU:HB2	1.97	0.47
1:H:450:PHE:CD1	1:H:454:ASN:ND2	2.83	0.47
1:J:209:LEU:HB3	1:K:34:PRO:HG3	1.97	0.47
1:J:316:THR:HG23	1:J:366:PRO:HA	1.96	0.47
1:N:260:PRO:HD3	1:N:369:SER:HB3	1.97	0.47
1:Q:313:LEU:HA	1:Q:316:THR:HB	1.97	0.47
1:Q:433:LEU:HB3	1:Q:439:PHE:HB2	1.95	0.47
1:U:404:LEU:O	1:U:405:PRO:C	2.58	0.47
1:X:236:ASP:OD1	1:X:373:TYR:OH	2.29	0.47
1:X:287:ASP:O	1:X:289:THR:N	2.48	0.47
1:X:425:ARG:HB3	1:X:425:ARG:NH2	2.30	0.47
1:B:335:ASN:HD22	1:B:401:LEU:HD13	1.80	0.47
1:F:260:PRO:HD3	1:F:369:SER:HB3	1.96	0.47
1:L:348:ARG:HD3	1:L:364:ARG:HD2	1.97	0.47
1:Q:455:GLU:C	1:Q:458:PRO:HD2	2.40	0.47
1:D:194:LEU:HD22	1:D:198:MET:HE3	1.97	0.46
1:O:272:HIS:CD2	1:O:364:ARG:HG2	2.50	0.46
1:Q:365:SER:N	1:Q:366:PRO:HD3	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:430:HIS:HB2	1:Q:444:ILE:HD13	1.97	0.46
1:T:140:PHE:O	1:T:141:ASP:CB	2.62	0.46
1:T:157:TRP:HB3	1:T:176:VAL:HA	1.95	0.46
1:V:70:ASP:HB2	1:V:90:PHE:CE1	2.50	0.46
1:C:42:VAL:O	1:C:46:GLY:HA2	2.15	0.46
1:E:1:THR:HG22	1:E:3:ASP:N	2.30	0.46
1:F:140:PHE:CE1	1:M:469:ALA:HA	2.50	0.46
1:H:226:TYR:OH	1:H:238:MET:HE2	2.16	0.46
1:H:376:PHE:HA	1:H:379:MET:HE3	1.97	0.46
1:J:332:ALA:O	1:J:334:ILE:N	2.48	0.46
1:M:276:SER:HB3	2:M:900:2K9:H11	1.97	0.46
1:W:65:MET:HE3	1:W:67:LEU:HD11	1.96	0.46
1:B:70:ASP:HB2	1:B:90:PHE:CE1	2.51	0.46
1:B:336:LEU:HB2	1:B:413:PRO:HG2	1.98	0.46
1:C:242:LYS:NZ	1:C:368:SER:O	2.43	0.46
1:C:464:HIS:HD2	1:C:466:TYR:H	1.62	0.46
1:F:382:ALA:HA	1:F:432:TYR:CD1	2.50	0.46
1:Q:232:LEU:HD23	1:Q:233:HIS:CE1	2.51	0.46
1:R:316:THR:C	1:R:318:PRO:HD3	2.40	0.46
1:U:271:MET:O	1:U:366:PRO:HB2	2.15	0.46
1:W:331:GLU:OE2	1:W:402:TYR:HB2	2.16	0.46
1:K:68:LEU:HD23	1:K:92:HIS:CD2	2.50	0.46
1:O:473:ASP:N	1:O:473:ASP:OD1	2.48	0.46
1:R:126:PHE:HA	1:R:274:HIS:O	2.15	0.46
1:U:331:GLU:HG3	1:U:331:GLU:O	2.15	0.46
1:A:246:LYS:NZ	1:R:473:ASP:O	2.42	0.46
1:F:38:PHE:CE1	1:F:42:VAL:HG11	2.50	0.46
1:G:279:LYS:HB3	1:G:284:LEU:HD11	1.97	0.46
1:G:321:ASN:ND2	1:G:324:LYS:HG3	2.31	0.46
1:L:75:ARG:HG3	1:L:240:LEU:HD11	1.97	0.46
1:E:299:ARG:NH2	1:E:392:GLU:OE2	2.48	0.46
1:F:146:GLY:HA2	1:M:149:TYR:CE1	2.51	0.46
1:F:455:GLU:C	1:F:458:PRO:HD2	2.39	0.46
1:L:454:ASN:C	1:L:458:PRO:HG2	2.40	0.46
1:R:316:THR:CG2	1:R:317:ASN:OD1	2.64	0.46
1:R:419:LEU:HG	1:R:456:ILE:HD11	1.97	0.46
1:U:129:GLU:HG2	1:U:225:ASN:CB	2.46	0.46
1:D:462:ARG:O	1:O:464:HIS:HE1	1.98	0.46
1:F:114:TYR:CD2	1:F:436:GLY:HA3	2.51	0.46
1:G:101:SER:O	1:G:107:ILE:HD11	2.16	0.46
1:M:214:HIS:HB3	1:N:33:ILE:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:100:TYR:CE2	1:N:102:ARG:HB2	2.51	0.46
1:Q:216:VAL:HG12	1:Q:223:GLU:HB3	1.98	0.46
1:W:106:ASN:HD21	1:W:109:ARG:NH1	2.13	0.46
1:C:275:GLN:NE2	1:C:301:TYR:OH	2.49	0.46
1:E:70:ASP:HA	1:E:71:PRO:HD2	1.81	0.46
1:G:314:ALA:CB	1:G:426:LEU:HD22	2.46	0.46
1:M:260:PRO:HD2	1:M:321:ASN:OD1	2.15	0.46
1:N:209:LEU:HD11	1:N:225:ASN:O	2.16	0.46
1:T:126:PHE:CE2	1:T:275:GLN:HG2	2.50	0.46
1:U:18:ASP:OD2	1:U:30:HIS:CD2	2.69	0.46
1:C:342:ASN:ND2	1:C:401:LEU:HD12	2.31	0.46
1:F:299:ARG:NH2	1:F:392:GLU:OE2	2.49	0.46
1:F:419:LEU:HG	1:F:456:ILE:HD11	1.97	0.46
1:M:90:PHE:HB3	1:M:106:ASN:HD21	1.81	0.46
1:O:311:SER:HB2	1:O:426:LEU:HA	1.98	0.46
1:P:83:LYS:HA	1:P:83:LYS:HD3	1.81	0.46
1:S:230:SER:O	1:S:231:LEU:C	2.58	0.46
1:V:207:PHE:CE1	1:V:240:LEU:HD13	2.51	0.46
1:X:18:ASP:CB	1:X:86:ASN:HD22	2.28	0.46
1:F:18:ASP:OD2	1:F:30:HIS:HD2	1.99	0.46
1:F:352:THR:HG21	1:F:359:LYS:HA	1.97	0.46
1:G:329:GLY:C	1:G:331:GLU:H	2.23	0.46
1:I:213:HIS:HA	1:I:225:ASN:ND2	2.31	0.46
1:J:74:ALA:O	1:J:75:ARG:HD3	2.16	0.46
1:O:128:ALA:HA	1:O:272:HIS:O	2.16	0.46
1:H:316:THR:HG23	1:H:366:PRO:HA	1.97	0.45
1:H:464:HIS:HD2	1:H:466:TYR:N	2.02	0.45
1:P:419:LEU:O	1:P:423:ILE:HG12	2.16	0.45
1:P:425:ARG:HB3	1:P:425:ARG:NH2	2.31	0.45
1:V:18:ASP:OD2	1:V:30:HIS:CD2	2.69	0.45
1:X:114:TYR:CD2	1:X:436:GLY:HA3	2.52	0.45
1:H:386:GLY:HA2	1:H:391:ILE:HD12	1.97	0.45
1:H:404:LEU:HD23	1:H:409:ALA:HB2	1.98	0.45
1:M:19:VAL:HG13	1:M:89:PHE:CE1	2.52	0.45
1:M:100:TYR:HD2	1:M:101:SER:N	2.13	0.45
1:P:102:ARG:NH2	1:P:446:THR:OG1	2.50	0.45
1:P:170:PRO:HB2	1:Q:137:SER:HB3	1.98	0.45
1:Q:265:GLY:O	1:Q:266:ASP:HB2	2.16	0.45
1:U:336:LEU:HD12	1:U:413:PRO:HB2	1.99	0.45
1:X:294:LEU:HD21	1:X:349:ILE:HG12	1.99	0.45
1:B:100:TYR:CZ	1:B:102:ARG:HB2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:ALA:HA	1:B:272:HIS:O	2.16	0.45
1:F:74:ALA:HB1	1:F:85:LEU:HD11	1.98	0.45
1:I:140:PHE:O	1:I:141:ASP:HB3	2.16	0.45
1:K:45:ASP:O	1:K:66:LEU:HD11	2.16	0.45
1:F:276:SER:HB3	2:F:900:2K9:C17	2.45	0.45
1:J:115:LEU:HD23	1:J:384:LEU:HD21	1.97	0.45
1:J:182:TYR:O	1:J:184:PRO:HD3	2.17	0.45
1:P:18:ASP:HB3	1:P:86:ASN:HD22	1.82	0.45
1:A:328:PRO:HD3	1:A:417:THR:HG21	1.98	0.45
1:C:302:ILE:HG12	1:C:361:LEU:HD22	1.98	0.45
1:E:417:THR:O	1:E:418:GLN:NE2	2.50	0.45
1:F:274:HIS:N	1:F:274:HIS:CD2	2.85	0.45
1:F:300:HIS:NE2	1:F:390:LYS:HB3	2.31	0.45
1:J:316:THR:CG2	1:J:317:ASN:OD1	2.64	0.45
1:O:129:GLU:HG2	1:O:225:ASN:HB3	1.98	0.45
1:O:189:ASP:OD1	1:O:192:VAL:HG13	2.17	0.45
1:E:462:ARG:O	1:N:464:HIS:HE1	1.99	0.45
1:F:210:GLU:H	1:F:213:HIS:HD2	1.63	0.45
1:G:367:ASP:C	1:G:369:SER:H	2.24	0.45
1:M:365:SER:N	1:M:366:PRO:CD	2.80	0.45
1:N:157:TRP:CB	1:N:176:VAL:HA	2.45	0.45
1:P:309:ALA:HB3	1:P:310:PRO:HD3	1.99	0.45
1:S:404:LEU:HD12	1:S:405:PRO:HD2	1.99	0.45
1:V:338:TYR:CE1	1:V:396:PRO:HB3	2.52	0.45
1:D:316:THR:HG23	1:D:366:PRO:HA	1.98	0.45
1:S:323:TYR:OH	1:S:422:VAL:HG21	2.17	0.45
1:T:8:LEU:HD22	1:T:76:ILE:HD11	1.99	0.45
1:U:126:PHE:CE2	1:U:275:GLN:HG2	2.52	0.45
1:V:18:ASP:HB3	1:V:86:ASN:HD22	1.81	0.45
1:V:210:GLU:HB3	1:V:211:LYS:H	1.45	0.45
1:X:316:THR:HG23	1:X:366:PRO:CA	2.45	0.45
1:B:386:GLY:HA2	1:B:391:ILE:HD12	1.98	0.45
1:E:181:GLY:HA3	1:F:29:GLN:OE1	2.16	0.45
1:G:90:PHE:HB3	1:G:106:ASN:HD21	1.82	0.45
1:H:115:LEU:HD23	1:H:384:LEU:HD11	1.99	0.45
1:H:140:PHE:CE1	1:W:469:ALA:HA	2.52	0.45
1:N:275:GLN:O	1:N:360:ARG:HB2	2.17	0.45
1:R:12:GLU:OE2	1:R:83:LYS:NZ	2.47	0.45
1:T:277:LEU:HB2	1:T:285:MET:HE3	1.98	0.45
1:U:271:MET:HE3	1:U:273:CYS:SG	2.57	0.45
1:A:18:ASP:OD2	1:A:30:HIS:HD2	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:TYR:O	1:B:184:PRO:HD3	2.16	0.45
1:B:213:HIS:HA	1:B:225:ASN:HD21	1.82	0.45
1:G:231:LEU:HD23	1:G:231:LEU:C	2.42	0.45
1:J:416:PRO:HB2	1:J:422:VAL:HG12	1.97	0.45
1:L:276:SER:HB2	1:L:285:MET:HG3	1.99	0.45
1:N:471:TYR:HA	1:N:474:VAL:HG13	1.97	0.45
1:O:23:ASP:C	1:O:23:ASP:OD1	2.60	0.45
1:R:329:GLY:C	1:R:331:GLU:H	2.24	0.45
1:S:471:TYR:O	1:S:472:TYR:C	2.59	0.45
1:V:299:ARG:HD2	1:V:392:GLU:OE1	2.17	0.45
1:X:108:ALA:HB3	1:X:232:LEU:HD13	1.99	0.45
1:X:335:ASN:ND2	1:X:401:LEU:HD13	2.32	0.45
1:C:68:LEU:HD23	1:C:92:HIS:CD2	2.52	0.45
1:C:329:GLY:C	1:C:331:GLU:H	2.23	0.45
1:D:469:ALA:HA	1:O:140:PHE:CE1	2.52	0.45
1:E:314:ALA:O	1:E:318:PRO:HB3	2.17	0.45
1:H:235:ALA:HB1	1:H:372:PRO:HB2	1.99	0.45
1:I:19:VAL:HG13	1:I:89:PHE:CE1	2.52	0.45
1:J:452:ARG:HA	1:J:456:ILE:HB	1.99	0.45
1:K:107:ILE:HD11	1:K:443:LEU:HD22	1.99	0.45
1:K:330:TYR:HD2	1:K:330:TYR:O	2.00	0.45
1:U:19:VAL:O	1:U:30:HIS:HA	2.17	0.45
1:V:210:GLU:O	1:V:211:LYS:C	2.58	0.45
1:W:18:ASP:OD2	1:W:30:HIS:HD2	1.99	0.45
1:E:216:VAL:HG12	1:E:223:GLU:HB3	1.98	0.44
1:F:286:TYR:O	1:F:287:ASP:HB2	2.16	0.44
1:G:18:ASP:HB3	1:G:86:ASN:ND2	2.33	0.44
1:H:342:ASN:ND2	1:H:401:LEU:HB2	2.31	0.44
1:H:405:PRO:HA	1:H:406:PRO:HD3	1.83	0.44
1:J:467:GLU:OE1	1:U:324:LYS:HE3	2.17	0.44
1:M:336:LEU:HD21	1:M:415:THR:HG22	1.99	0.44
1:N:70:ASP:HA	1:N:71:PRO:HD2	1.85	0.44
1:V:457:GLU:O	1:V:461:ILE:HG23	2.17	0.44
1:F:133:TYR:CD1	1:F:262:PRO:HG2	2.52	0.44
1:F:146:GLY:HA2	1:M:149:TYR:CZ	2.53	0.44
1:F:211:LYS:C	1:F:213:HIS:H	2.26	0.44
1:G:314:ALA:HB3	1:G:426:LEU:HD22	1.99	0.44
1:I:24:LEU:HD21	1:I:443:LEU:HD11	1.99	0.44
1:I:309:ALA:HB3	1:I:310:PRO:HD3	1.99	0.44
1:M:126:PHE:CE2	1:M:275:GLN:HG2	2.52	0.44
1:N:157:TRP:CD1	1:N:157:TRP:H	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:126:PHE:CE2	1:O:275:GLN:HG2	2.52	0.44
1:O:294:LEU:HD21	1:O:349:ILE:HG12	1.99	0.44
1:B:207:PHE:CE1	1:B:240:LEU:HD13	2.51	0.44
1:C:70:ASP:HB2	1:C:90:PHE:CE1	2.52	0.44
1:D:102:ARG:O	1:D:104:PRO:HD3	2.17	0.44
1:E:313:LEU:HG	1:E:317:ASN:ND2	2.31	0.44
1:F:464:HIS:HE1	1:M:462:ARG:O	2.01	0.44
1:S:202:LEU:O	1:S:207:PHE:HB2	2.18	0.44
1:V:330:TYR:O	1:V:331:GLU:HB2	2.17	0.44
1:A:210:GLU:H	1:A:213:HIS:HD2	1.64	0.44
1:B:405:PRO:C	1:B:407:GLU:H	2.24	0.44
1:D:256:VAL:HG12	1:D:257:THR:N	2.33	0.44
1:H:365:SER:N	1:H:366:PRO:CD	2.81	0.44
1:O:404:LEU:HG	1:O:405:PRO:HD2	1.99	0.44
1:R:18:ASP:HB3	1:R:86:ASN:HD22	1.83	0.44
1:U:464:HIS:CD2	1:U:465:PRO:HD2	2.53	0.44
1:W:43:PHE:CD2	1:W:69:PRO:HG2	2.53	0.44
1:C:8:LEU:O	1:C:12:GLU:HG2	2.18	0.44
1:C:421:ASP:O	1:C:424:ASP:HB2	2.18	0.44
1:G:464:HIS:CD2	1:G:466:TYR:H	2.29	0.44
1:H:106:ASN:HD21	1:H:109:ARG:NH1	2.16	0.44
1:R:318:PRO:HB2	1:R:319:THR:HG23	1.99	0.44
1:S:18:ASP:OD2	1:S:30:HIS:CD2	2.62	0.44
1:A:114:TYR:CD2	1:A:436:GLY:HA3	2.53	0.44
1:B:311:SER:HB2	1:B:426:LEU:HA	2.00	0.44
1:H:210:GLU:H	1:H:213:HIS:CD2	2.32	0.44
1:I:389:ASN:O	1:I:390:LYS:C	2.61	0.44
1:N:96:THR:OG1	1:N:98:GLU:HB2	2.18	0.44
1:N:226:TYR:OH	1:N:238:MET:HE2	2.17	0.44
1:O:405:PRO:HB2	1:O:408:GLU:HB2	1.98	0.44
1:P:464:HIS:CD2	1:P:466:TYR:H	2.34	0.44
1:T:309:ALA:HB3	1:T:336:LEU:HD21	2.00	0.44
1:U:439:PHE:HB3	1:U:444:ILE:HD11	1.99	0.44
1:V:1:THR:O	1:V:4:ASP:HB2	2.17	0.44
1:B:351:ILE:H	1:B:351:ILE:HG13	1.56	0.44
1:B:450:PHE:O	1:B:454:ASN:HB2	2.17	0.44
1:J:165:GLU:OE1	1:J:171:ASN:HA	2.18	0.44
1:K:106:ASN:HD21	1:K:109:ARG:HH11	1.64	0.44
1:N:196:ASP:OD1	1:O:80:ARG:NH2	2.51	0.44
1:Q:365:SER:N	1:Q:366:PRO:CD	2.81	0.44
1:T:423:ILE:CG2	1:T:448:ILE:HG23	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:121:ALA:HB1	1:W:278:TRP:O	2.18	0.44
1:X:209:LEU:HD13	1:X:213:HIS:HB3	1.99	0.44
1:C:464:HIS:CD2	1:C:466:TYR:H	2.35	0.44
1:D:207:PHE:HE1	1:D:240:LEU:HD13	1.81	0.44
1:G:467:GLU:OE2	1:X:324:LYS:HE3	2.17	0.44
1:H:1:THR:HG22	1:H:3:ASP:H	1.83	0.44
1:H:140:PHE:O	1:H:141:ASP:CB	2.65	0.44
1:Q:335:ASN:ND2	1:Q:401:LEU:HD13	2.33	0.44
1:Q:456:ILE:O	1:Q:460:ASN:HB2	2.18	0.44
1:S:213:HIS:CE1	1:S:227:GLN:HA	2.52	0.44
1:T:338:TYR:HA	1:T:347:VAL:O	2.17	0.44
1:V:184:PRO:O	1:V:189:ASP:HB2	2.17	0.44
1:B:66:LEU:HB3	1:B:92:HIS:HB2	2.00	0.44
1:B:299:ARG:HD2	1:B:392:GLU:OE1	2.18	0.44
1:C:105:ARG:HG2	1:C:373:TYR:CE2	2.53	0.44
1:C:114:TYR:CD2	1:C:436:GLY:HA3	2.53	0.44
1:C:471:TYR:CZ	1:P:319:THR:HB	2.53	0.44
1:G:170:PRO:HB3	1:H:137:SER:HB3	1.99	0.44
1:L:140:PHE:CE1	1:S:469:ALA:HA	2.53	0.44
1:N:450:PHE:O	1:N:454:ASN:HB2	2.17	0.44
1:T:464:HIS:CD2	1:T:466:TYR:H	2.12	0.44
1:V:114:TYR:O	1:V:117:SER:HB2	2.18	0.44
1:V:179:LYS:HB2	1:W:450:PHE:CZ	2.52	0.44
1:W:452:ARG:O	1:W:457:GLU:HB2	2.18	0.44
1:A:279:LYS:HB3	1:A:284:LEU:HD11	2.00	0.43
1:A:311:SER:HB2	1:A:426:LEU:HA	1.99	0.43
1:B:178:HIS:CE1	1:P:473:ASP:HB2	2.52	0.43
1:C:90:PHE:HB3	1:C:106:ASN:HD21	1.82	0.43
1:F:103:ASP:O	1:F:106:ASN:HB2	2.18	0.43
1:I:115:LEU:HD23	1:I:384:LEU:HD11	2.00	0.43
1:N:83:LYS:HA	1:N:83:LYS:HD3	1.83	0.43
1:X:435:GLU:C	1:X:437:GLY:H	2.26	0.43
1:A:230:SER:O	1:A:231:LEU:C	2.61	0.43
1:D:68:LEU:HA	1:D:69:PRO:HD3	1.87	0.43
1:D:210:GLU:H	1:D:213:HIS:CD2	2.36	0.43
1:G:70:ASP:HA	1:G:71:PRO:HD2	1.86	0.43
1:G:301:TYR:CD1	1:G:383:GLY:HA3	2.54	0.43
1:I:70:ASP:HB2	1:I:90:PHE:CE1	2.53	0.43
1:I:365:SER:N	1:I:366:PRO:CD	2.81	0.43
1:K:231:LEU:C	1:K:231:LEU:HD23	2.43	0.43
1:M:389:ASN:N	1:M:389:ASN:HD22	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:75:ARG:HG3	1:Q:240:LEU:HD11	2.00	0.43
1:V:115:LEU:HD23	1:V:384:LEU:HD11	2.00	0.43
1:D:112:GLU:HG3	1:D:231:LEU:HB3	1.99	0.43
1:F:311:SER:HB2	1:F:426:LEU:HD12	2.00	0.43
1:F:423:ILE:HG22	1:F:452:ARG:HH11	1.84	0.43
1:H:352:THR:HG21	1:H:358:ALA:O	2.18	0.43
1:N:214:HIS:HB3	1:O:33:ILE:HG22	2.00	0.43
1:O:86:ASN:C	1:O:87:ILE:HG13	2.43	0.43
1:O:123:THR:HG21	1:O:125:TYR:CZ	2.54	0.43
1:T:276:SER:HB2	1:T:285:MET:HG3	2.00	0.43
1:F:24:LEU:HD21	1:F:443:LEU:HD11	2.01	0.43
1:G:194:LEU:HD22	1:G:198:MET:HE3	2.00	0.43
1:H:471:TYR:HA	1:H:474:VAL:HG13	2.00	0.43
1:M:34:PRO:HG3	1:R:209:LEU:HB3	2.01	0.43
1:O:405:PRO:HA	1:O:406:PRO:HD3	1.87	0.43
1:T:114:TYR:O	1:T:118:THR:HG23	2.18	0.43
1:V:8:LEU:O	1:V:8:LEU:HD23	2.17	0.43
1:X:210:GLU:H	1:X:213:HIS:HD2	1.65	0.43
1:A:157:TRP:HB3	1:A:176:VAL:HA	2.01	0.43
1:I:68:LEU:HA	1:I:69:PRO:HD2	1.77	0.43
1:N:319:THR:O	1:N:322:SER:HB2	2.18	0.43
1:P:291:TYR:O	1:P:294:LEU:HB2	2.18	0.43
1:U:210:GLU:H	1:U:213:HIS:CD2	2.35	0.43
1:V:140:PHE:O	1:V:141:ASP:CB	2.66	0.43
1:X:140:PHE:O	1:X:141:ASP:HB3	2.17	0.43
1:B:276:SER:HB2	1:B:285:MET:HG3	1.99	0.43
1:L:49:PHE:HD1	1:L:65:MET:CE	2.32	0.43
1:T:73:THR:HG21	1:T:88:ASN:HB2	2.00	0.43
1:T:471:TYR:O	1:T:474:VAL:HG22	2.19	0.43
1:X:230:SER:O	1:X:231:LEU:C	2.61	0.43
1:A:169:SER:HB2	1:A:170:PRO:HD2	2.00	0.43
1:F:70:ASP:HA	1:F:71:PRO:HD2	1.91	0.43
1:F:230:SER:O	1:F:231:LEU:C	2.60	0.43
1:G:340:GLN:HB3	1:G:351:ILE:HD11	2.01	0.43
1:G:405:PRO:HA	1:G:406:PRO:HD3	1.74	0.43
1:I:70:ASP:HA	1:I:71:PRO:HD2	1.71	0.43
1:I:276:SER:HB2	1:I:285:MET:HG3	1.99	0.43
1:J:435:GLU:C	1:J:437:GLY:H	2.27	0.43
1:O:464:HIS:HD2	1:O:466:TYR:N	2.09	0.43
1:Q:96:THR:C	1:Q:98:GLU:N	2.77	0.43
1:Q:160:THR:OG1	1:R:140:PHE:CE1	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:238:MET:HE3	1:Q:271:MET:SD	2.59	0.43
1:B:154:ILE:C	1:B:156:GLY:H	2.27	0.43
1:B:420:SER:HB3	1:B:456:ILE:HG21	2.00	0.43
1:K:328:PRO:HD3	1:K:417:THR:HG21	2.01	0.43
1:N:330:TYR:CD1	1:N:330:TYR:N	2.86	0.43
1:R:207:PHE:CE1	1:R:240:LEU:HD13	2.53	0.43
1:U:129:GLU:HG2	1:U:225:ASN:HB3	2.01	0.43
1:X:451:LYS:HD3	1:X:451:LYS:HA	1.89	0.43
1:B:306:LEU:HD13	1:B:336:LEU:O	2.18	0.43
1:B:471:TYR:CZ	1:Q:319:THR:HB	2.54	0.43
1:D:171:ASN:C	1:D:171:ASN:OD1	2.61	0.43
1:E:276:SER:HB2	1:E:285:MET:HG3	2.01	0.43
1:E:464:HIS:CD2	1:E:465:PRO:HD2	2.53	0.43
1:E:464:HIS:HE1	1:N:462:ARG:O	2.02	0.43
1:H:77:ASP:HA	1:H:78:PRO:HD3	1.87	0.43
1:I:467:GLU:OE2	1:V:321:ASN:ND2	2.50	0.43
1:N:65:MET:HE3	1:N:67:LEU:HD11	2.01	0.43
1:U:173:GLY:O	1:U:174:TYR:HB2	2.19	0.43
1:W:74:ALA:HB1	1:W:85:LEU:HD11	2.00	0.43
1:X:213:HIS:CE1	1:X:227:GLN:HA	2.54	0.43
1:F:382:ALA:HB2	1:F:432:TYR:HE1	1.83	0.43
1:H:209:LEU:HB3	1:I:34:PRO:HG3	1.99	0.43
1:J:213:HIS:HA	1:J:225:ASN:HD21	1.83	0.43
1:M:18:ASP:OD1	1:M:30:HIS:HD2	2.01	0.43
1:N:336:LEU:HD12	1:N:413:PRO:HB2	2.00	0.43
1:P:68:LEU:CD2	1:P:92:HIS:HD2	2.30	0.43
1:Q:445:GLU:HA	1:Q:448:ILE:HD12	2.00	0.43
1:W:380:LEU:O	1:W:384:LEU:HG	2.19	0.43
1:W:405:PRO:C	1:W:407:GLU:H	2.27	0.43
1:B:90:PHE:HB3	1:B:106:ASN:HD21	1.84	0.42
1:C:19:VAL:HG22	1:C:89:PHE:CZ	2.54	0.42
1:I:23:ASP:OD1	1:I:27:ILE:N	2.51	0.42
1:M:154:ILE:C	1:M:156:GLY:H	2.25	0.42
1:O:309:ALA:HA	1:O:312:LEU:HB2	2.01	0.42
1:Q:16:TYR:O	1:Q:84:THR:HA	2.19	0.42
1:V:18:ASP:CG	1:V:30:HIS:HD2	2.25	0.42
1:X:421:ASP:O	1:X:425:ARG:HG2	2.18	0.42
1:X:425:ARG:HB3	1:X:425:ARG:HH21	1.84	0.42
1:A:464:HIS:HD2	1:A:466:TYR:N	2.04	0.42
1:B:432:TYR:CE1	1:B:433:LEU:HD13	2.54	0.42
1:H:238:MET:O	1:H:241:TYR:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:430:HIS:CD2	1:H:444:ILE:HG21	2.53	0.42
1:H:455:GLU:C	1:H:458:PRO:HD2	2.45	0.42
1:J:100:TYR:CE2	1:J:102:ARG:HB2	2.54	0.42
1:M:23:ASP:C	1:M:23:ASP:OD1	2.62	0.42
1:M:276:SER:CB	2:M:900:2K9:H11	2.49	0.42
1:P:209:LEU:HD13	1:P:213:HIS:HB3	2.00	0.42
1:Q:336:LEU:HD12	1:Q:413:PRO:HB2	2.00	0.42
1:S:286:TYR:O	1:S:287:ASP:HB2	2.19	0.42
1:U:182:TYR:O	1:U:184:PRO:HD3	2.19	0.42
1:W:336:LEU:HD21	1:W:415:THR:HG22	2.01	0.42
1:B:140:PHE:CE1	1:Q:469:ALA:HA	2.55	0.42
1:F:327:VAL:HG21	1:M:461:ILE:HG22	2.01	0.42
1:G:311:SER:HB2	1:G:426:LEU:HA	2.00	0.42
1:H:464:HIS:CD2	1:H:466:TYR:H	2.17	0.42
1:H:472:TYR:CE2	1:W:138:VAL:HG11	2.55	0.42
1:L:317:ASN:OD1	1:L:366:PRO:HA	2.20	0.42
1:M:19:VAL:HG13	1:M:89:PHE:CD1	2.54	0.42
1:M:470:LEU:HD12	1:M:470:LEU:HA	1.78	0.42
1:P:105:ARG:HG2	1:P:373:TYR:CZ	2.53	0.42
1:R:209:LEU:CD1	1:R:213:HIS:HB3	2.38	0.42
1:R:332:ALA:O	1:R:334:ILE:N	2.52	0.42
1:S:260:PRO:HD2	1:S:321:ASN:OD1	2.19	0.42
1:A:106:ASN:ND2	1:A:109:ARG:NH1	2.67	0.42
1:B:18:ASP:OD2	1:B:30:HIS:HD2	2.01	0.42
1:C:425:ARG:NH2	1:C:425:ARG:HB3	2.33	0.42
1:D:146:GLY:HA2	1:O:149:TYR:CE1	2.55	0.42
1:G:24:LEU:HD22	1:G:24:LEU:HA	1.90	0.42
1:G:278:TRP:HH2	1:G:357:LYS:HG2	1.84	0.42
1:G:332:ALA:O	1:G:334:ILE:N	2.53	0.42
1:I:231:LEU:C	1:I:231:LEU:HD23	2.44	0.42
1:K:308:HIS:O	1:K:312:LEU:HB2	2.18	0.42
1:L:18:ASP:CB	1:L:86:ASN:HD22	2.31	0.42
1:L:23:ASP:OD1	1:L:27:ILE:N	2.52	0.42
1:Q:18:ASP:OD2	1:Q:30:HIS:HD2	2.01	0.42
1:S:276:SER:HB2	1:S:285:MET:HG3	2.02	0.42
1:T:416:PRO:HB2	1:T:422:VAL:HG12	2.02	0.42
1:U:462:ARG:HA	1:U:463:PRO:HD3	1.88	0.42
1:A:274:HIS:HB3	1:A:360:ARG:HD2	2.02	0.42
1:B:195:ARG:O	1:B:198:MET:HB2	2.20	0.42
1:B:332:ALA:HA	1:B:333:PRO:HD3	1.87	0.42
1:F:471:TYR:CE1	1:M:319:THR:HB	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:18:ASP:OD1	1:G:30:HIS:HD2	2.02	0.42
1:G:75:ARG:O	1:G:85:LEU:HD12	2.20	0.42
1:G:189:ASP:O	1:G:192:VAL:HG22	2.19	0.42
1:G:464:HIS:HD2	1:G:466:TYR:N	2.14	0.42
1:M:207:PHE:CE1	1:M:240:LEU:HD13	2.54	0.42
1:X:271:MET:HE3	1:X:273:CYS:SG	2.60	0.42
1:X:432:TYR:CD1	1:X:433:LEU:HD13	2.54	0.42
1:D:186:ALA:HB1	1:E:247:ASN:HD21	1.85	0.42
1:F:75:ARG:HG3	1:F:240:LEU:HD11	2.01	0.42
1:F:101:SER:HB2	1:F:440:THR:HG21	2.01	0.42
1:F:451:LYS:HD2	1:F:451:LYS:HA	1.96	0.42
1:K:49:PHE:CG	1:K:50:ASP:N	2.87	0.42
1:L:106:ASN:ND2	1:L:109:ARG:HH11	2.18	0.42
1:O:70:ASP:HA	1:O:71:PRO:HD2	1.77	0.42
1:Q:210:GLU:H	1:Q:213:HIS:CD2	2.38	0.42
1:Q:355:ASN:HA	1:Q:356:PRO:HD3	1.81	0.42
1:U:3:ASP:C	1:U:5:VAL:N	2.78	0.42
1:B:184:PRO:O	1:B:189:ASP:HB2	2.19	0.42
1:H:179:LYS:H	1:H:179:LYS:HD3	1.83	0.42
1:J:91:VAL:HG23	1:J:103:ASP:OD2	2.20	0.42
1:J:231:LEU:HD23	1:J:231:LEU:C	2.45	0.42
1:K:92:HIS:CE1	1:K:99:PRO:HG3	2.55	0.42
1:L:241:TYR:O	1:L:245:ILE:HG12	2.20	0.42
1:M:214:HIS:HB3	1:N:33:ILE:CG2	2.49	0.42
1:O:300:HIS:HB3	1:O:386:GLY:O	2.20	0.42
1:R:75:ARG:HG3	1:R:240:LEU:HD11	2.00	0.42
1:X:342:ASN:HD22	1:X:401:LEU:HD12	1.85	0.42
1:B:70:ASP:HA	1:B:71:PRO:HD2	1.90	0.42
1:D:160:THR:CG2	1:D:176:VAL:HG13	2.50	0.42
1:G:390:LYS:HE3	1:G:390:LYS:HB2	1.94	0.42
1:J:19:VAL:HG13	1:J:89:PHE:CE1	2.55	0.42
1:J:213:HIS:HA	1:J:225:ASN:ND2	2.35	0.42
1:O:229:ASN:OD1	1:O:230:SER:N	2.52	0.42
1:Q:312:LEU:HD21	1:Q:378:ALA:C	2.45	0.42
1:Q:454:ASN:O	1:Q:458:PRO:HG2	2.20	0.42
1:C:316:THR:HG23	1:C:366:PRO:CA	2.50	0.42
1:G:309:ALA:HB3	1:G:310:PRO:HD3	2.01	0.42
1:I:395:ALA:HA	1:I:396:PRO:HD2	1.86	0.42
1:K:468:PHE:CZ	1:T:149:TYR:CE1	3.08	0.42
1:N:294:LEU:HD11	1:N:349:ILE:HG12	2.01	0.42
1:N:335:ASN:HD22	1:N:401:LEU:HD13	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:455:GLU:O	1:Q:456:ILE:C	2.62	0.42
1:R:230:SER:O	1:R:231:LEU:C	2.62	0.42
1:S:329:GLY:C	1:S:331:GLU:H	2.27	0.42
1:S:367:ASP:C	1:S:369:SER:H	2.27	0.42
1:B:74:ALA:HB1	1:B:85:LEU:HD11	2.01	0.42
1:B:194:LEU:HD22	1:B:198:MET:HE3	2.02	0.42
1:D:435:GLU:C	1:D:437:GLY:H	2.27	0.42
1:E:294:LEU:HD11	1:E:349:ILE:HG12	2.02	0.42
1:E:316:THR:HG23	1:E:366:PRO:HA	2.02	0.42
1:I:85:LEU:HD23	1:I:87:ILE:HD11	2.02	0.42
1:J:195:ARG:CZ	1:J:217:GLY:HA3	2.49	0.42
1:L:106:ASN:HD21	1:L:109:ARG:NH1	2.18	0.42
1:N:16:TYR:O	1:N:84:THR:HA	2.20	0.42
1:N:70:ASP:HB2	1:N:90:PHE:CE1	2.55	0.42
1:N:317:ASN:OD1	1:N:366:PRO:HA	2.19	0.42
1:P:78:PRO:HG2	1:P:79:PHE:CE2	2.55	0.42
1:Q:371:ASN:HA	1:Q:372:PRO:HD2	1.87	0.42
1:R:90:PHE:HB3	1:R:106:ASN:HD21	1.85	0.42
1:R:228:PHE:HB3	2:R:900:2K9:C16	2.49	0.42
1:T:106:ASN:HD22	1:T:106:ASN:HA	1.74	0.42
1:T:248:THR:O	1:T:252:ASN:ND2	2.53	0.42
1:U:19:VAL:HG13	1:U:89:PHE:CE1	2.55	0.42
1:U:115:LEU:HD23	1:U:384:LEU:HD21	2.00	0.42
1:V:106:ASN:HD21	1:V:109:ARG:NH1	2.17	0.42
1:W:189:ASP:OD2	1:X:30:HIS:HE1	2.03	0.42
1:C:231:LEU:C	1:C:231:LEU:HD23	2.45	0.41
1:D:249:ALA:CB	1:D:256:VAL:HG23	2.49	0.41
1:E:149:TYR:CE1	1:N:468:PHE:CZ	3.07	0.41
1:G:189:ASP:CG	1:G:195:ARG:HH12	2.28	0.41
1:K:464:HIS:CD2	1:K:465:PRO:HD2	2.55	0.41
1:L:184:PRO:O	1:L:189:ASP:HB2	2.19	0.41
1:N:129:GLU:O	1:N:271:MET:HA	2.20	0.41
1:Q:392:GLU:HA	1:Q:393:PRO:HD2	1.91	0.41
1:R:126:PHE:CE1	1:R:231:LEU:HD12	2.55	0.41
1:R:425:ARG:HG2	1:R:425:ARG:H	1.70	0.41
1:T:65:MET:HE3	1:T:67:LEU:HD11	2.02	0.41
1:A:18:ASP:HB3	1:A:86:ASN:ND2	2.28	0.41
1:B:19:VAL:O	1:B:30:HIS:HA	2.20	0.41
1:B:108:ALA:HA	1:B:377:SER:OG	2.20	0.41
1:H:134:ILE:HD13	1:H:194:LEU:HD13	2.00	0.41
1:I:464:HIS:CD2	1:I:465:PRO:HD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:452:ARG:O	1:J:457:GLU:HB2	2.19	0.41
1:L:173:GLY:O	1:L:174:TYR:HB2	2.20	0.41
1:L:226:TYR:OH	1:L:238:MET:HE2	2.20	0.41
1:O:462:ARG:HA	1:O:463:PRO:HD3	1.93	0.41
1:Q:313:LEU:HG	1:Q:317:ASN:HD22	1.85	0.41
1:Q:444:ILE:O	1:Q:448:ILE:HG13	2.20	0.41
1:V:230:SER:O	1:V:231:LEU:C	2.62	0.41
1:W:439:PHE:HB3	1:W:444:ILE:HD11	2.01	0.41
1:X:106:ASN:HD22	1:X:106:ASN:HA	1.73	0.41
1:C:19:VAL:HG13	1:C:89:PHE:CD1	2.55	0.41
1:D:274:HIS:C	1:D:275:GLN:HG3	2.44	0.41
1:D:327:VAL:CG2	1:D:328:PRO:HD2	2.50	0.41
1:E:231:LEU:HD23	1:E:231:LEU:C	2.45	0.41
1:G:16:TYR:HD2	1:G:34:PRO:HA	1.86	0.41
1:K:207:PHE:HE1	1:K:240:LEU:HD13	1.84	0.41
1:K:319:THR:HB	1:T:471:TYR:CE1	2.55	0.41
1:R:450:PHE:CB	1:R:451:LYS:HB2	2.38	0.41
1:B:336:LEU:HD12	1:B:413:PRO:HB2	2.03	0.41
1:B:365:SER:N	1:B:366:PRO:CD	2.83	0.41
1:D:119:GLY:O	1:D:279:LYS:NZ	2.47	0.41
1:H:455:GLU:O	1:H:458:PRO:HD2	2.20	0.41
1:N:128:ALA:HB3	1:N:238:MET:HE3	2.02	0.41
1:N:338:TYR:HA	1:N:347:VAL:O	2.21	0.41
1:Q:70:ASP:C	1:Q:70:ASP:OD1	2.64	0.41
1:S:405:PRO:HA	1:S:406:PRO:HD3	1.85	0.41
1:A:172:ARG:NH2	1:B:253:GLY:HA2	2.36	0.41
1:C:226:TYR:OH	1:C:238:MET:HE2	2.20	0.41
1:C:327:VAL:CG2	1:C:328:PRO:HD2	2.51	0.41
1:D:423:ILE:HG23	1:D:448:ILE:HG23	2.02	0.41
1:H:412:ILE:HA	1:H:413:PRO:HD3	1.93	0.41
1:J:19:VAL:O	1:J:30:HIS:HA	2.21	0.41
1:J:90:PHE:HB3	1:J:106:ASN:HD21	1.86	0.41
1:M:405:PRO:HA	1:M:406:PRO:HD3	1.87	0.41
1:O:129:GLU:HB3	1:O:223:GLU:OE2	2.20	0.41
1:R:352:THR:O	1:R:353:GLY:O	2.38	0.41
1:U:471:TYR:O	1:U:472:TYR:C	2.62	0.41
1:B:452:ARG:O	1:B:457:GLU:HB2	2.19	0.41
1:D:317:ASN:OD1	1:D:366:PRO:HA	2.20	0.41
1:E:77:ASP:HA	1:E:78:PRO:HD2	1.96	0.41
1:G:209:LEU:HB2	1:H:34:PRO:HG3	2.01	0.41
1:I:464:HIS:O	1:I:467:GLU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:380:LEU:HD13	1:L:384:LEU:CD1	2.50	0.41
1:L:425:ARG:NH2	1:L:425:ARG:HB3	2.35	0.41
1:M:47:LEU:O	1:M:66:LEU:HA	2.20	0.41
1:M:312:LEU:HD11	1:M:379:MET:HA	2.02	0.41
1:N:50:ASP:OD2	1:N:50:ASP:N	2.53	0.41
1:N:358:ALA:HA	2:N:900:2K9:C12	2.51	0.41
1:O:105:ARG:HG2	1:O:373:TYR:CE2	2.54	0.41
1:O:122:ASP:OD2	1:O:279:LYS:HA	2.19	0.41
1:Q:245:ILE:HG22	1:Q:256:VAL:HG11	2.02	0.41
1:X:328:PRO:HD3	1:X:417:THR:HG21	2.03	0.41
1:B:130:ALA:HB3	1:B:241:TYR:HE1	1.86	0.41
1:C:70:ASP:HA	1:C:71:PRO:HD2	1.76	0.41
1:K:211:LYS:HB2	1:K:211:LYS:HE3	1.79	0.41
1:L:210:GLU:HB3	1:L:211:LYS:H	1.58	0.41
1:U:121:ALA:HB1	1:U:278:TRP:O	2.19	0.41
1:V:434:THR:HA	1:V:439:PHE:O	2.20	0.41
1:A:67:LEU:HB3	1:A:89:PHE:CD2	2.56	0.41
1:H:24:LEU:HD21	1:H:443:LEU:HD11	2.03	0.41
1:L:185:VAL:CB	1:L:186:ALA:HB3	2.43	0.41
1:L:316:THR:HG22	1:L:317:ASN:ND2	2.36	0.41
1:M:19:VAL:O	1:M:30:HIS:HA	2.20	0.41
1:M:336:LEU:HD12	1:M:413:PRO:HB2	2.03	0.41
1:N:470:LEU:HB3	1:N:471:TYR:CE1	2.55	0.41
1:Q:462:ARG:HA	1:Q:463:PRO:HD3	1.96	0.41
1:R:409:ALA:C	1:R:411:SER:H	2.29	0.41
1:S:65:MET:HB2	1:S:91:VAL:HG13	2.03	0.41
1:T:210:GLU:HB3	1:T:211:LYS:H	1.64	0.41
1:U:210:GLU:H	1:U:213:HIS:HD2	1.69	0.41
1:W:93:ASP:HB3	1:W:96:THR:OG1	2.20	0.41
1:A:182:TYR:O	1:A:184:PRO:HD3	2.20	0.41
1:B:74:ALA:O	1:B:75:ARG:HD3	2.21	0.41
1:B:104:PRO:HA	1:B:107:ILE:HG12	2.02	0.41
1:B:291:TYR:C	1:B:293:GLY:N	2.79	0.41
1:C:140:PHE:CE1	1:P:469:ALA:HA	2.56	0.41
1:C:209:LEU:HB2	1:D:34:PRO:HG3	2.02	0.41
1:C:389:ASN:O	1:C:390:LYS:C	2.64	0.41
1:D:209:LEU:HB3	1:E:34:PRO:HG3	2.03	0.41
1:D:241:TYR:O	1:D:245:ILE:HG12	2.21	0.41
1:E:115:LEU:HD23	1:E:384:LEU:HD21	2.03	0.41
1:F:392:GLU:HA	1:F:393:PRO:HD3	1.94	0.41
1:G:302:ILE:HG13	1:G:361:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:371:ASN:HA	1:H:372:PRO:HD2	1.86	0.41
1:H:471:TYR:O	1:H:474:VAL:HG22	2.21	0.41
1:I:67:LEU:HB3	1:I:89:PHE:HD2	1.84	0.41
1:I:342:ASN:ND2	1:I:401:LEU:HD12	2.36	0.41
1:J:171:ASN:OD1	1:J:171:ASN:C	2.64	0.41
1:J:331:GLU:HB3	1:J:344:SER:HB3	2.02	0.41
1:M:96:THR:OG1	1:M:98:GLU:HB2	2.21	0.41
1:M:209:LEU:HB3	1:N:34:PRO:HG3	2.02	0.41
1:O:39:ASP:HB2	1:O:40:LYS:H	1.73	0.41
1:P:101:SER:O	1:P:107:ILE:HD11	2.20	0.41
1:P:188:ASN:O	1:P:190:GLN:N	2.54	0.41
1:U:172:ARG:HH21	1:V:253:GLY:HA2	1.85	0.41
1:U:405:PRO:HA	1:U:406:PRO:HD3	1.83	0.41
1:V:213:HIS:HA	1:V:225:ASN:HD21	1.86	0.41
1:V:464:HIS:CD2	1:V:466:TYR:H	2.21	0.41
1:X:106:ASN:ND2	1:X:109:ARG:HH11	2.18	0.41
1:X:286:TYR:HA	1:X:293:GLY:O	2.20	0.41
1:A:300:HIS:HB3	1:A:386:GLY:O	2.20	0.41
1:B:4:ASP:OD2	1:B:4:ASP:N	2.52	0.41
1:E:210:GLU:N	1:E:213:HIS:HD2	2.12	0.41
1:F:471:TYR:O	1:F:472:TYR:C	2.62	0.41
1:G:114:TYR:CD2	1:G:436:GLY:HA3	2.55	0.41
1:J:169:SER:HB2	1:J:170:PRO:HD2	2.02	0.41
1:K:10:LYS:HD2	1:K:10:LYS:HA	1.89	0.41
1:K:196:ASP:OD1	1:L:80:ARG:NH2	2.53	0.41
1:L:434:THR:HA	1:L:439:PHE:O	2.21	0.41
1:M:207:PHE:HE1	1:M:240:LEU:HD13	1.85	0.41
1:N:386:GLY:HA2	1:N:391:ILE:HD12	2.02	0.41
1:P:90:PHE:HB3	1:P:106:ASN:HD21	1.86	0.41
1:P:300:HIS:HB3	1:P:387:ILE:HA	2.03	0.41
1:U:7:LYS:HG2	1:U:11:ASP:OD2	2.20	0.41
1:X:330:TYR:O	1:X:331:GLU:HB2	2.21	0.41
1:X:355:ASN:HA	1:X:356:PRO:HD3	1.78	0.41
1:D:114:TYR:HA	1:D:117:SER:OG	2.21	0.40
1:D:173:GLY:O	1:D:174:TYR:HB2	2.21	0.40
1:G:425:ARG:NH2	1:G:425:ARG:HB3	2.36	0.40
1:L:98:GLU:HG2	1:L:99:PRO:HD2	2.04	0.40
1:T:274:HIS:HB3	1:T:360:ARG:CD	2.46	0.40
1:U:106:ASN:HD21	1:U:109:ARG:HH11	1.68	0.40
1:W:365:SER:N	1:W:366:PRO:CD	2.84	0.40
1:X:286:TYR:CE2	1:X:288:GLU:HG3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:316:THR:HG22	1:E:317:ASN:CG	2.47	0.40
1:E:330:TYR:O	1:E:331:GLU:HB2	2.20	0.40
1:H:327:VAL:HG21	1:W:461:ILE:HG22	2.02	0.40
1:L:0:LYS:HG2	1:L:72:GLU:OE1	2.22	0.40
1:N:209:LEU:CD1	1:N:213:HIS:HB3	2.51	0.40
1:R:312:LEU:O	1:R:316:THR:HB	2.22	0.40
1:S:209:LEU:HB3	1:T:34:PRO:HG3	2.03	0.40
1:S:277:LEU:C	1:S:278:TRP:HD1	2.29	0.40
1:V:171:ASN:OD1	1:V:171:ASN:C	2.64	0.40
1:W:286:TYR:CE2	1:W:288:GLU:HG2	2.56	0.40
1:B:302:ILE:HG13	1:B:361:LEU:HD22	2.04	0.40
1:E:313:LEU:HG	1:E:317:ASN:HD22	1.86	0.40
1:G:316:THR:HG22	1:G:317:ASN:CG	2.45	0.40
1:G:412:ILE:HA	1:G:413:PRO:HD3	1.91	0.40
1:I:376:PHE:N	1:I:376:PHE:CD2	2.89	0.40
1:Q:471:TYR:O	1:Q:472:TYR:C	2.61	0.40
1:R:371:ASN:HA	1:R:372:PRO:HD2	1.90	0.40
1:T:42:VAL:HG13	1:T:47:LEU:HD21	2.02	0.40
1:T:231:LEU:C	1:T:231:LEU:HD23	2.47	0.40
1:A:301:TYR:CE1	1:A:383:GLY:HA3	2.57	0.40
1:B:18:ASP:OD2	1:B:30:HIS:CD2	2.75	0.40
1:B:135:PHE:HB3	1:B:152:ASP:O	2.22	0.40
1:B:238:MET:HG2	1:B:372:PRO:HB3	2.04	0.40
1:C:45:ASP:O	1:C:66:LEU:HD11	2.21	0.40
1:D:12:GLU:OE2	1:D:83:LYS:NZ	2.55	0.40
1:F:149:TYR:CE1	1:M:146:GLY:HA2	2.57	0.40
1:G:130:ALA:HB3	1:G:241:TYR:CE1	2.56	0.40
1:G:196:ASP:OD1	1:H:80:ARG:NH2	2.55	0.40
1:G:196:ASP:OD2	1:H:80:ARG:HD3	2.21	0.40
1:L:297:THR:HG22	1:L:387:ILE:HD13	2.04	0.40
1:P:70:ASP:HB2	1:P:90:PHE:HE1	1.84	0.40
1:P:339:SER:OG	1:P:340:GLN:N	2.55	0.40
1:Q:274:HIS:CE1	1:Q:362:GLU:HB2	2.57	0.40
1:R:316:THR:HG23	1:R:366:PRO:HA	2.03	0.40
1:T:351:ILE:H	1:T:351:ILE:HG13	1.60	0.40
1:X:74:ALA:HA	1:X:86:ASN:O	2.21	0.40
1:X:447:TRP:O	1:X:448:ILE:C	2.65	0.40
1:A:138:VAL:HG11	1:R:472:TYR:CZ	2.56	0.40
1:F:157:TRP:CD1	1:F:157:TRP:H	2.39	0.40
1:I:73:THR:O	1:I:75:ARG:HG2	2.22	0.40
1:L:1:THR:HB	1:L:2:PRO:HD2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:-1:GLU:HG2	1:P:0:LYS:N	2.36	0.40
1:P:93:ASP:HA	1:P:94:PRO:HD2	1.95	0.40
1:P:302:ILE:HG12	1:P:361:LEU:HD22	2.00	0.40
1:Q:96:THR:C	1:Q:98:GLU:H	2.29	0.40
1:Q:210:GLU:H	1:Q:213:HIS:HD2	1.69	0.40
1:Q:350:PRO:HG2	1:Q:360:ARG:NH2	2.36	0.40
1:S:50:ASP:HB2	1:X:343:ARG:NH1	2.35	0.40
1:S:70:ASP:HA	1:S:71:PRO:HD2	1.82	0.40
1:T:68:LEU:HD23	1:T:92:HIS:CD2	2.57	0.40
1:W:365:SER:N	1:W:366:PRO:HD3	2.37	0.40
1:X:98:GLU:HA	1:X:99:PRO:HD3	1.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	462/478 (97%)	432 (94%)	25 (5%)	5 (1%)	11	39
1	B	460/478 (96%)	414 (90%)	40 (9%)	6 (1%)	9	35
1	C	456/478 (95%)	408 (90%)	44 (10%)	4 (1%)	14	43
1	D	462/478 (97%)	430 (93%)	30 (6%)	2 (0%)	30	60
1	E	459/478 (96%)	421 (92%)	32 (7%)	6 (1%)	9	35
1	F	463/478 (97%)	419 (90%)	38 (8%)	6 (1%)	9	35
1	G	462/478 (97%)	426 (92%)	28 (6%)	8 (2%)	7	30
1	H	460/478 (96%)	424 (92%)	30 (6%)	6 (1%)	9	35
1	I	456/478 (95%)	421 (92%)	30 (7%)	5 (1%)	11	39
1	J	462/478 (97%)	432 (94%)	26 (6%)	4 (1%)	14	43
1	K	459/478 (96%)	418 (91%)	34 (7%)	7 (2%)	8	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	463/478 (97%)	424 (92%)	29 (6%)	10 (2%)	5	26
1	M	462/478 (97%)	425 (92%)	32 (7%)	5 (1%)	11	39
1	N	460/478 (96%)	422 (92%)	34 (7%)	4 (1%)	14	43
1	O	456/478 (95%)	421 (92%)	29 (6%)	6 (1%)	9	35
1	P	462/478 (97%)	418 (90%)	35 (8%)	9 (2%)	6	28
1	Q	459/478 (96%)	420 (92%)	31 (7%)	8 (2%)	7	30
1	R	463/478 (97%)	422 (91%)	32 (7%)	9 (2%)	6	28
1	S	462/478 (97%)	424 (92%)	32 (7%)	6 (1%)	9	35
1	T	460/478 (96%)	420 (91%)	34 (7%)	6 (1%)	9	35
1	U	456/478 (95%)	425 (93%)	27 (6%)	4 (1%)	14	43
1	V	462/478 (97%)	429 (93%)	26 (6%)	7 (2%)	8	32
1	W	459/478 (96%)	426 (93%)	29 (6%)	4 (1%)	14	43
1	X	463/478 (97%)	428 (92%)	28 (6%)	7 (2%)	8	32
All	All	11048/11472 (96%)	10149 (92%)	755 (7%)	144 (1%)	9	35

All (144) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	211	LYS
1	C	330	TYR
1	D	-1	GLU
1	F	287	ASP
1	F	451	LYS
1	G	330	TYR
1	H	231	LEU
1	J	-1	GLU
1	K	1	THR
1	K	330	TYR
1	L	63	SER
1	L	211	LYS
1	L	353	GLY
1	L	451	LYS
1	O	405	PRO
1	P	189	ASP
1	P	231	LEU
1	Q	211	LYS
1	R	353	GLY

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Mol	Chain	Res	Type
1	R	451	LYS
1	S	231	LEU
1	S	330	TYR
1	T	330	TYR
1	V	-1	GLU
1	W	211	LYS
1	W	330	TYR
1	X	288	GLU
1	X	451	LYS
1	B	155	SER
1	B	428	ALA
1	F	211	LYS
1	F	330	TYR
1	G	63	SER
1	G	405	PRO
1	K	211	LYS
1	L	228	PHE
1	M	330	TYR
1	M	405	PRO
1	O	13	LYS
1	O	211	LYS
1	P	330	TYR
1	Q	231	LEU
1	Q	402	TYR
1	R	329	GLY
1	S	287	ASP
1	S	405	PRO
1	U	4	ASP
1	U	405	PRO
1	V	211	LYS
1	X	353	GLY
1	A	1	THR
1	B	292	ALA
1	C	4	ASP
1	C	331	GLU
1	E	1	THR
1	E	211	LYS
1	F	63	SER
1	F	405	PRO
1	H	141	ASP
1	H	292	ALA
1	H	329	GLY

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Mol	Chain	Res	Type
1	H	336	LEU
1	I	211	LYS
1	J	211	LYS
1	L	330	TYR
1	M	211	LYS
1	M	228	PHE
1	N	330	TYR
1	O	287	ASP
1	P	428	ALA
1	R	450	PHE
1	S	211	LYS
1	T	141	ASP
1	T	288	GLU
1	V	231	LEU
1	W	333	PRO
1	X	354	SER
1	A	231	LEU
1	A	330	TYR
1	E	231	LEU
1	G	368	SER
1	I	262	PRO
1	I	390	LYS
1	N	228	PHE
1	O	166	ALA
1	P	-1	GLU
1	P	211	LYS
1	P	438	VAL
1	Q	1	THR
1	Q	266	ASP
1	U	231	LEU
1	X	228	PHE
1	X	231	LEU
1	A	287	ASP
1	B	390	LYS
1	E	438	VAL
1	G	287	ASP
1	J	331	GLU
1	O	5	VAL
1	Q	330	TYR
1	Q	356	PRO
1	R	319	THR
1	R	333	PRO

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Mol	Chain	Res	Type
1	R	354	SER
1	S	1	THR
1	T	63	SER
1	G	1	THR
1	G	328	PRO
1	K	155	SER
1	K	328	PRO
1	L	331	GLU
1	N	428	ALA
1	Q	287	ASP
1	R	318	PRO
1	T	333	PRO
1	V	1	THR
1	V	201	ASN
1	V	438	VAL
1	E	456	ILE
1	I	333	PRO
1	K	329	GLY
1	P	1	THR
1	P	333	PRO
1	D	1	THR
1	H	333	PRO
1	J	333	PRO
1	L	333	PRO
1	N	333	PRO
1	T	329	GLY
1	U	406	PRO
1	W	329	GLY
1	C	438	VAL
1	G	262	PRO
1	M	438	VAL
1	V	318	PRO
1	B	406	PRO
1	E	329	GLY
1	K	438	VAL
1	L	186	ALA
1	L	351	ILE
1	X	438	VAL
1	B	329	GLY
1	I	406	PRO
1	R	405	PRO

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	394/405 (97%)	368 (93%)	26 (7%)	15	43
1	B	392/405 (97%)	351 (90%)	41 (10%)	6	25
1	C	388/405 (96%)	344 (89%)	44 (11%)	5	21
1	D	394/405 (97%)	360 (91%)	34 (9%)	10	33
1	E	392/405 (97%)	355 (91%)	37 (9%)	8	30
1	F	395/405 (98%)	352 (89%)	43 (11%)	6	23
1	G	394/405 (97%)	357 (91%)	37 (9%)	8	30
1	H	392/405 (97%)	353 (90%)	39 (10%)	7	27
1	I	388/405 (96%)	359 (92%)	29 (8%)	12	38
1	J	394/405 (97%)	356 (90%)	38 (10%)	8	29
1	K	392/405 (97%)	353 (90%)	39 (10%)	7	27
1	L	395/405 (98%)	356 (90%)	39 (10%)	7	27
1	M	394/405 (97%)	354 (90%)	40 (10%)	7	26
1	N	392/405 (97%)	352 (90%)	40 (10%)	7	26
1	O	388/405 (96%)	350 (90%)	38 (10%)	7	28
1	P	394/405 (97%)	359 (91%)	35 (9%)	9	32
1	Q	392/405 (97%)	350 (89%)	42 (11%)	6	24
1	R	395/405 (98%)	359 (91%)	36 (9%)	9	31
1	S	394/405 (97%)	362 (92%)	32 (8%)	11	36
1	T	392/405 (97%)	360 (92%)	32 (8%)	10	35
1	U	388/405 (96%)	352 (91%)	36 (9%)	8	30
1	V	394/405 (97%)	360 (91%)	34 (9%)	10	33
1	W	392/405 (97%)	353 (90%)	39 (10%)	7	27
1	X	395/405 (98%)	359 (91%)	36 (9%)	9	31
All	All	9420/9720 (97%)	8534 (91%)	886 (9%)	8	30

All (886) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	40	LYS
1	A	62	GLU
1	A	83	LYS
1	A	97	LEU
1	A	115	LEU
1	A	141	ASP
1	A	176	VAL
1	A	192	VAL
1	A	194	LEU
1	A	209	LEU
1	A	215	GLU
1	A	240	LEU
1	A	256	VAL
1	A	297	THR
1	A	312	LEU
1	A	316	THR
1	A	330	TYR
1	A	361	LEU
1	A	368	SER
1	A	380	LEU
1	A	418	GLN
1	A	425	ARG
1	A	433	LEU
1	A	442	ASP
1	A	470	LEU
1	B	4	ASP
1	B	8	LEU
1	B	24	LEU
1	B	42	VAL
1	B	47	LEU
1	B	62	GLU
1	B	63	SER
1	B	72	GLU
1	B	97	LEU
1	B	115	LEU
1	B	141	ASP
1	B	176	VAL
1	B	185	VAL
1	B	190	GLN
1	B	192	VAL
1	B	194	LEU
1	B	200	THR

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Mol	Chain	Res	Type
1	B	215	GLU
1	B	216	VAL
1	B	240	LEU
1	B	251	GLN
1	B	256	VAL
1	B	288	GLU
1	B	312	LEU
1	B	316	THR
1	B	351	ILE
1	B	360	ARG
1	B	361	LEU
1	B	368	SER
1	B	380	LEU
1	B	390	LYS
1	B	397	VAL
1	B	400	ASP
1	B	403	GLU
1	B	408	GLU
1	B	418	GLN
1	B	425	ARG
1	B	431	GLU
1	B	433	LEU
1	B	449	SER
1	B	470	LEU
1	C	4	ASP
1	C	8	LEU
1	C	24	LEU
1	C	40	LYS
1	C	64	ASP
1	C	93	ASP
1	C	115	LEU
1	C	139	SER
1	C	141	ASP
1	C	147	SER
1	C	148	PHE
1	C	176	VAL
1	C	177	ARG
1	C	182	TYR
1	C	192	VAL
1	C	194	LEU
1	C	209	LEU
1	C	210	GLU

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Mol	Chain	Res	Type
1	C	211	LYS
1	C	216	VAL
1	C	240	LEU
1	C	255	THR
1	C	256	VAL
1	C	267	ASN
1	C	297	THR
1	C	312	LEU
1	C	313	LEU
1	C	316	THR
1	C	330	TYR
1	C	334	ILE
1	C	342	ASN
1	C	343	ARG
1	C	360	ARG
1	C	368	SER
1	C	380	LEU
1	C	401	LEU
1	C	403	GLU
1	C	404	LEU
1	C	418	GLN
1	C	431	GLU
1	C	433	LEU
1	C	440	THR
1	C	442	ASP
1	C	470	LEU
1	D	-2	THR
1	D	-1	GLU
1	D	24	LEU
1	D	27	ILE
1	D	30	HIS
1	D	32	THR
1	D	83	LYS
1	D	115	LEU
1	D	117	SER
1	D	141	ASP
1	D	142	SER
1	D	147	SER
1	D	154	ILE
1	D	176	VAL
1	D	178	HIS
1	D	194	LEU

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Mol	Chain	Res	Type
1	D	205	SER
1	D	240	LEU
1	D	251	GLN
1	D	255	THR
1	D	284	LEU
1	D	296	ASP
1	D	297	THR
1	D	312	LEU
1	D	316	THR
1	D	360	ARG
1	D	361	LEU
1	D	368	SER
1	D	380	LEU
1	D	418	GLN
1	D	425	ARG
1	D	433	LEU
1	D	442	ASP
1	D	470	LEU
1	E	8	LEU
1	E	24	LEU
1	E	27	ILE
1	E	36	SER
1	E	45	ASP
1	E	64	ASP
1	E	65	MET
1	E	68	LEU
1	E	97	LEU
1	E	98	GLU
1	E	106	ASN
1	E	115	LEU
1	E	116	ILE
1	E	141	ASP
1	E	154	ILE
1	E	176	VAL
1	E	185	VAL
1	E	192	VAL
1	E	194	LEU
1	E	205	SER
1	E	240	LEU
1	E	267	ASN
1	E	285	MET
1	E	312	LEU

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Mol	Chain	Res	Type
1	E	316	THR
1	E	330	TYR
1	E	351	ILE
1	E	360	ARG
1	E	368	SER
1	E	380	LEU
1	E	407	GLU
1	E	418	GLN
1	E	429	ASP
1	E	433	LEU
1	E	442	ASP
1	E	443	LEU
1	E	470	LEU
1	F	-1	GLU
1	F	0	LYS
1	F	7	LYS
1	F	8	LEU
1	F	24	LEU
1	F	50	ASP
1	F	62	GLU
1	F	64	ASP
1	F	97	LEU
1	F	115	LEU
1	F	138	VAL
1	F	141	ASP
1	F	154	ILE
1	F	176	VAL
1	F	190	GLN
1	F	192	VAL
1	F	194	LEU
1	F	205	SER
1	F	209	LEU
1	F	210	GLU
1	F	232	LEU
1	F	240	LEU
1	F	255	THR
1	F	256	VAL
1	F	267	ASN
1	F	276	SER
1	F	285	MET
1	F	294	LEU
1	F	312	LEU

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Mol	Chain	Res	Type
1	F	316	THR
1	F	337	VAL
1	F	343	ARG
1	F	355	ASN
1	F	361	LEU
1	F	368	SER
1	F	390	LYS
1	F	400	ASP
1	F	403	GLU
1	F	418	GLN
1	F	433	LEU
1	F	442	ASP
1	F	446	THR
1	F	470	LEU
1	G	24	LEU
1	G	27	ILE
1	G	30	HIS
1	G	32	THR
1	G	39	ASP
1	G	40	LYS
1	G	41	SER
1	G	98	GLU
1	G	115	LEU
1	G	116	ILE
1	G	141	ASP
1	G	176	VAL
1	G	185	VAL
1	G	192	VAL
1	G	194	LEU
1	G	209	LEU
1	G	214	HIS
1	G	240	LEU
1	G	251	GLN
1	G	267	ASN
1	G	297	THR
1	G	310	PRO
1	G	312	LEU
1	G	316	THR
1	G	330	TYR
1	G	337	VAL
1	G	342	ASN
1	G	361	LEU

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Mol	Chain	Res	Type
1	G	368	SER
1	G	380	LEU
1	G	401	LEU
1	G	415	THR
1	G	429	ASP
1	G	431	GLU
1	G	433	LEU
1	G	442	ASP
1	G	444	ILE
1	H	8	LEU
1	H	11	ASP
1	H	13	LYS
1	H	24	LEU
1	H	32	THR
1	H	63	SER
1	H	83	LYS
1	H	85	LEU
1	H	115	LEU
1	H	141	ASP
1	H	147	SER
1	H	148	PHE
1	H	160	THR
1	H	176	VAL
1	H	179	LYS
1	H	190	GLN
1	H	192	VAL
1	H	194	LEU
1	H	209	LEU
1	H	240	LEU
1	H	255	THR
1	H	256	VAL
1	H	288	GLU
1	H	289	THR
1	H	312	LEU
1	H	316	THR
1	H	343	ARG
1	H	360	ARG
1	H	368	SER
1	H	380	LEU
1	H	401	LEU
1	H	404	LEU
1	H	418	GLN

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Mol	Chain	Res	Type
1	H	429	ASP
1	H	431	GLU
1	H	433	LEU
1	H	440	THR
1	H	442	ASP
1	H	470	LEU
1	I	4	ASP
1	I	8	LEU
1	I	14	VAL
1	I	27	ILE
1	I	50	ASP
1	I	72	GLU
1	I	115	LEU
1	I	141	ASP
1	I	176	VAL
1	I	192	VAL
1	I	194	LEU
1	I	209	LEU
1	I	240	LEU
1	I	267	ASN
1	I	284	LEU
1	I	312	LEU
1	I	316	THR
1	I	327	VAL
1	I	331	GLU
1	I	357	LYS
1	I	360	ARG
1	I	368	SER
1	I	380	LEU
1	I	389	ASN
1	I	418	GLN
1	I	433	LEU
1	I	440	THR
1	I	442	ASP
1	I	470	LEU
1	J	1	THR
1	J	8	LEU
1	J	10	LYS
1	J	14	VAL
1	J	24	LEU
1	J	27	ILE
1	J	30	HIS

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Mol	Chain	Res	Type
1	J	68	LEU
1	J	80	ARG
1	J	83	LYS
1	J	115	LEU
1	J	141	ASP
1	J	150	GLU
1	J	154	ILE
1	J	176	VAL
1	J	192	VAL
1	J	194	LEU
1	J	211	LYS
1	J	215	GLU
1	J	230	SER
1	J	240	LEU
1	J	255	THR
1	J	256	VAL
1	J	284	LEU
1	J	285	MET
1	J	312	LEU
1	J	316	THR
1	J	331	GLU
1	J	343	ARG
1	J	360	ARG
1	J	361	LEU
1	J	368	SER
1	J	380	LEU
1	J	425	ARG
1	J	429	ASP
1	J	433	LEU
1	J	442	ASP
1	J	470	LEU
1	K	1	THR
1	K	24	LEU
1	K	27	ILE
1	K	40	LYS
1	K	64	ASP
1	K	68	LEU
1	K	72	GLU
1	K	80	ARG
1	K	83	LYS
1	K	97	LEU
1	K	98	GLU

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Mol	Chain	Res	Type
1	K	103	ASP
1	K	106	ASN
1	K	115	LEU
1	K	138	VAL
1	K	141	ASP
1	K	175	LYS
1	K	179	LYS
1	K	192	VAL
1	K	194	LEU
1	K	208	ILE
1	K	209	LEU
1	K	216	VAL
1	K	240	LEU
1	K	255	THR
1	K	267	ASN
1	K	285	MET
1	K	288	GLU
1	K	312	LEU
1	K	316	THR
1	K	343	ARG
1	K	360	ARG
1	K	368	SER
1	K	380	LEU
1	K	418	GLN
1	K	429	ASP
1	K	431	GLU
1	K	433	LEU
1	K	470	LEU
1	L	8	LEU
1	L	10	LYS
1	L	14	VAL
1	L	24	LEU
1	L	27	ILE
1	L	40	LYS
1	L	50	ASP
1	L	62	GLU
1	L	64	ASP
1	L	83	LYS
1	L	97	LEU
1	L	115	LEU
1	L	138	VAL
1	L	141	ASP

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Mol	Chain	Res	Type
1	L	160	THR
1	L	176	VAL
1	L	192	VAL
1	L	194	LEU
1	L	209	LEU
1	L	211	LYS
1	L	232	LEU
1	L	240	LEU
1	L	256	VAL
1	L	284	LEU
1	L	297	THR
1	L	312	LEU
1	L	316	THR
1	L	330	TYR
1	L	351	ILE
1	L	354	SER
1	L	360	ARG
1	L	361	LEU
1	L	368	SER
1	L	390	LYS
1	L	414	GLN
1	L	431	GLU
1	L	433	LEU
1	L	442	ASP
1	L	470	LEU
1	M	24	LEU
1	M	30	HIS
1	M	32	THR
1	M	40	LYS
1	M	65	MET
1	M	80	ARG
1	M	98	GLU
1	M	115	LEU
1	M	117	SER
1	M	123	THR
1	M	139	SER
1	M	141	ASP
1	M	142	SER
1	M	154	ILE
1	M	176	VAL
1	M	178	HIS
1	M	192	VAL

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Mol	Chain	Res	Type
1	M	194	LEU
1	M	215	GLU
1	M	216	VAL
1	M	225	ASN
1	M	240	LEU
1	M	256	VAL
1	M	267	ASN
1	M	285	MET
1	M	312	LEU
1	M	316	THR
1	M	331	GLU
1	M	351	ILE
1	M	360	ARG
1	M	361	LEU
1	M	368	SER
1	M	389	ASN
1	M	400	ASP
1	M	418	GLN
1	M	423	ILE
1	M	429	ASP
1	M	431	GLU
1	M	433	LEU
1	M	470	LEU
1	N	8	LEU
1	N	24	LEU
1	N	27	ILE
1	N	30	HIS
1	N	50	ASP
1	N	62	GLU
1	N	80	ARG
1	N	115	LEU
1	N	141	ASP
1	N	142	SER
1	N	160	THR
1	N	176	VAL
1	N	190	GLN
1	N	192	VAL
1	N	194	LEU
1	N	205	SER
1	N	208	ILE
1	N	225	ASN
1	N	240	LEU

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Mol	Chain	Res	Type
1	N	255	THR
1	N	267	ASN
1	N	276	SER
1	N	296	ASP
1	N	312	LEU
1	N	316	THR
1	N	330	TYR
1	N	331	GLU
1	N	351	ILE
1	N	360	ARG
1	N	361	LEU
1	N	368	SER
1	N	380	LEU
1	N	403	GLU
1	N	418	GLN
1	N	425	ARG
1	N	431	GLU
1	N	433	LEU
1	N	444	ILE
1	N	449	SER
1	N	470	LEU
1	O	4	ASP
1	O	8	LEU
1	O	14	VAL
1	O	24	LEU
1	O	83	LYS
1	O	97	LEU
1	O	98	GLU
1	O	115	LEU
1	O	138	VAL
1	O	141	ASP
1	O	157	TRP
1	O	176	VAL
1	O	192	VAL
1	O	194	LEU
1	O	208	ILE
1	O	209	LEU
1	O	211	LYS
1	O	215	GLU
1	O	225	ASN
1	O	240	LEU
1	O	251	GLN

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Mol	Chain	Res	Type
1	O	255	THR
1	O	256	VAL
1	O	296	ASP
1	O	297	THR
1	O	312	LEU
1	O	330	TYR
1	O	331	GLU
1	O	360	ARG
1	O	361	LEU
1	O	368	SER
1	O	407	GLU
1	O	418	GLN
1	O	433	LEU
1	O	440	THR
1	O	457	GLU
1	O	470	LEU
1	O	473	ASP
1	P	-2	THR
1	P	-1	GLU
1	P	0	LYS
1	P	7	LYS
1	P	8	LEU
1	P	24	LEU
1	P	27	ILE
1	P	45	ASP
1	P	63	SER
1	P	64	ASP
1	P	68	LEU
1	P	83	LYS
1	P	95	PHE
1	P	141	ASP
1	P	176	VAL
1	P	177	ARG
1	P	183	PHE
1	P	185	VAL
1	P	192	VAL
1	P	194	LEU
1	P	205	SER
1	P	211	LYS
1	P	240	LEU
1	P	297	THR
1	P	312	LEU

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Mol	Chain	Res	Type
1	P	316	THR
1	P	342	ASN
1	P	368	SER
1	P	380	LEU
1	P	418	GLN
1	P	429	ASP
1	P	431	GLU
1	P	433	LEU
1	P	442	ASP
1	P	470	LEU
1	Q	8	LEU
1	Q	14	VAL
1	Q	24	LEU
1	Q	45	ASP
1	Q	50	ASP
1	Q	68	LEU
1	Q	83	LYS
1	Q	97	LEU
1	Q	115	LEU
1	Q	117	SER
1	Q	141	ASP
1	Q	142	SER
1	Q	154	ILE
1	Q	179	LYS
1	Q	183	PHE
1	Q	190	GLN
1	Q	192	VAL
1	Q	194	LEU
1	Q	227	GLN
1	Q	240	LEU
1	Q	251	GLN
1	Q	255	THR
1	Q	256	VAL
1	Q	266	ASP
1	Q	296	ASP
1	Q	297	THR
1	Q	312	LEU
1	Q	316	THR
1	Q	360	ARG
1	Q	361	LEU
1	Q	367	ASP
1	Q	368	SER

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Mol	Chain	Res	Type
1	Q	415	THR
1	Q	418	GLN
1	Q	422	VAL
1	Q	424	ASP
1	Q	425	ARG
1	Q	431	GLU
1	Q	433	LEU
1	Q	441	ASN
1	Q	442	ASP
1	Q	470	LEU
1	R	24	LEU
1	R	27	ILE
1	R	32	THR
1	R	61	HIS
1	R	62	GLU
1	R	68	LEU
1	R	97	LEU
1	R	115	LEU
1	R	141	ASP
1	R	154	ILE
1	R	160	THR
1	R	176	VAL
1	R	178	HIS
1	R	190	GLN
1	R	192	VAL
1	R	205	SER
1	R	240	LEU
1	R	256	VAL
1	R	284	LEU
1	R	312	LEU
1	R	316	THR
1	R	338	TYR
1	R	343	ARG
1	R	347	VAL
1	R	354	SER
1	R	360	ARG
1	R	361	LEU
1	R	368	SER
1	R	380	LEU
1	R	400	ASP
1	R	403	GLU
1	R	418	GLN

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Mol	Chain	Res	Type
1	R	420	SER
1	R	425	ARG
1	R	433	LEU
1	R	470	LEU
1	S	14	VAL
1	S	24	LEU
1	S	87	ILE
1	S	97	LEU
1	S	115	LEU
1	S	141	ASP
1	S	150	GLU
1	S	167	ASP
1	S	176	VAL
1	S	192	VAL
1	S	194	LEU
1	S	205	SER
1	S	240	LEU
1	S	256	VAL
1	S	267	ASN
1	S	296	ASP
1	S	312	LEU
1	S	316	THR
1	S	330	TYR
1	S	360	ARG
1	S	368	SER
1	S	380	LEU
1	S	400	ASP
1	S	402	TYR
1	S	403	GLU
1	S	417	THR
1	S	418	GLN
1	S	429	ASP
1	S	432	TYR
1	S	433	LEU
1	S	446	THR
1	S	470	LEU
1	T	8	LEU
1	T	14	VAL
1	T	24	LEU
1	T	27	ILE
1	T	115	LEU
1	T	123	THR

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Mol	Chain	Res	Type
1	T	138	VAL
1	T	141	ASP
1	T	160	THR
1	T	176	VAL
1	T	192	VAL
1	T	194	LEU
1	T	205	SER
1	T	240	LEU
1	T	284	LEU
1	T	297	THR
1	T	312	LEU
1	T	316	THR
1	T	343	ARG
1	T	351	ILE
1	T	361	LEU
1	T	368	SER
1	T	380	LEU
1	T	400	ASP
1	T	403	GLU
1	T	407	GLU
1	T	418	GLN
1	T	422	VAL
1	T	425	ARG
1	T	431	GLU
1	T	433	LEU
1	T	470	LEU
1	U	4	ASP
1	U	8	LEU
1	U	24	LEU
1	U	27	ILE
1	U	40	LYS
1	U	97	LEU
1	U	115	LEU
1	U	138	VAL
1	U	141	ASP
1	U	147	SER
1	U	154	ILE
1	U	176	VAL
1	U	192	VAL
1	U	194	LEU
1	U	209	LEU
1	U	211	LYS

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Mol	Chain	Res	Type
1	U	231	LEU
1	U	240	LEU
1	U	256	VAL
1	U	312	LEU
1	U	316	THR
1	U	331	GLU
1	U	343	ARG
1	U	351	ILE
1	U	361	LEU
1	U	368	SER
1	U	380	LEU
1	U	390	LYS
1	U	400	ASP
1	U	403	GLU
1	U	407	GLU
1	U	418	GLN
1	U	431	GLU
1	U	433	LEU
1	U	442	ASP
1	U	470	LEU
1	V	13	LYS
1	V	24	LEU
1	V	30	HIS
1	V	64	ASP
1	V	80	ARG
1	V	83	LYS
1	V	85	LEU
1	V	115	LEU
1	V	141	ASP
1	V	160	THR
1	V	176	VAL
1	V	182	TYR
1	V	190	GLN
1	V	192	VAL
1	V	194	LEU
1	V	205	SER
1	V	209	LEU
1	V	240	LEU
1	V	251	GLN
1	V	284	LEU
1	V	285	MET
1	V	296	ASP

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Mol	Chain	Res	Type
1	V	312	LEU
1	V	316	THR
1	V	330	TYR
1	V	360	ARG
1	V	368	SER
1	V	380	LEU
1	V	403	GLU
1	V	418	GLN
1	V	431	GLU
1	V	433	LEU
1	V	442	ASP
1	V	470	LEU
1	W	0	LYS
1	W	8	LEU
1	W	14	VAL
1	W	24	LEU
1	W	27	ILE
1	W	45	ASP
1	W	68	LEU
1	W	97	LEU
1	W	115	LEU
1	W	138	VAL
1	W	141	ASP
1	W	160	THR
1	W	192	VAL
1	W	194	LEU
1	W	210	GLU
1	W	240	LEU
1	W	255	THR
1	W	256	VAL
1	W	267	ASN
1	W	289	THR
1	W	297	THR
1	W	312	LEU
1	W	316	THR
1	W	330	TYR
1	W	342	ASN
1	W	351	ILE
1	W	357	LYS
1	W	361	LEU
1	W	368	SER
1	W	380	LEU

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Mol	Chain	Res	Type
1	W	389	ASN
1	W	398	ASP
1	W	401	LEU
1	W	418	GLN
1	W	425	ARG
1	W	431	GLU
1	W	433	LEU
1	W	449	SER
1	W	470	LEU
1	X	-1	GLU
1	X	14	VAL
1	X	24	LEU
1	X	62	GLU
1	X	64	ASP
1	X	65	MET
1	X	68	LEU
1	X	83	LYS
1	X	97	LEU
1	X	98	GLU
1	X	115	LEU
1	X	141	ASP
1	X	154	ILE
1	X	157	TRP
1	X	176	VAL
1	X	190	GLN
1	X	192	VAL
1	X	194	LEU
1	X	205	SER
1	X	240	LEU
1	X	256	VAL
1	X	267	ASN
1	X	312	LEU
1	X	316	THR
1	X	330	TYR
1	X	352	THR
1	X	360	ARG
1	X	361	LEU
1	X	368	SER
1	X	380	LEU
1	X	407	GLU
1	X	418	GLN
1	X	425	ARG

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Mol	Chain	Res	Type
1	X	433	LEU
1	X	444	ILE
1	X	470	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (371) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	A	86	ASN
1	A	106	ASN
1	A	113	ASN
1	A	178	HIS
1	A	190	GLN
1	A	213	HIS
1	A	221	GLN
1	A	225	ASN
1	A	247	ASN
1	A	267	ASN
1	A	275	GLN
1	A	418	GLN
1	A	464	HIS
1	B	30	HIS
1	B	106	ASN
1	B	113	ASN
1	B	178	HIS
1	B	213	HIS
1	B	221	GLN
1	B	225	ASN
1	B	267	ASN
1	B	275	GLN
1	B	317	ASN
1	B	335	ASN
1	B	342	ASN
1	B	464	HIS
1	C	30	HIS
1	C	86	ASN
1	C	92	HIS
1	C	106	ASN
1	C	113	ASN
1	C	190	GLN
1	C	213	HIS
1	C	221	GLN

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Mol	Chain	Res	Type
1	C	225	ASN
1	C	247	ASN
1	C	274	HIS
1	C	275	GLN
1	C	342	ASN
1	C	414	GLN
1	C	464	HIS
1	D	86	ASN
1	D	106	ASN
1	D	113	ASN
1	D	190	GLN
1	D	213	HIS
1	D	214	HIS
1	D	221	GLN
1	D	247	ASN
1	D	267	ASN
1	D	275	GLN
1	D	307	HIS
1	D	317	ASN
1	D	335	ASN
1	D	414	GLN
1	D	464	HIS
1	E	30	HIS
1	E	86	ASN
1	E	113	ASN
1	E	190	GLN
1	E	213	HIS
1	E	214	HIS
1	E	247	ASN
1	E	251	GLN
1	E	275	GLN
1	E	342	ASN
1	E	418	GLN
1	E	460	ASN
1	E	464	HIS
1	F	30	HIS
1	F	86	ASN
1	F	92	HIS
1	F	106	ASN
1	F	113	ASN
1	F	213	HIS
1	F	221	GLN

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Mol	Chain	Res	Type
1	F	267	ASN
1	F	317	ASN
1	F	342	ASN
1	F	389	ASN
1	F	418	GLN
1	F	464	HIS
1	G	30	HIS
1	G	86	ASN
1	G	106	ASN
1	G	113	ASN
1	G	178	HIS
1	G	213	HIS
1	G	221	GLN
1	G	247	ASN
1	G	267	ASN
1	G	275	GLN
1	G	342	ASN
1	G	394	GLN
1	G	414	GLN
1	G	418	GLN
1	G	441	ASN
1	G	464	HIS
1	H	30	HIS
1	H	86	ASN
1	H	92	HIS
1	H	106	ASN
1	H	113	ASN
1	H	190	GLN
1	H	201	ASN
1	H	213	HIS
1	H	214	HIS
1	H	221	GLN
1	H	227	GLN
1	H	247	ASN
1	H	251	GLN
1	H	267	ASN
1	H	275	GLN
1	H	317	ASN
1	H	342	ASN
1	H	414	GLN
1	H	418	GLN
1	H	441	ASN

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Mol	Chain	Res	Type
1	H	464	HIS
1	I	30	HIS
1	I	86	ASN
1	I	88	ASN
1	I	92	HIS
1	I	106	ASN
1	I	113	ASN
1	I	190	GLN
1	I	213	HIS
1	I	225	ASN
1	I	247	ASN
1	I	272	HIS
1	I	317	ASN
1	I	335	ASN
1	I	342	ASN
1	I	389	ASN
1	I	394	GLN
1	I	464	HIS
1	J	30	HIS
1	J	86	ASN
1	J	106	ASN
1	J	113	ASN
1	J	190	GLN
1	J	213	HIS
1	J	221	GLN
1	J	225	ASN
1	J	247	ASN
1	J	267	ASN
1	J	272	HIS
1	J	275	GLN
1	J	307	HIS
1	J	335	ASN
1	J	394	GLN
1	J	414	GLN
1	J	418	GLN
1	J	464	HIS
1	K	30	HIS
1	K	86	ASN
1	K	106	ASN
1	K	113	ASN
1	K	178	HIS
1	K	188	ASN

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Mol	Chain	Res	Type
1	K	190	GLN
1	K	213	HIS
1	K	225	ASN
1	K	247	ASN
1	K	252	ASN
1	K	272	HIS
1	K	300	HIS
1	K	307	HIS
1	K	342	ASN
1	K	418	GLN
1	K	464	HIS
1	L	30	HIS
1	L	106	ASN
1	L	113	ASN
1	L	178	HIS
1	L	221	GLN
1	L	247	ASN
1	L	267	ASN
1	L	275	GLN
1	L	335	ASN
1	L	430	HIS
1	L	441	ASN
1	L	460	ASN
1	L	464	HIS
1	M	30	HIS
1	M	86	ASN
1	M	106	ASN
1	M	113	ASN
1	M	178	HIS
1	M	190	GLN
1	M	213	HIS
1	M	221	GLN
1	M	225	ASN
1	M	227	GLN
1	M	247	ASN
1	M	267	ASN
1	M	275	GLN
1	M	340	GLN
1	M	342	ASN
1	M	371	ASN
1	M	389	ASN
1	M	394	GLN

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Mol	Chain	Res	Type
1	M	464	HIS
1	N	86	ASN
1	N	106	ASN
1	N	113	ASN
1	N	178	HIS
1	N	190	GLN
1	N	213	HIS
1	N	221	GLN
1	N	247	ASN
1	N	275	GLN
1	N	335	ASN
1	N	394	GLN
1	N	418	GLN
1	N	464	HIS
1	O	86	ASN
1	O	106	ASN
1	O	113	ASN
1	O	178	HIS
1	O	213	HIS
1	O	221	GLN
1	O	247	ASN
1	O	251	GLN
1	O	272	HIS
1	O	275	GLN
1	O	307	HIS
1	O	317	ASN
1	O	340	GLN
1	O	342	ASN
1	O	418	GLN
1	O	430	HIS
1	O	441	ASN
1	O	464	HIS
1	P	86	ASN
1	P	92	HIS
1	P	106	ASN
1	P	113	ASN
1	P	178	HIS
1	P	221	GLN
1	P	247	ASN
1	P	267	ASN
1	P	300	HIS
1	P	335	ASN

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Mol	Chain	Res	Type
1	P	340	GLN
1	P	464	HIS
1	Q	30	HIS
1	Q	92	HIS
1	Q	106	ASN
1	Q	113	ASN
1	Q	213	HIS
1	Q	221	GLN
1	Q	225	ASN
1	Q	233	HIS
1	Q	247	ASN
1	Q	335	ASN
1	Q	342	ASN
1	Q	418	GLN
1	Q	460	ASN
1	R	30	HIS
1	R	86	ASN
1	R	106	ASN
1	R	113	ASN
1	R	190	GLN
1	R	213	HIS
1	R	221	GLN
1	R	225	ASN
1	R	233	HIS
1	R	247	ASN
1	R	267	ASN
1	R	275	GLN
1	R	300	HIS
1	R	418	GLN
1	R	464	HIS
1	S	30	HIS
1	S	86	ASN
1	S	106	ASN
1	S	113	ASN
1	S	178	HIS
1	S	188	ASN
1	S	190	GLN
1	S	213	HIS
1	S	272	HIS
1	S	275	GLN
1	S	300	HIS
1	S	342	ASN

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Mol	Chain	Res	Type
1	S	418	GLN
1	S	464	HIS
1	T	30	HIS
1	T	86	ASN
1	T	92	HIS
1	T	106	ASN
1	T	113	ASN
1	T	188	ASN
1	T	213	HIS
1	T	214	HIS
1	T	221	GLN
1	T	225	ASN
1	T	233	HIS
1	T	247	ASN
1	T	267	ASN
1	T	275	GLN
1	T	317	ASN
1	T	342	ASN
1	T	418	GLN
1	T	430	HIS
1	T	464	HIS
1	U	30	HIS
1	U	86	ASN
1	U	106	ASN
1	U	113	ASN
1	U	190	GLN
1	U	213	HIS
1	U	214	HIS
1	U	221	GLN
1	U	225	ASN
1	U	275	GLN
1	U	307	HIS
1	U	418	GLN
1	U	460	ASN
1	U	464	HIS
1	V	29	GLN
1	V	30	HIS
1	V	86	ASN
1	V	92	HIS
1	V	106	ASN
1	V	113	ASN
1	V	178	HIS

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Mol	Chain	Res	Type
1	V	190	GLN
1	V	213	HIS
1	V	221	GLN
1	V	225	ASN
1	V	233	HIS
1	V	247	ASN
1	V	267	ASN
1	V	272	HIS
1	V	275	GLN
1	V	342	ASN
1	V	394	GLN
1	V	414	GLN
1	V	418	GLN
1	V	464	HIS
1	W	30	HIS
1	W	86	ASN
1	W	92	HIS
1	W	106	ASN
1	W	190	GLN
1	W	213	HIS
1	W	214	HIS
1	W	221	GLN
1	W	227	GLN
1	W	247	ASN
1	W	275	GLN
1	W	342	ASN
1	W	389	ASN
1	W	464	HIS
1	X	30	HIS
1	X	86	ASN
1	X	92	HIS
1	X	106	ASN
1	X	178	HIS
1	X	190	GLN
1	X	213	HIS
1	X	214	HIS
1	X	233	HIS
1	X	247	ASN
1	X	275	GLN
1	X	317	ASN
1	X	389	ASN
1	X	464	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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	2K9	D	900	-	25,27,27	2.02	6 (24%)	28,40,40	2.37	6 (21%)
2	2K9	P	900	-	25,27,27	1.98	5 (20%)	28,40,40	2.24	6 (21%)
2	2K9	V	900	-	25,27,27	1.89	5 (20%)	28,40,40	2.32	6 (21%)
2	2K9	B	900	-	25,27,27	2.04	5 (20%)	28,40,40	2.28	5 (17%)
2	2K9	G	900	-	25,27,27	2.00	5 (20%)	28,40,40	2.39	8 (28%)
2	2K9	H	900	-	25,27,27	2.06	5 (20%)	28,40,40	2.49	7 (25%)
2	2K9	M	900	-	25,27,27	1.92	5 (20%)	28,40,40	2.34	6 (21%)
2	2K9	Q	900	-	25,27,27	1.96	5 (20%)	28,40,40	2.19	5 (17%)
2	2K9	A	900	-	25,27,27	1.95	5 (20%)	28,40,40	2.38	6 (21%)
2	2K9	F	900	-	25,27,27	1.97	5 (20%)	28,40,40	2.37	9 (32%)
2	2K9	U	900	-	25,27,27	1.98	5 (20%)	28,40,40	2.39	7 (25%)
2	2K9	C	900	-	25,27,27	2.01	6 (24%)	28,40,40	2.40	8 (28%)
2	2K9	R	900	-	25,27,27	1.94	5 (20%)	28,40,40	2.32	6 (21%)
2	2K9	I	900	-	25,27,27	1.97	5 (20%)	28,40,40	2.42	7 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	2K9	E	900	-	25,27,27	1.99	5 (20%)	28,40,40	2.36	8 (28%)
2	2K9	O	900	-	25,27,27	1.96	5 (20%)	28,40,40	2.39	6 (21%)
2	2K9	K	900	-	25,27,27	1.93	5 (20%)	28,40,40	2.16	6 (21%)
2	2K9	J	900	-	25,27,27	1.98	5 (20%)	28,40,40	2.40	7 (25%)
2	2K9	S	900	-	25,27,27	1.89	5 (20%)	28,40,40	2.24	6 (21%)
2	2K9	W	900	-	25,27,27	1.97	5 (20%)	28,40,40	2.18	5 (17%)
2	2K9	X	900	-	25,27,27	1.95	5 (20%)	28,40,40	2.25	5 (17%)
2	2K9	T	900	-	25,27,27	1.93	5 (20%)	28,40,40	2.28	5 (17%)
2	2K9	N	900	-	25,27,27	2.03	5 (20%)	28,40,40	2.44	6 (21%)
2	2K9	L	900	-	25,27,27	1.98	5 (20%)	28,40,40	2.14	5 (17%)

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	2K9	D	900	-	-	0/4/12/12	0/5/5/5
2	2K9	P	900	-	-	0/4/12/12	0/5/5/5
2	2K9	V	900	-	-	0/4/12/12	0/5/5/5
2	2K9	B	900	-	-	2/4/12/12	0/5/5/5
2	2K9	G	900	-	-	0/4/12/12	0/5/5/5
2	2K9	H	900	-	-	1/4/12/12	0/5/5/5
2	2K9	M	900	-	-	0/4/12/12	0/5/5/5
2	2K9	Q	900	-	-	0/4/12/12	0/5/5/5
2	2K9	A	900	-	-	0/4/12/12	0/5/5/5
2	2K9	F	900	-	-	0/4/12/12	0/5/5/5
2	2K9	U	900	-	-	0/4/12/12	0/5/5/5
2	2K9	C	900	-	-	0/4/12/12	0/5/5/5
2	2K9	R	900	-	-	0/4/12/12	0/5/5/5
2	2K9	I	900	-	-	0/4/12/12	0/5/5/5
2	2K9	E	900	-	-	0/4/12/12	0/5/5/5
2	2K9	O	900	-	-	0/4/12/12	0/5/5/5
2	2K9	K	900	-	-	0/4/12/12	0/5/5/5
2	2K9	J	900	-	-	0/4/12/12	0/5/5/5
2	2K9	S	900	-	-	0/4/12/12	0/5/5/5
2	2K9	W	900	-	-	0/4/12/12	0/5/5/5
2	2K9	X	900	-	-	0/4/12/12	0/5/5/5
2	2K9	T	900	-	-	0/4/12/12	0/5/5/5
2	2K9	N	900	-	-	0/4/12/12	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2K9	L	900	-	-	0/4/12/12	0/5/5/5

All (122) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	900	2K9	C3-C1	5.56	1.48	1.37
2	C	900	2K9	C3-C1	5.46	1.47	1.37
2	W	900	2K9	C3-C1	5.37	1.47	1.37
2	Q	900	2K9	C3-C1	5.36	1.47	1.37
2	U	900	2K9	C3-C1	5.33	1.47	1.37
2	T	900	2K9	C3-C1	5.32	1.47	1.37
2	V	900	2K9	C3-C1	5.31	1.47	1.37
2	N	900	2K9	C3-C1	5.28	1.47	1.37
2	R	900	2K9	C3-C1	5.27	1.47	1.37
2	J	900	2K9	C3-C1	5.26	1.47	1.37
2	M	900	2K9	C3-C1	5.25	1.47	1.37
2	S	900	2K9	C3-C1	5.22	1.47	1.37
2	F	900	2K9	C3-C1	5.21	1.47	1.37
2	B	900	2K9	C3-C1	5.17	1.47	1.37
2	L	900	2K9	C3-C1	5.17	1.47	1.37
2	K	900	2K9	C3-C1	5.13	1.47	1.37
2	D	900	2K9	C3-C1	5.09	1.47	1.37
2	X	900	2K9	C3-C1	5.07	1.47	1.37
2	O	900	2K9	C3-C1	5.07	1.47	1.37
2	G	900	2K9	C3-C1	4.94	1.46	1.37
2	I	900	2K9	C3-C1	4.92	1.46	1.37
2	H	900	2K9	C5-N1	-4.91	1.33	1.39
2	E	900	2K9	C3-C1	4.90	1.46	1.37
2	B	900	2K9	C5-N1	-4.73	1.33	1.39
2	H	900	2K9	C3-C1	4.71	1.46	1.37
2	A	900	2K9	C5-N1	-4.67	1.33	1.39
2	N	900	2K9	C5-N1	-4.62	1.33	1.39
2	J	900	2K9	C5-N1	-4.61	1.33	1.39
2	D	900	2K9	C5-N1	-4.60	1.33	1.39
2	E	900	2K9	C5-N1	-4.59	1.33	1.39
2	A	900	2K9	C3-C1	4.58	1.46	1.37
2	G	900	2K9	C5-N1	-4.58	1.33	1.39
2	L	900	2K9	C5-N1	-4.55	1.33	1.39
2	X	900	2K9	C5-N1	-4.48	1.33	1.39
2	F	900	2K9	C5-N1	-4.48	1.33	1.39
2	Q	900	2K9	C5-N1	-4.41	1.33	1.39
2	W	900	2K9	C5-N1	-4.37	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	900	2K9	C5-N1	-4.31	1.33	1.39
2	T	900	2K9	C5-N1	-4.27	1.34	1.39
2	C	900	2K9	C4-C2	-4.23	1.37	1.45
2	R	900	2K9	C5-N1	-4.23	1.34	1.39
2	U	900	2K9	C5-N1	-4.23	1.34	1.39
2	I	900	2K9	C5-N1	-4.19	1.34	1.39
2	P	900	2K9	C5-N1	-4.17	1.34	1.39
2	K	900	2K9	C5-N1	-4.12	1.34	1.39
2	O	900	2K9	C4-C2	-4.09	1.37	1.45
2	C	900	2K9	C5-N1	-4.07	1.34	1.39
2	M	900	2K9	C5-N1	-4.03	1.34	1.39
2	H	900	2K9	C4-C2	-4.01	1.37	1.45
2	V	900	2K9	C5-N1	-4.00	1.34	1.39
2	S	900	2K9	C5-N1	-3.97	1.34	1.39
2	I	900	2K9	C4-C2	-3.95	1.37	1.45
2	E	900	2K9	C4-C2	-3.92	1.37	1.45
2	P	900	2K9	C4-C2	-3.89	1.37	1.45
2	U	900	2K9	C4-C2	-3.82	1.38	1.45
2	W	900	2K9	C6-N1	-3.80	1.33	1.39
2	J	900	2K9	C4-C2	-3.80	1.38	1.45
2	K	900	2K9	C6-N1	-3.79	1.33	1.39
2	N	900	2K9	C4-C2	-3.78	1.38	1.45
2	D	900	2K9	C4-C2	-3.73	1.38	1.45
2	G	900	2K9	C4-C2	-3.72	1.38	1.45
2	B	900	2K9	C4-C2	-3.70	1.38	1.45
2	B	900	2K9	C6-N1	-3.69	1.33	1.39
2	Q	900	2K9	C6-N1	-3.67	1.33	1.39
2	E	900	2K9	C6-N1	-3.66	1.33	1.39
2	X	900	2K9	C6-N1	-3.66	1.33	1.39
2	H	900	2K9	C1-N1	-3.64	1.34	1.39
2	L	900	2K9	C6-N1	-3.63	1.33	1.39
2	M	900	2K9	C4-C2	-3.62	1.38	1.45
2	R	900	2K9	C4-C2	-3.62	1.38	1.45
2	V	900	2K9	C4-C2	-3.61	1.38	1.45
2	U	900	2K9	C6-N1	-3.60	1.33	1.39
2	T	900	2K9	C4-C2	-3.59	1.38	1.45
2	I	900	2K9	C6-N1	-3.58	1.33	1.39
2	H	900	2K9	C6-N1	-3.57	1.33	1.39
2	S	900	2K9	C4-C2	-3.57	1.38	1.45
2	A	900	2K9	C4-C2	-3.56	1.38	1.45
2	N	900	2K9	C6-N1	-3.55	1.33	1.39
2	F	900	2K9	C6-N1	-3.54	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	900	2K9	C6-N1	-3.51	1.33	1.39
2	R	900	2K9	C6-N1	-3.51	1.33	1.39
2	W	900	2K9	C4-C2	-3.49	1.38	1.45
2	D	900	2K9	C6-N1	-3.45	1.33	1.39
2	C	900	2K9	C6-N1	-3.44	1.33	1.39
2	M	900	2K9	C6-N1	-3.40	1.33	1.39
2	P	900	2K9	C6-N1	-3.39	1.33	1.39
2	F	900	2K9	C1-N1	-3.32	1.34	1.39
2	L	900	2K9	C4-C2	-3.32	1.39	1.45
2	D	900	2K9	C1-N1	-3.26	1.34	1.39
2	A	900	2K9	C6-N1	-3.25	1.34	1.39
2	B	900	2K9	C1-N1	-3.25	1.34	1.39
2	X	900	2K9	C1-N1	-3.23	1.34	1.39
2	G	900	2K9	C1-N1	-3.22	1.34	1.39
2	I	900	2K9	C1-N1	-3.22	1.34	1.39
2	O	900	2K9	C6-N1	-3.21	1.34	1.39
2	Q	900	2K9	C4-C2	-3.19	1.39	1.45
2	J	900	2K9	C6-N1	-3.16	1.34	1.39
2	A	900	2K9	C1-N1	-3.16	1.34	1.39
2	T	900	2K9	C6-N1	-3.16	1.34	1.39
2	E	900	2K9	C1-N1	-3.14	1.34	1.39
2	S	900	2K9	C6-N1	-3.13	1.34	1.39
2	K	900	2K9	C4-C2	-3.09	1.39	1.45
2	F	900	2K9	C4-C2	-3.06	1.39	1.45
2	L	900	2K9	C1-N1	-3.03	1.34	1.39
2	X	900	2K9	C4-C2	-3.02	1.39	1.45
2	V	900	2K9	C6-N1	-3.02	1.34	1.39
2	R	900	2K9	C1-N1	-2.99	1.35	1.39
2	K	900	2K9	C1-N1	-2.94	1.35	1.39
2	N	900	2K9	C1-N1	-2.92	1.35	1.39
2	Q	900	2K9	C1-N1	-2.86	1.35	1.39
2	O	900	2K9	C1-N1	-2.78	1.35	1.39
2	W	900	2K9	C1-N1	-2.68	1.35	1.39
2	J	900	2K9	C1-N1	-2.67	1.35	1.39
2	U	900	2K9	C1-N1	-2.58	1.35	1.39
2	M	900	2K9	C1-N1	-2.57	1.35	1.39
2	T	900	2K9	C1-N1	-2.54	1.35	1.39
2	V	900	2K9	C1-N1	-2.49	1.35	1.39
2	S	900	2K9	C1-N1	-2.46	1.35	1.39
2	C	900	2K9	C1-N1	-2.40	1.35	1.39
2	P	900	2K9	C1-N1	-2.29	1.36	1.39
2	C	900	2K9	C9-N2	-2.20	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	900	2K9	C9-N2	-2.01	1.34	1.38

All (151) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	900	2K9	C7-C3-C1	-9.94	99.65	107.50
2	O	900	2K9	C7-C3-C1	-9.49	100.01	107.50
2	E	900	2K9	C7-C3-C1	-9.33	100.13	107.50
2	I	900	2K9	C7-C3-C1	-9.14	100.28	107.50
2	A	900	2K9	C7-C3-C1	-9.10	100.31	107.50
2	M	900	2K9	C7-C3-C1	-9.09	100.32	107.50
2	G	900	2K9	C7-C3-C1	-9.09	100.32	107.50
2	U	900	2K9	C7-C3-C1	-9.07	100.34	107.50
2	B	900	2K9	C7-C3-C1	-9.01	100.39	107.50
2	J	900	2K9	C7-C3-C1	-9.00	100.39	107.50
2	R	900	2K9	C7-C3-C1	-8.99	100.40	107.50
2	N	900	2K9	C7-C3-C1	-8.88	100.49	107.50
2	D	900	2K9	C7-C3-C1	-8.87	100.50	107.50
2	F	900	2K9	C7-C3-C1	-8.73	100.61	107.50
2	V	900	2K9	C7-C3-C1	-8.57	100.73	107.50
2	T	900	2K9	C7-C3-C1	-8.57	100.73	107.50
2	X	900	2K9	C7-C3-C1	-8.54	100.76	107.50
2	S	900	2K9	C7-C3-C1	-8.48	100.80	107.50
2	P	900	2K9	C7-C3-C1	-8.47	100.81	107.50
2	C	900	2K9	C7-C3-C1	-8.44	100.83	107.50
2	K	900	2K9	C7-C3-C1	-8.44	100.84	107.50
2	Q	900	2K9	C7-C3-C1	-8.41	100.86	107.50
2	L	900	2K9	C7-C3-C1	-8.31	100.94	107.50
2	W	900	2K9	C7-C3-C1	-8.24	101.00	107.50
2	N	900	2K9	C10-N3-C5	4.63	109.66	105.08
2	V	900	2K9	C10-N3-C5	4.33	109.36	105.08
2	T	900	2K9	C10-N3-C5	4.14	109.17	105.08
2	X	900	2K9	C10-N3-C5	4.11	109.14	105.08
2	N	900	2K9	N1-C5-N3	-4.05	103.67	111.83
2	H	900	2K9	C10-N3-C5	4.02	109.05	105.08
2	X	900	2K9	N1-C5-N3	-3.99	103.80	111.83
2	M	900	2K9	C10-N3-C5	3.97	109.01	105.08
2	V	900	2K9	N1-C5-N3	-3.97	103.84	111.83
2	P	900	2K9	C10-N3-C5	3.96	109.00	105.08
2	A	900	2K9	C10-N3-C5	3.90	108.94	105.08
2	R	900	2K9	N1-C5-N3	-3.80	104.17	111.83
2	I	900	2K9	N1-C5-N3	-3.78	104.22	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	900	2K9	N1-C5-N3	-3.77	104.25	111.83
2	M	900	2K9	N1-C5-N3	-3.76	104.26	111.83
2	G	900	2K9	N1-C5-N3	-3.76	104.26	111.83
2	J	900	2K9	C10-N3-C5	3.74	108.78	105.08
2	H	900	2K9	N1-C5-N3	-3.71	104.35	111.83
2	G	900	2K9	C10-N3-C5	3.70	108.74	105.08
2	R	900	2K9	C10-N3-C5	3.69	108.73	105.08
2	A	900	2K9	N1-C5-N3	-3.66	104.45	111.83
2	E	900	2K9	N1-C5-N3	-3.66	104.46	111.83
2	I	900	2K9	C10-N3-C5	3.65	108.69	105.08
2	U	900	2K9	N1-C5-N3	-3.64	104.49	111.83
2	B	900	2K9	N1-C5-N3	-3.63	104.53	111.83
2	S	900	2K9	C10-N3-C5	3.62	108.66	105.08
2	S	900	2K9	N1-C5-N3	-3.62	104.55	111.83
2	U	900	2K9	C10-N3-C5	3.61	108.65	105.08
2	B	900	2K9	C10-N3-C5	3.61	108.65	105.08
2	C	900	2K9	C8-C4-C2	-3.58	126.66	133.76
2	P	900	2K9	N1-C5-N3	-3.58	104.62	111.83
2	C	900	2K9	C5-C9-N2	3.56	121.19	116.94
2	F	900	2K9	N1-C5-N3	-3.55	104.68	111.83
2	E	900	2K9	C10-N3-C5	3.49	108.53	105.08
2	W	900	2K9	N1-C5-N3	-3.47	104.85	111.83
2	Q	900	2K9	N1-C5-N3	-3.43	104.93	111.83
2	O	900	2K9	C10-N3-C5	3.39	108.44	105.08
2	D	900	2K9	N1-C5-N3	-3.38	105.03	111.83
2	J	900	2K9	N1-C5-N3	-3.37	105.04	111.83
2	W	900	2K9	C10-N3-C5	3.36	108.41	105.08
2	Q	900	2K9	C10-N3-C5	3.34	108.39	105.08
2	J	900	2K9	C5-C9-N2	3.33	120.91	116.94
2	C	900	2K9	C16-C13-C11	-3.32	115.40	120.91
2	D	900	2K9	C16-C13-C11	-3.31	115.42	120.91
2	N	900	2K9	C8-C4-C2	-3.31	127.21	133.76
2	D	900	2K9	C10-N3-C5	3.27	108.32	105.08
2	O	900	2K9	N1-C5-N3	-3.27	105.25	111.83
2	F	900	2K9	C10-N3-C5	3.26	108.31	105.08
2	L	900	2K9	N1-C5-N3	-3.22	105.35	111.83
2	K	900	2K9	N1-C5-N3	-3.20	105.39	111.83
2	O	900	2K9	C8-C4-C2	-3.19	127.45	133.76
2	U	900	2K9	C8-C4-C2	-3.17	127.47	133.76
2	D	900	2K9	C5-C9-N2	3.15	120.69	116.94
2	C	900	2K9	N1-C5-N3	-3.13	105.52	111.83
2	T	900	2K9	C5-C9-N2	3.11	120.65	116.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	900	2K9	C10-N3-C5	3.08	108.13	105.08
2	A	900	2K9	C5-C9-N2	3.08	120.61	116.94
2	H	900	2K9	C5-C9-N2	3.03	120.56	116.94
2	G	900	2K9	C8-C4-C2	-3.00	127.83	133.76
2	I	900	2K9	C5-C9-N2	2.98	120.50	116.94
2	P	900	2K9	C8-C4-C2	-2.96	127.89	133.76
2	J	900	2K9	C16-C13-C11	-2.96	116.00	120.91
2	R	900	2K9	C8-C4-C2	-2.94	127.94	133.76
2	B	900	2K9	C5-C9-N2	2.91	120.41	116.94
2	I	900	2K9	C8-C4-C2	-2.91	128.01	133.76
2	V	900	2K9	C8-C4-C2	-2.90	128.01	133.76
2	W	900	2K9	C8-C4-C2	-2.90	128.02	133.76
2	O	900	2K9	C5-C9-N2	2.85	120.34	116.94
2	K	900	2K9	C10-N3-C5	2.84	107.89	105.08
2	C	900	2K9	C10-N3-C5	2.84	107.89	105.08
2	S	900	2K9	C5-C9-N2	2.80	120.28	116.94
2	F	900	2K9	C8-C4-C2	-2.80	128.22	133.76
2	D	900	2K9	C8-C4-C2	-2.79	128.24	133.76
2	M	900	2K9	C8-C4-C2	-2.79	128.24	133.76
2	T	900	2K9	C8-C4-C2	-2.78	128.26	133.76
2	B	900	2K9	C8-C4-C2	-2.75	128.32	133.76
2	P	900	2K9	C5-C9-N2	2.74	120.21	116.94
2	E	900	2K9	C8-C4-C2	-2.71	128.40	133.76
2	J	900	2K9	C8-C4-C2	-2.70	128.41	133.76
2	Q	900	2K9	C8-C4-C2	-2.65	128.51	133.76
2	U	900	2K9	C5-C9-N2	2.65	120.10	116.94
2	S	900	2K9	C8-C4-C2	-2.65	128.52	133.76
2	E	900	2K9	C5-C9-N2	2.65	120.10	116.94
2	N	900	2K9	C5-C9-N2	2.65	120.10	116.94
2	L	900	2K9	C5-C9-N2	2.64	120.09	116.94
2	F	900	2K9	C15-C13-C11	2.62	125.25	120.91
2	W	900	2K9	C5-C9-N2	2.62	120.07	116.94
2	H	900	2K9	C8-C4-C2	-2.62	128.57	133.76
2	F	900	2K9	C16-C13-C11	-2.60	116.60	120.91
2	G	900	2K9	C5-C9-N2	2.58	120.02	116.94
2	I	900	2K9	C16-C13-C11	-2.56	116.66	120.91
2	C	900	2K9	C8-C4-C7	2.53	123.65	120.10
2	K	900	2K9	C16-C13-C11	-2.52	116.73	120.91
2	L	900	2K9	C8-C4-C2	-2.50	128.81	133.76
2	K	900	2K9	C5-C9-N2	2.50	119.92	116.94
2	O	900	2K9	C8-C4-C7	2.49	123.59	120.10
2	V	900	2K9	C5-C9-N2	2.48	119.90	116.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	900	2K9	C8-C4-C7	2.46	123.56	120.10
2	F	900	2K9	C10-C6-N1	-2.46	102.36	105.02
2	X	900	2K9	C8-C4-C2	-2.46	128.89	133.76
2	K	900	2K9	C8-C4-C2	-2.44	128.93	133.76
2	Q	900	2K9	C5-C9-N2	2.42	119.83	116.94
2	R	900	2K9	C5-C9-N2	2.34	119.74	116.94
2	N	900	2K9	C8-C4-C7	2.33	123.37	120.10
2	A	900	2K9	C8-C4-C2	-2.32	129.16	133.76
2	R	900	2K9	C10-C6-N1	-2.31	102.53	105.02
2	M	900	2K9	C5-C9-N2	2.28	119.66	116.94
2	G	900	2K9	C8-C4-C7	2.23	123.23	120.10
2	H	900	2K9	C8-C4-C7	2.23	123.23	120.10
2	A	900	2K9	C11-C7-C3	-2.23	125.59	133.48
2	C	900	2K9	C7-C11-C13	2.22	124.83	122.10
2	V	900	2K9	C8-C4-C7	2.20	123.18	120.10
2	M	900	2K9	C16-C13-C11	-2.17	117.32	120.91
2	S	900	2K9	C16-C13-C11	-2.15	117.34	120.91
2	F	900	2K9	C5-C9-N2	2.12	119.47	116.94
2	U	900	2K9	C16-C13-C11	-2.11	117.42	120.91
2	G	900	2K9	C10-C6-N1	-2.09	102.76	105.02
2	G	900	2K9	C11-C7-C3	-2.09	126.09	133.48
2	E	900	2K9	C10-C6-N1	-2.08	102.77	105.02
2	P	900	2K9	C8-C4-C7	2.07	123.01	120.10
2	J	900	2K9	C17-C15-C13	-2.05	118.20	120.54
2	I	900	2K9	C10-C6-N1	-2.04	102.82	105.02
2	E	900	2K9	C8-C4-C7	2.04	122.96	120.10
2	E	900	2K9	C11-C7-C3	-2.03	126.31	133.48
2	F	900	2K9	C6-N1-C1	-2.02	125.19	129.72
2	X	900	2K9	C5-C9-N2	2.01	119.34	116.94
2	H	900	2K9	C11-C7-C3	-2.00	126.39	133.48

There are no chirality outliers.

All (3) torsion outliers are listed below:

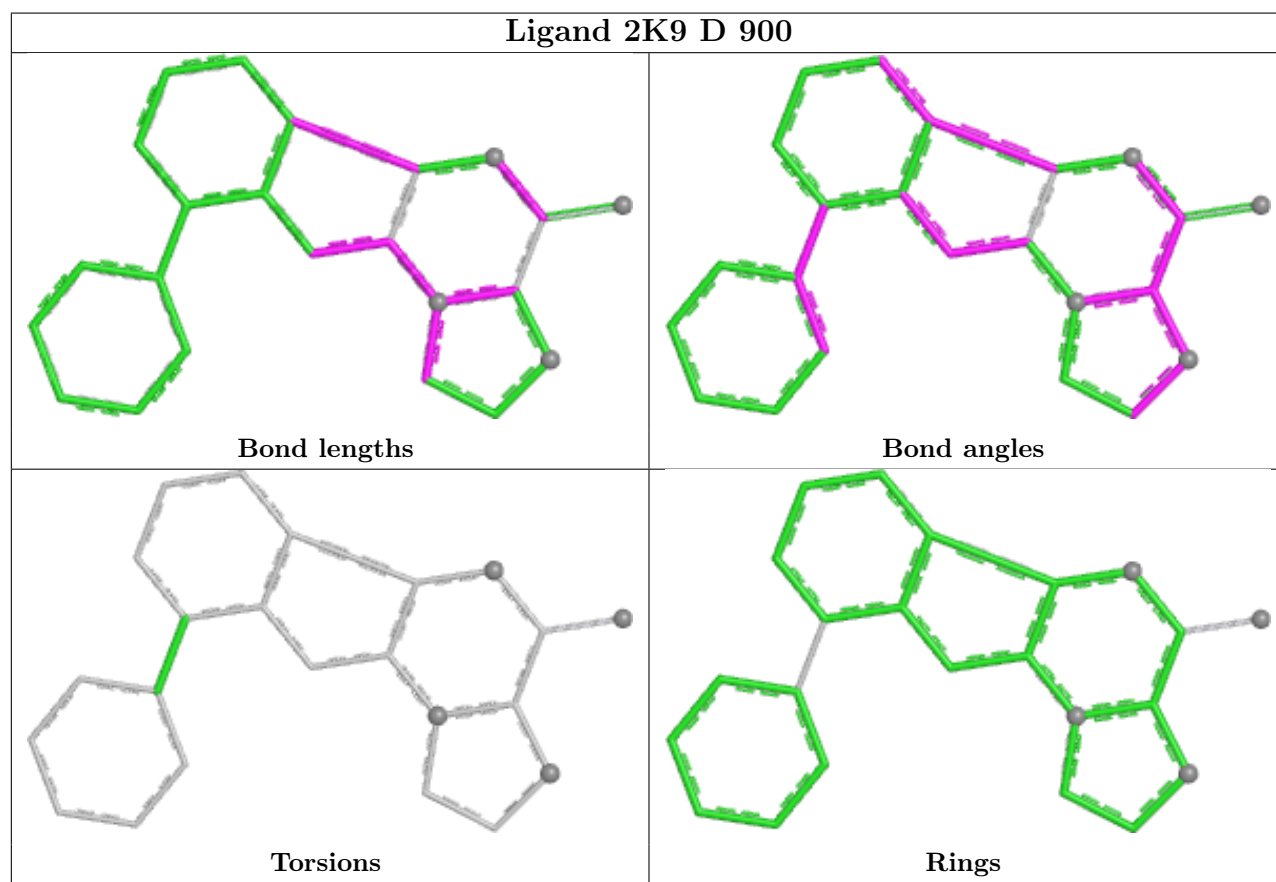
Mol	Chain	Res	Type	Atoms
2	B	900	2K9	C7-C11-C13-C16
2	H	900	2K9	C7-C11-C13-C16
2	B	900	2K9	C7-C11-C13-C15

There are no ring outliers.

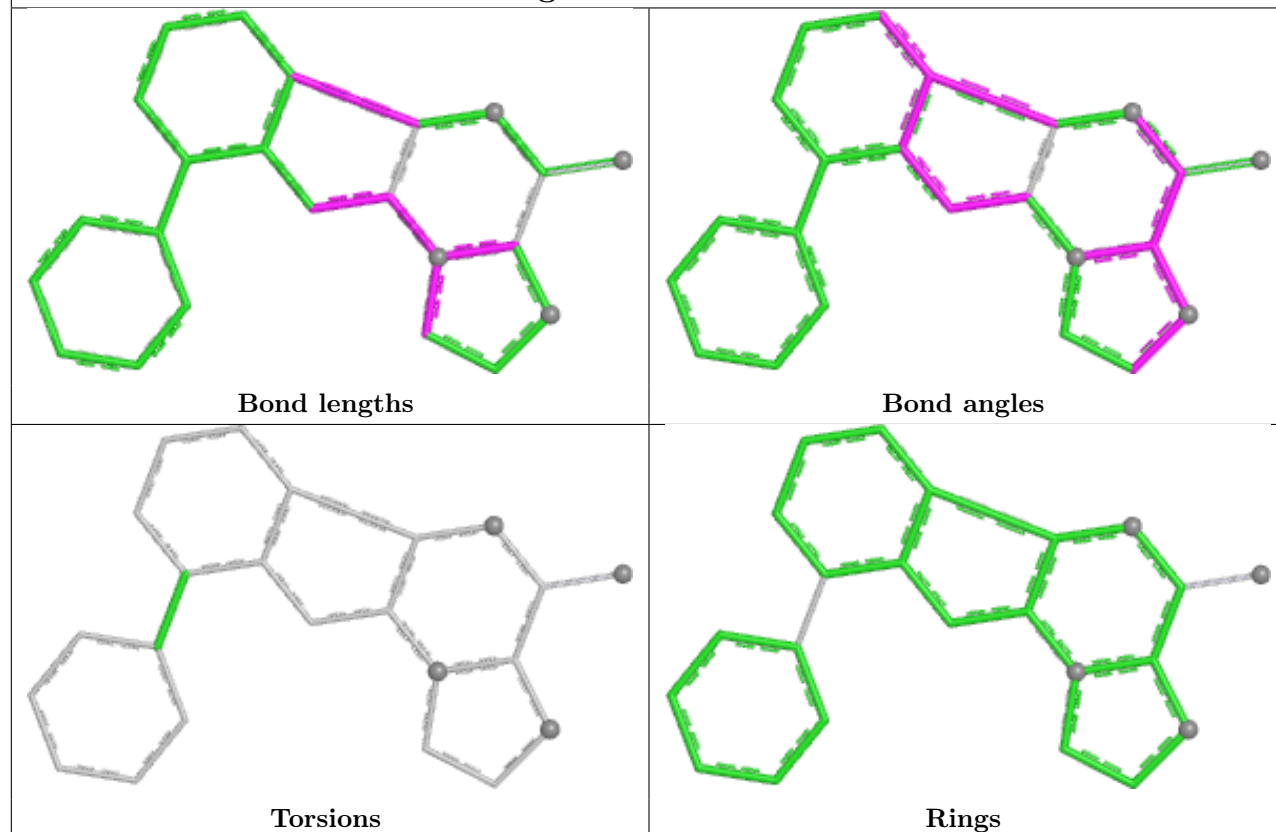
6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	900	2K9	1	0
2	B	900	2K9	1	0
2	M	900	2K9	2	0
2	F	900	2K9	2	0
2	R	900	2K9	1	0
2	N	900	2K9	1	0

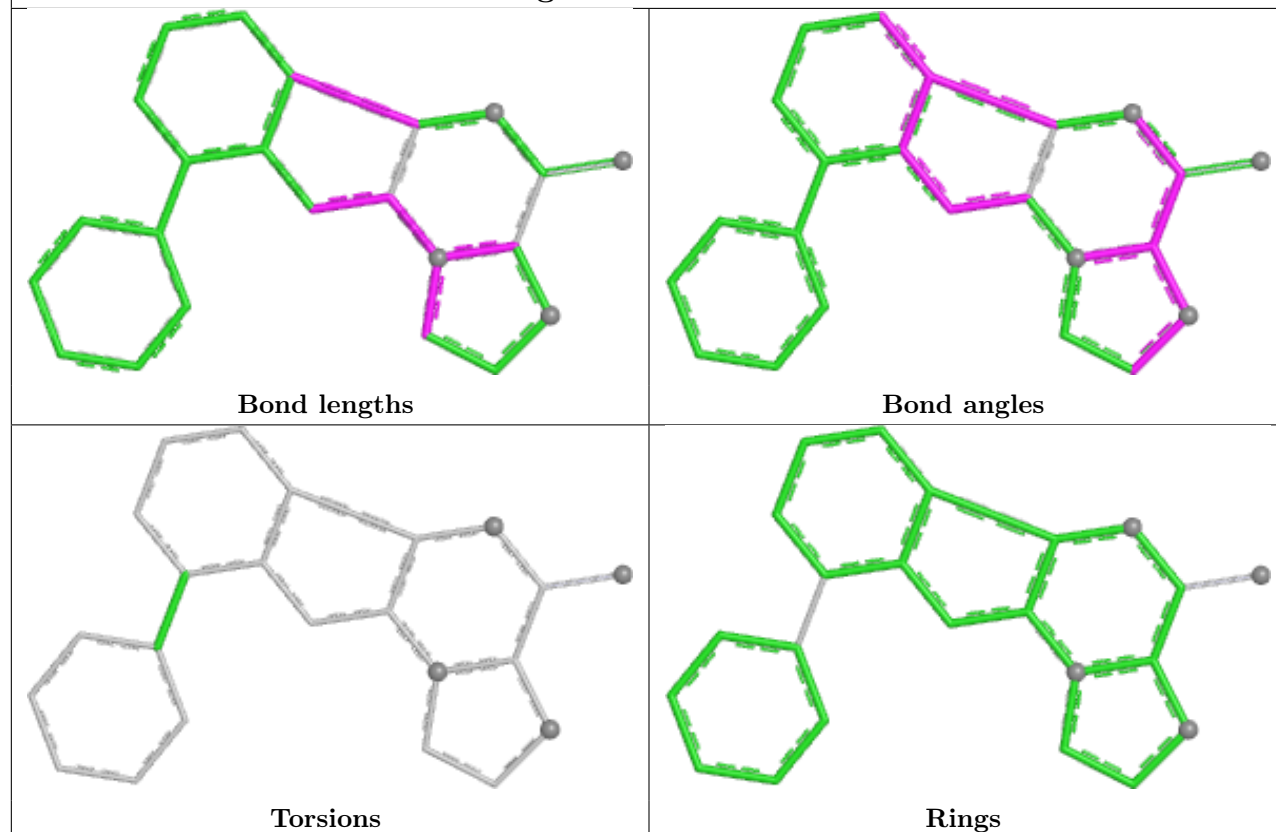
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



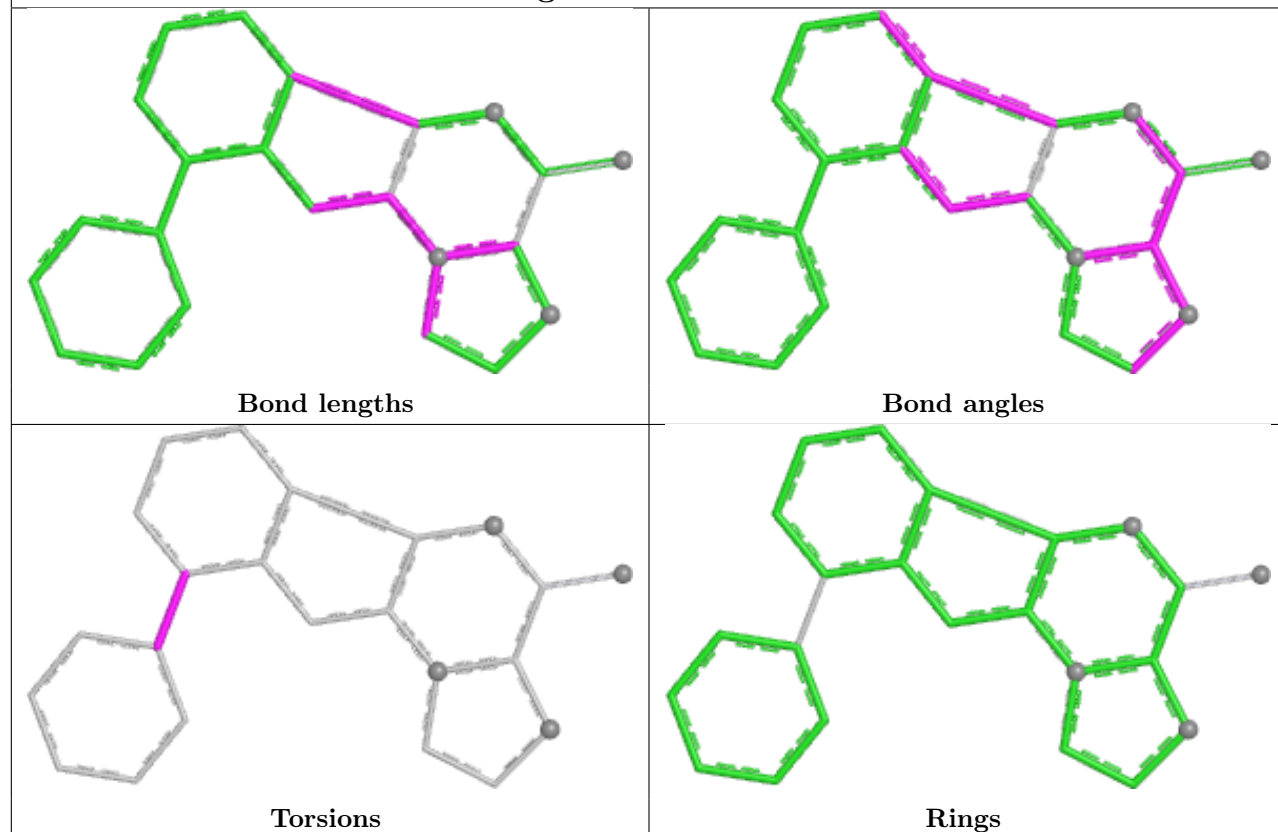
Ligand 2K9 P 900



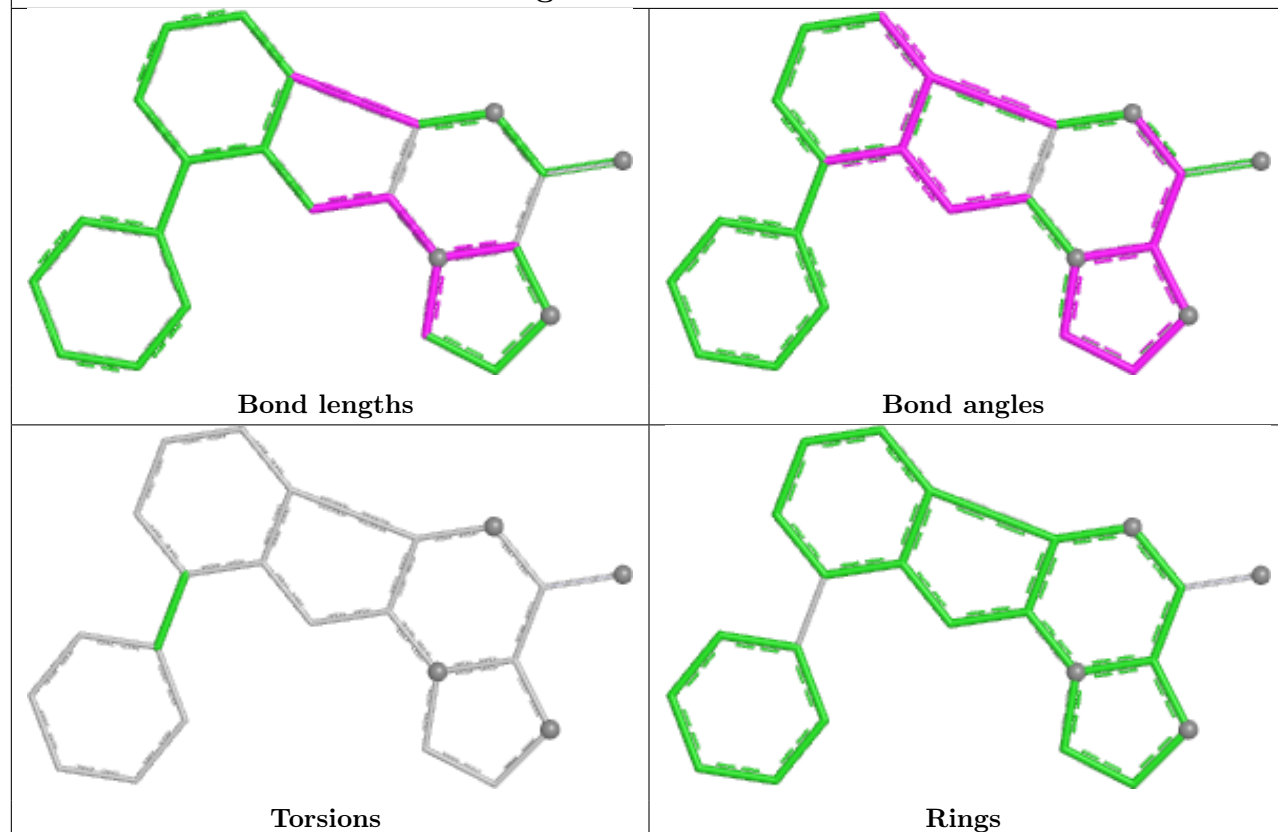
Ligand 2K9 V 900



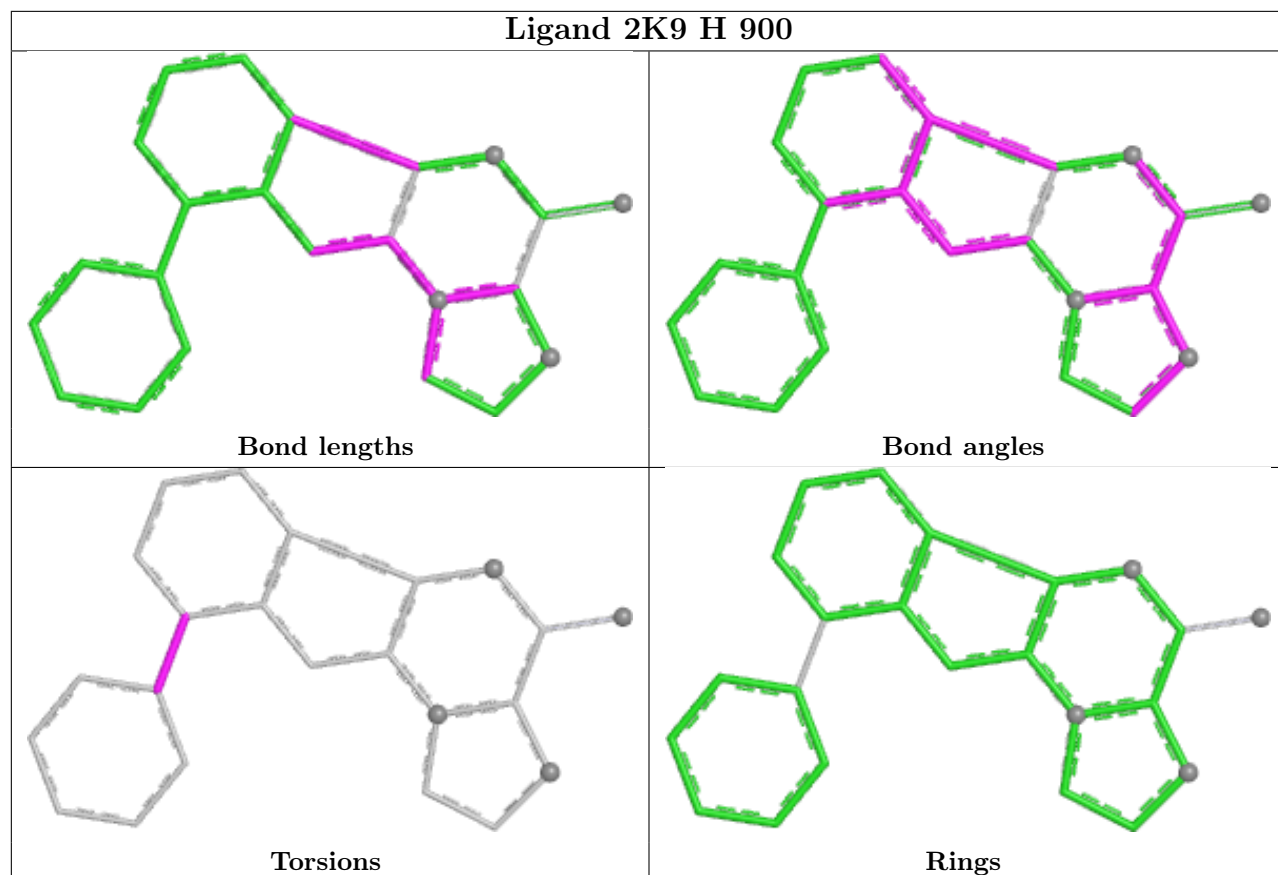
Ligand 2K9 B 900



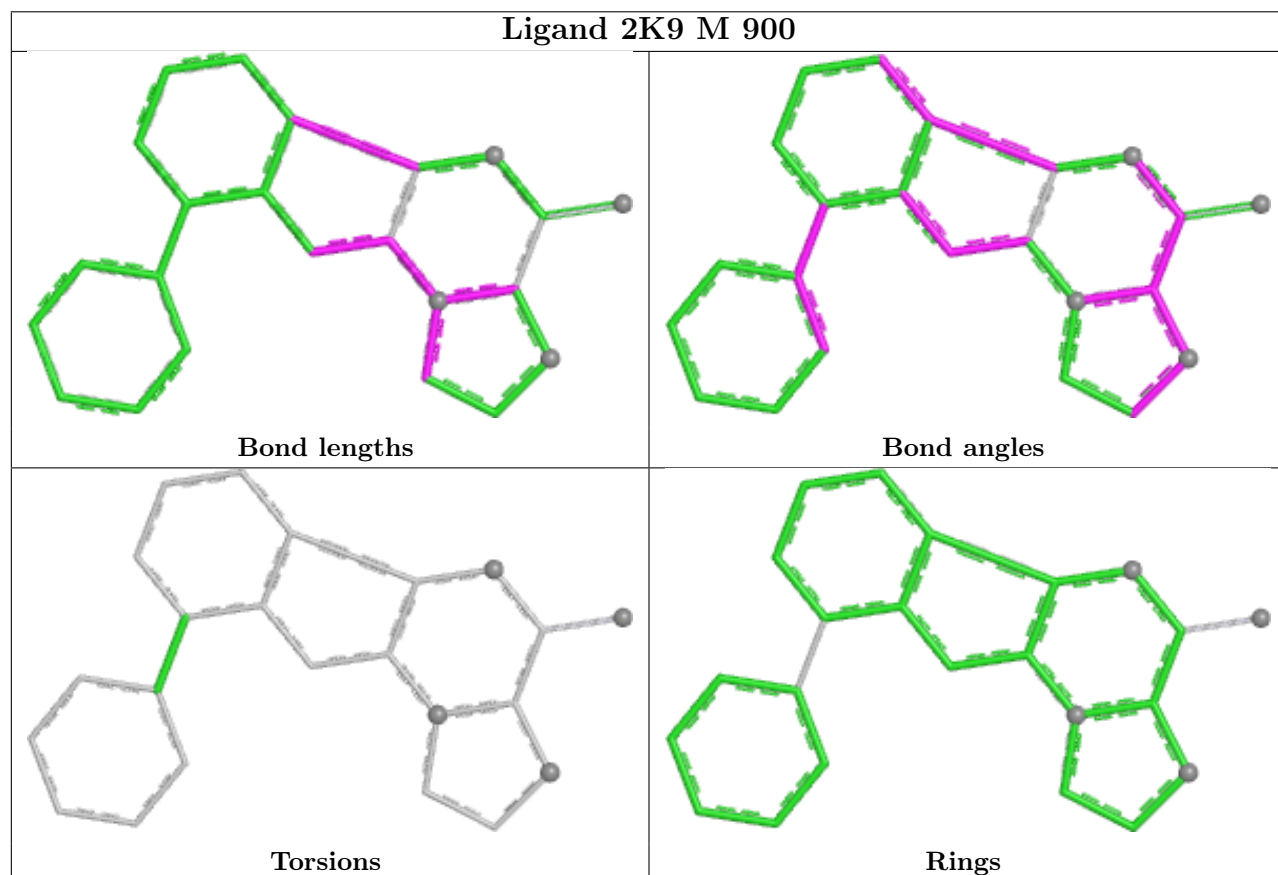
Ligand 2K9 G 900



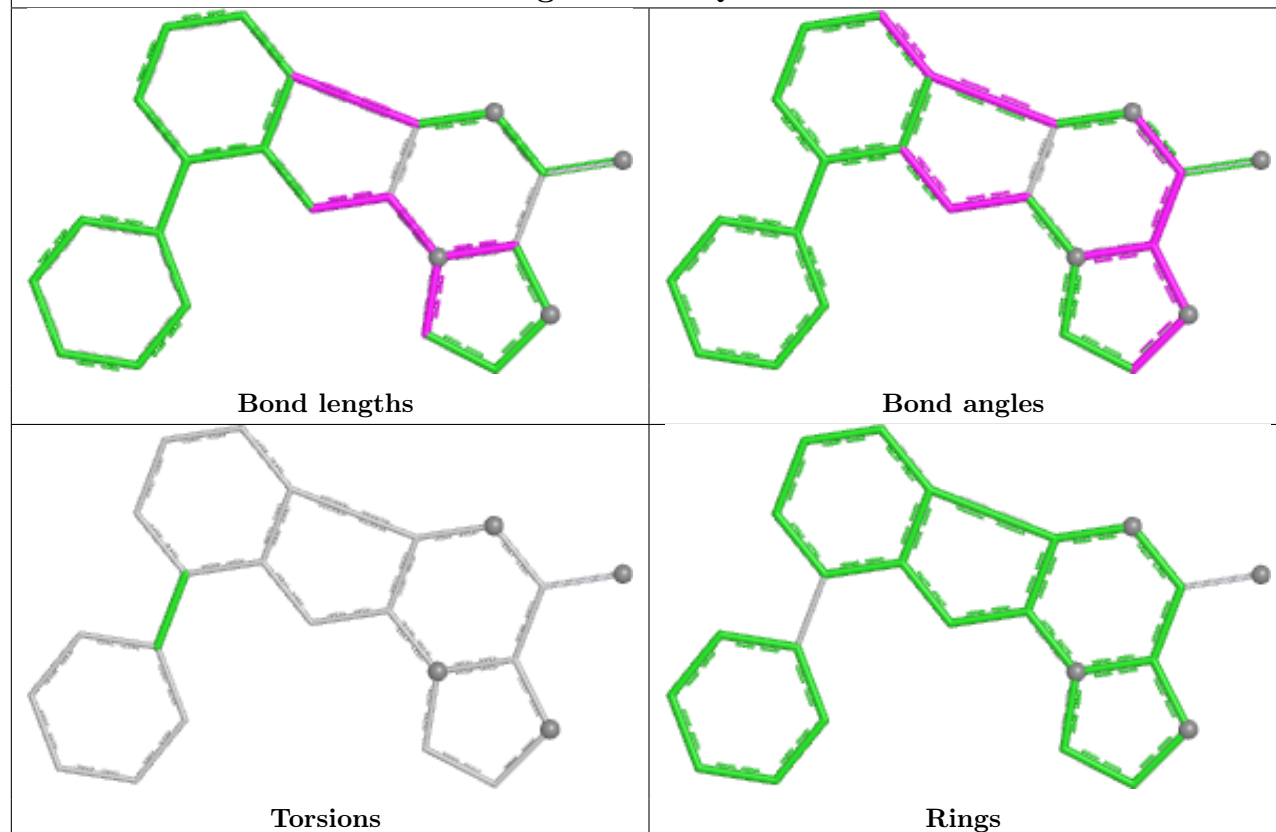
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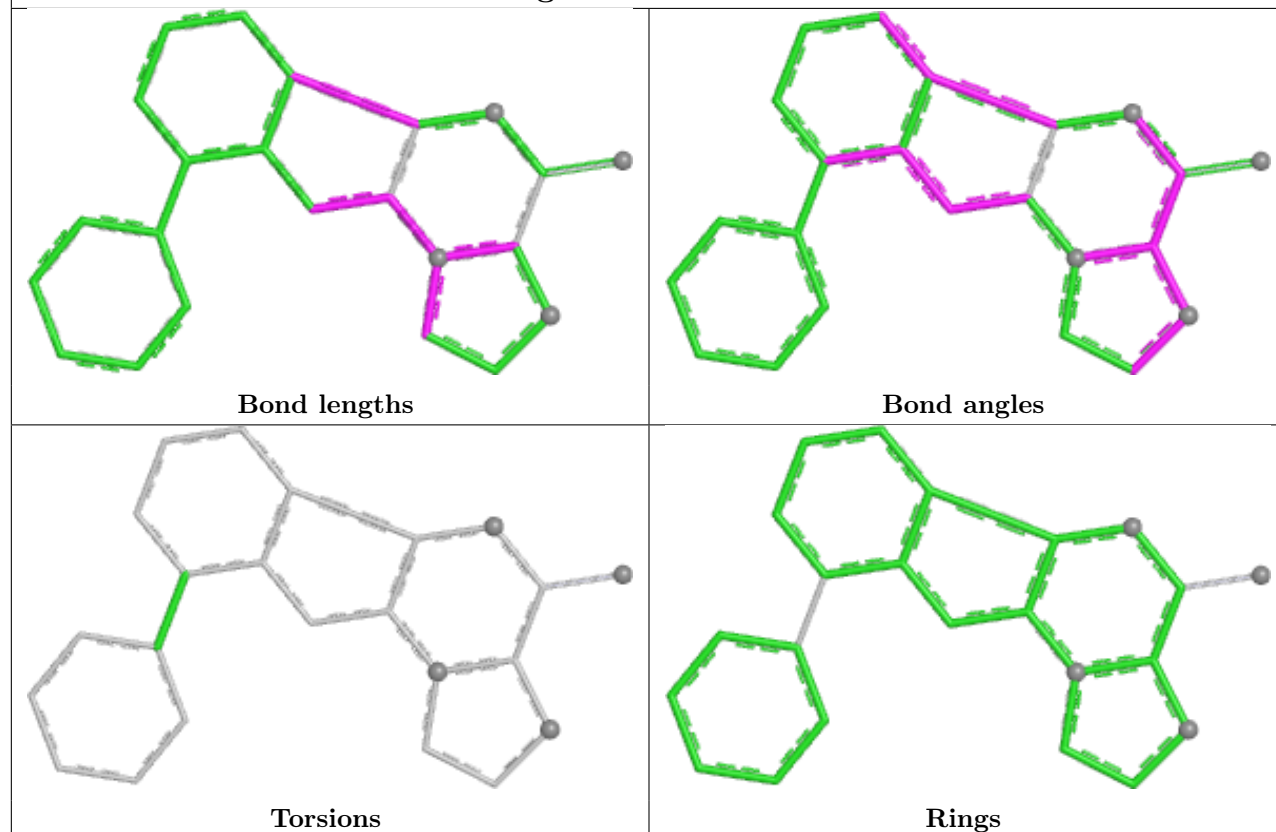
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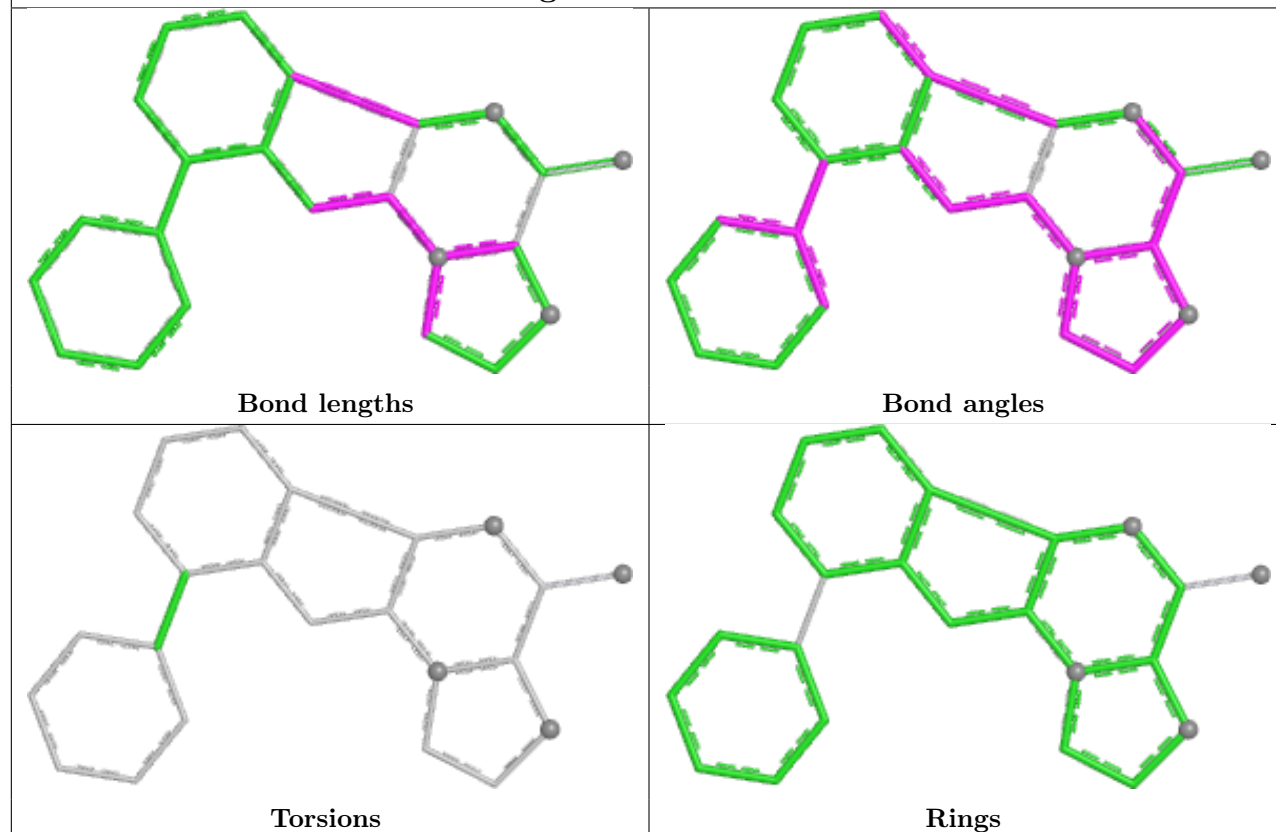
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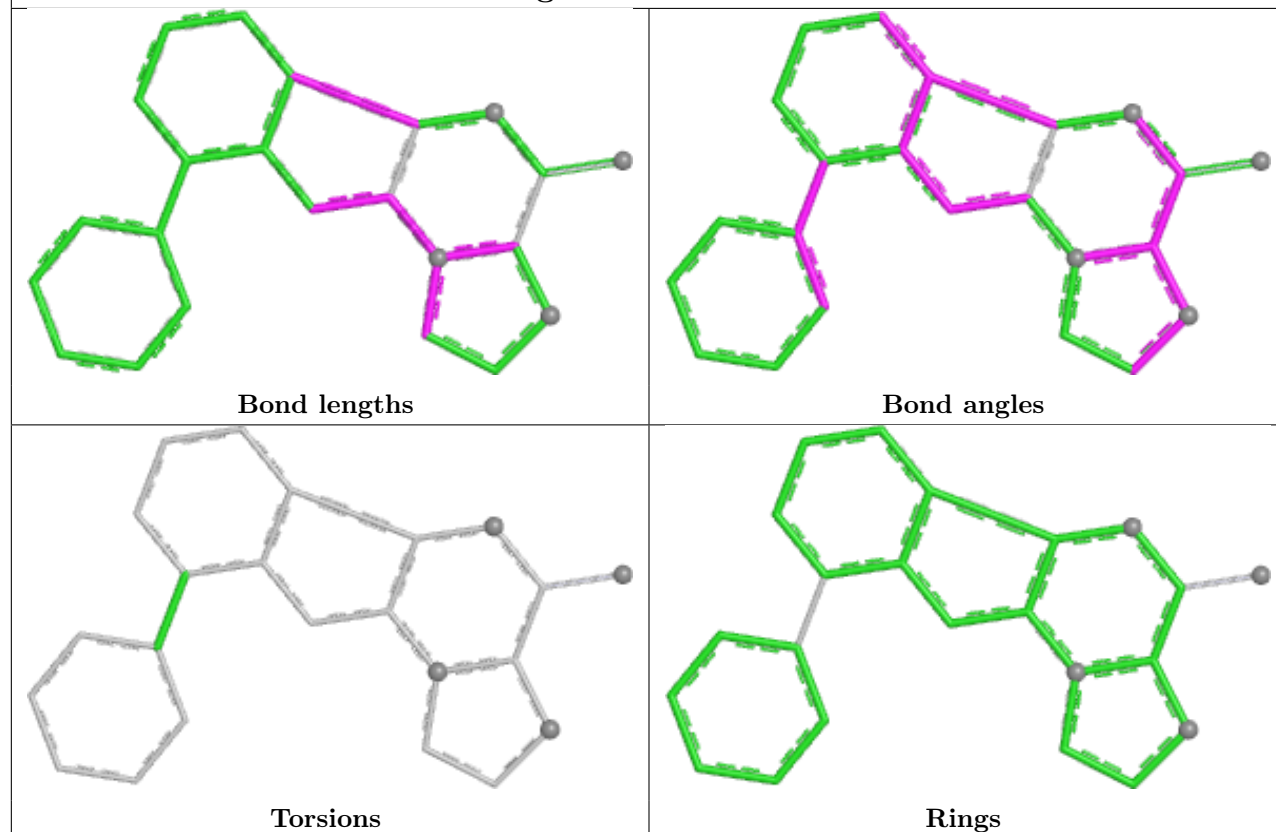
Ligand 2K9 A 900



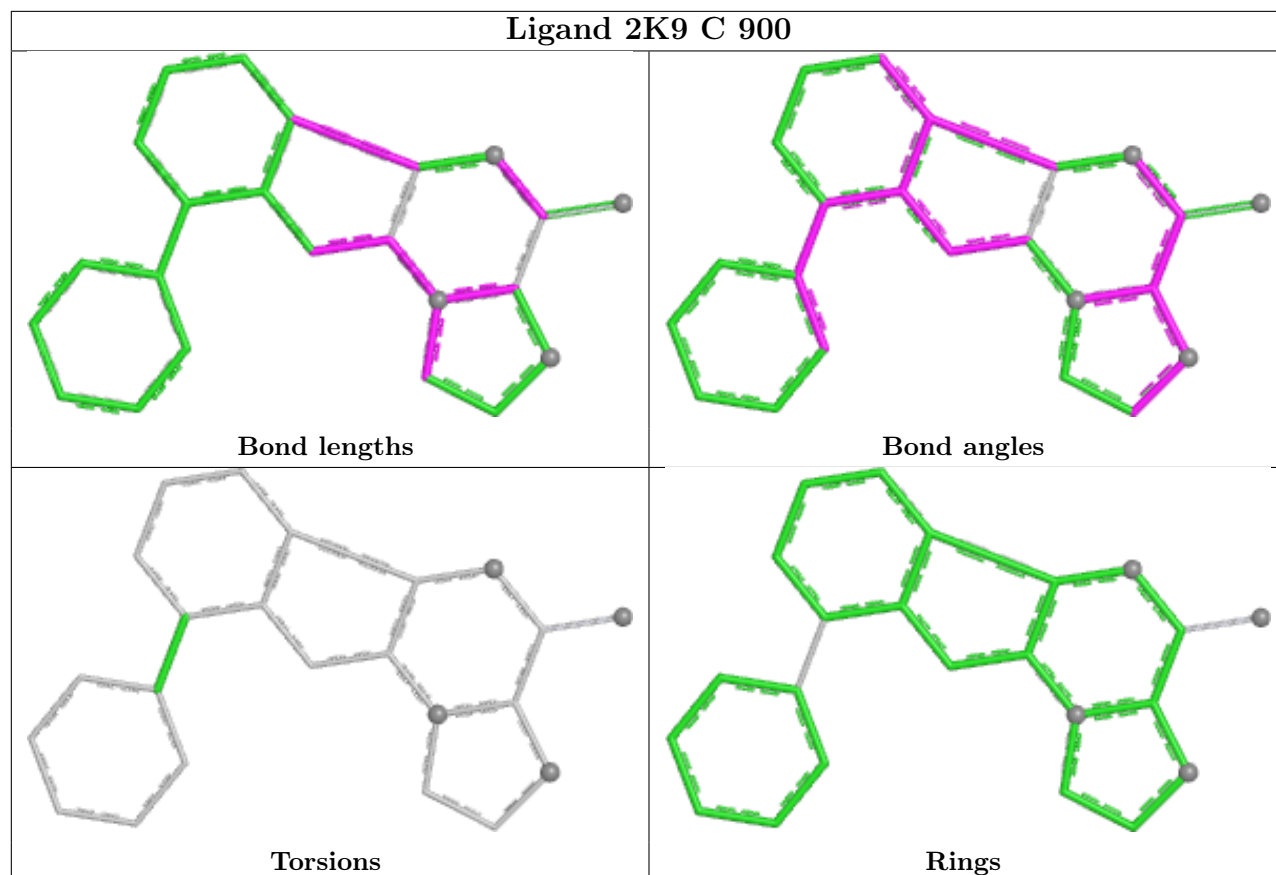
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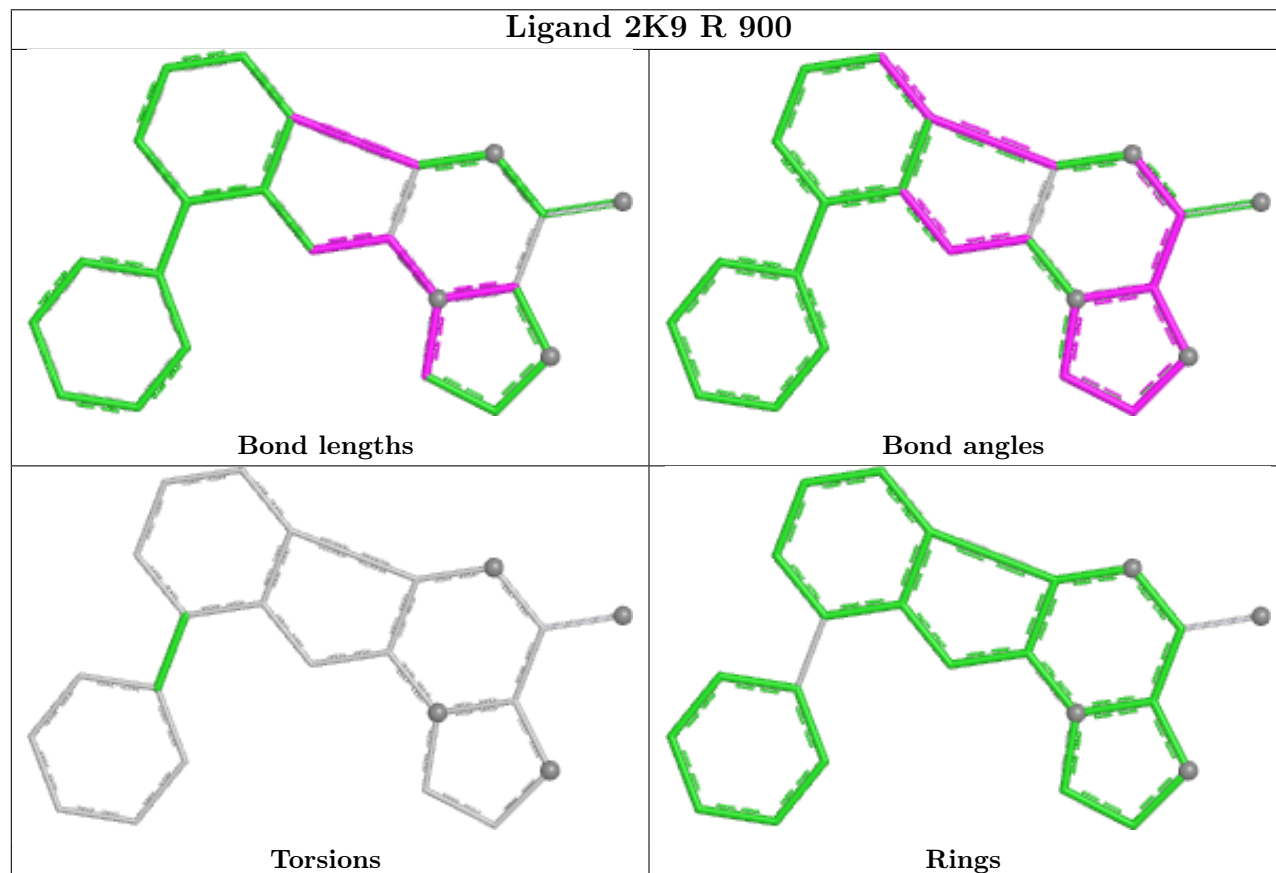
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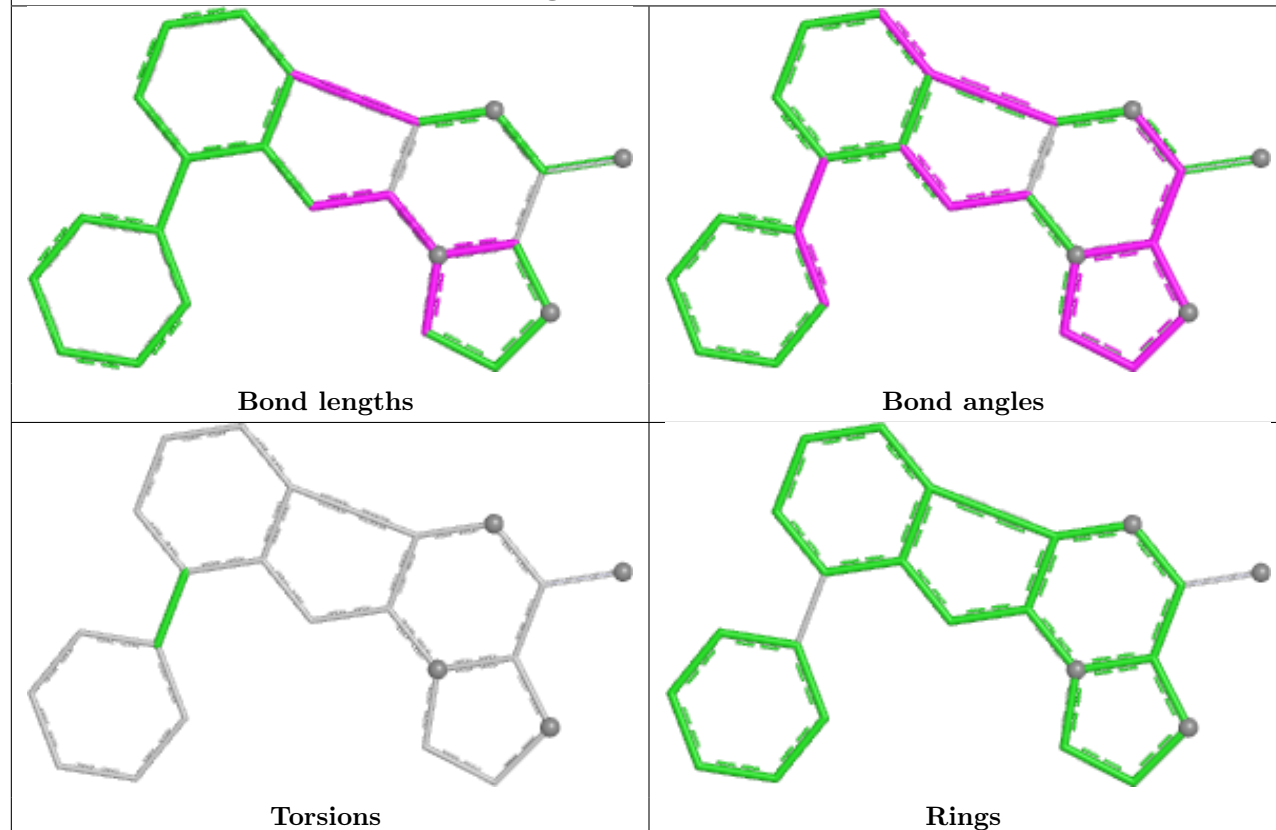
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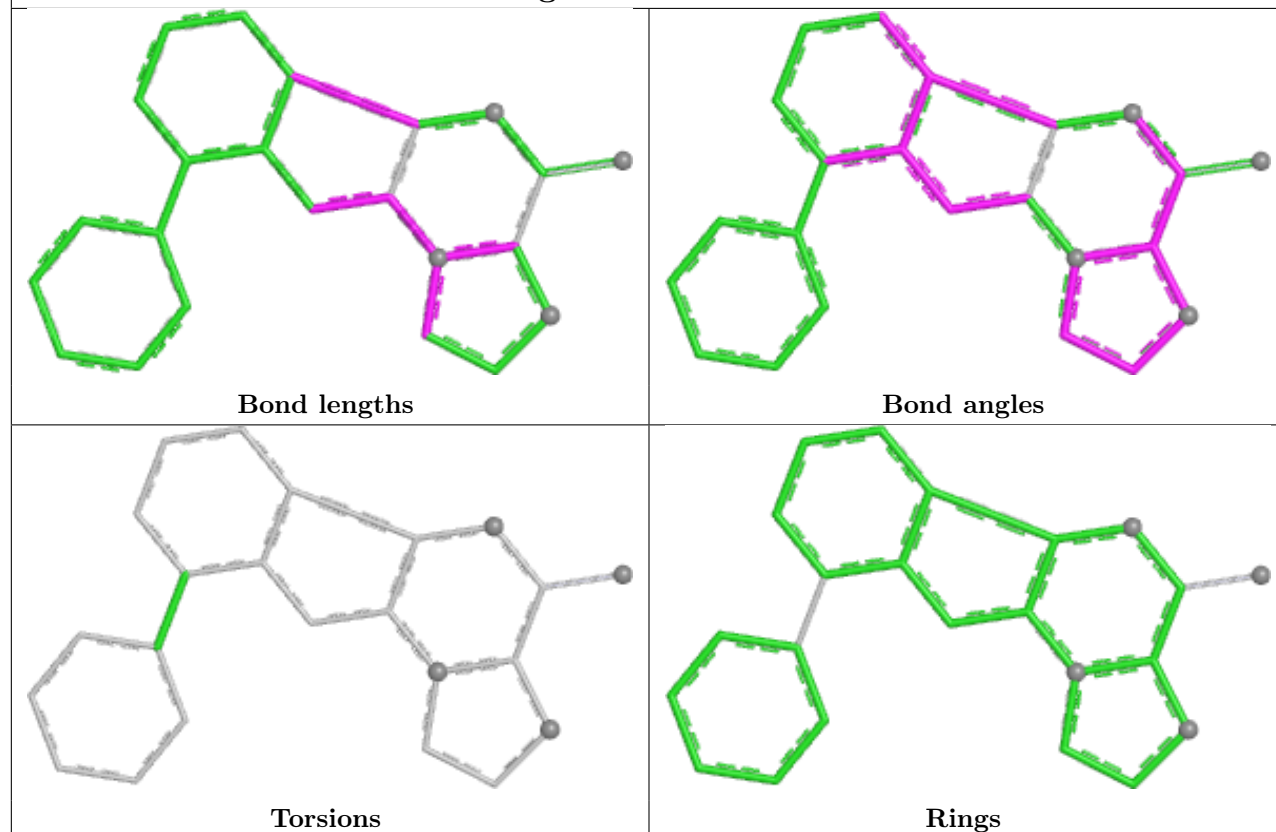
Ligand 2K9 R 900



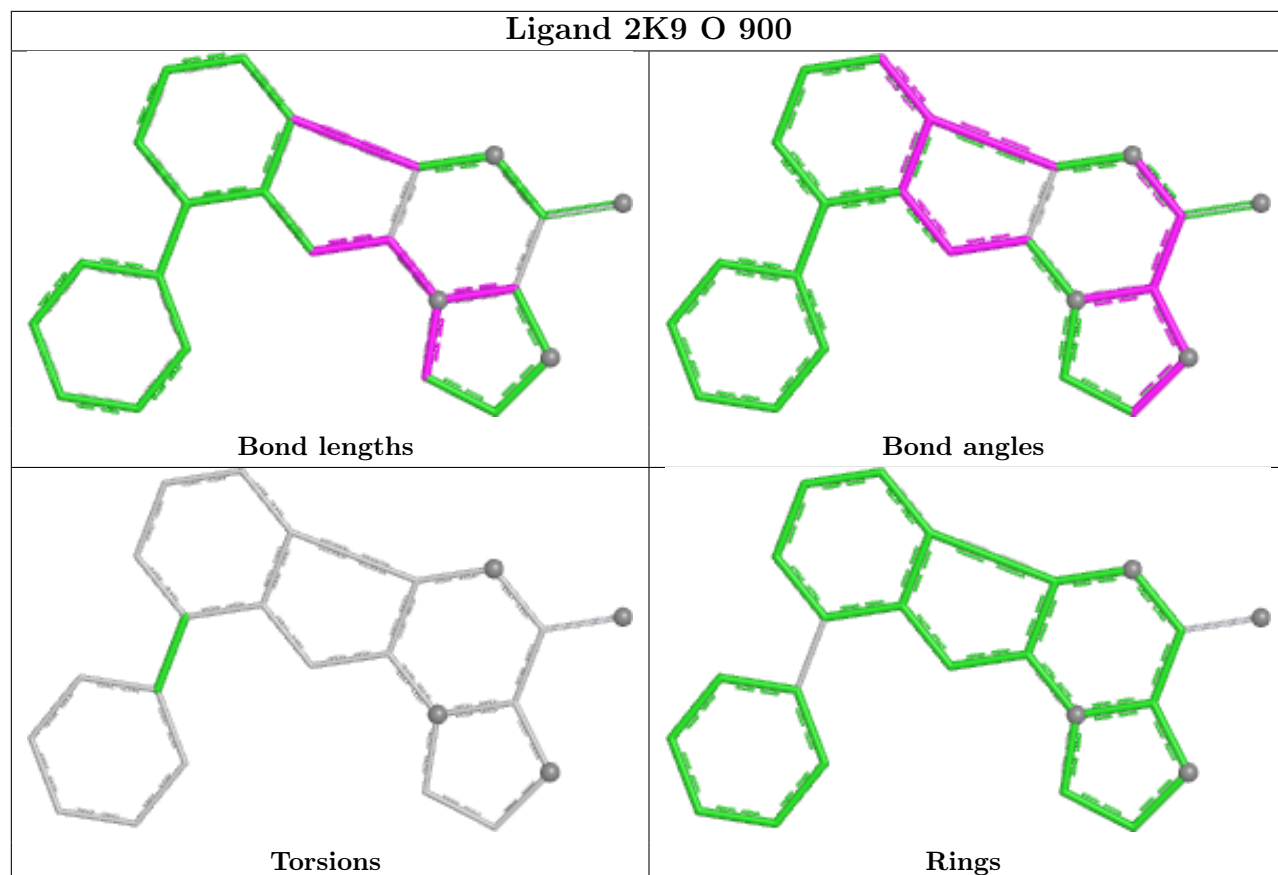
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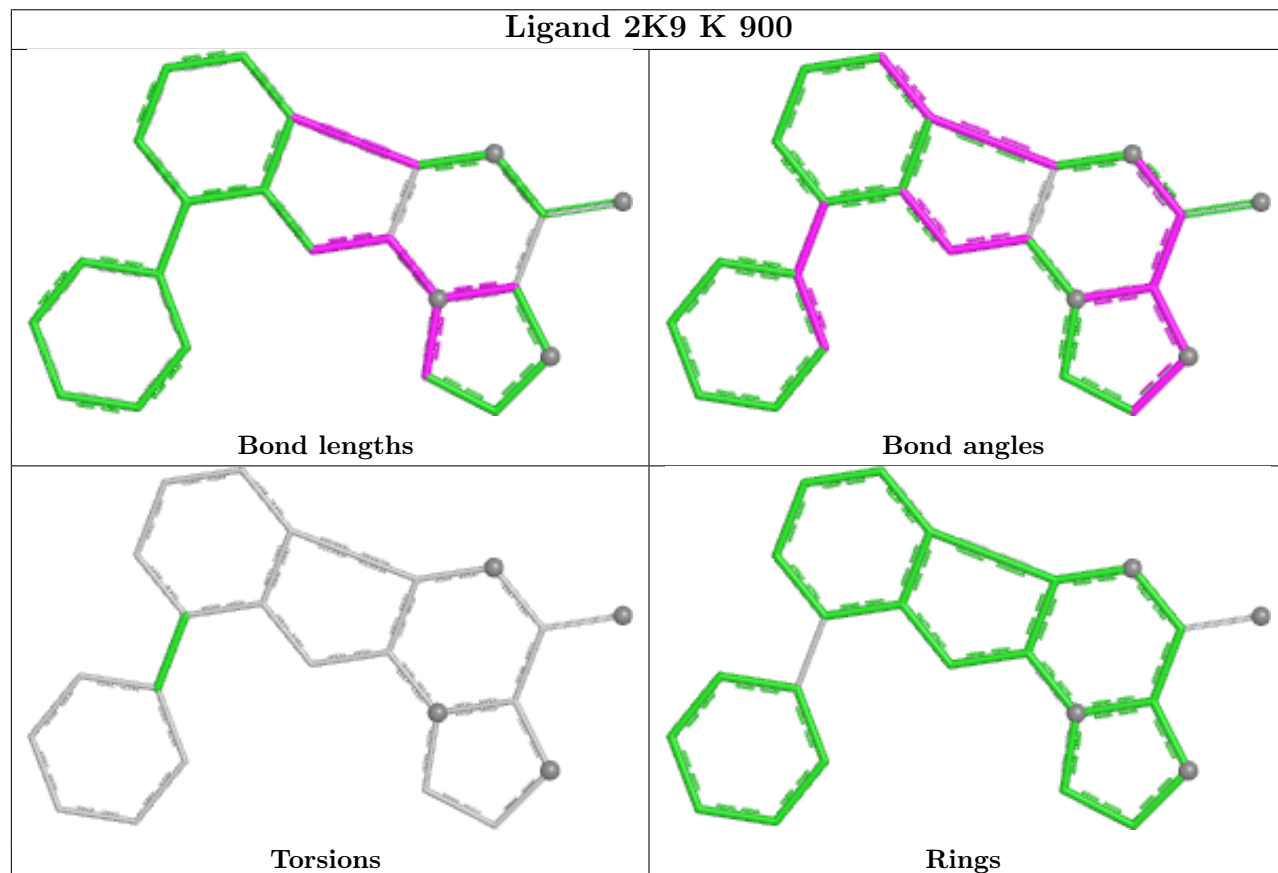
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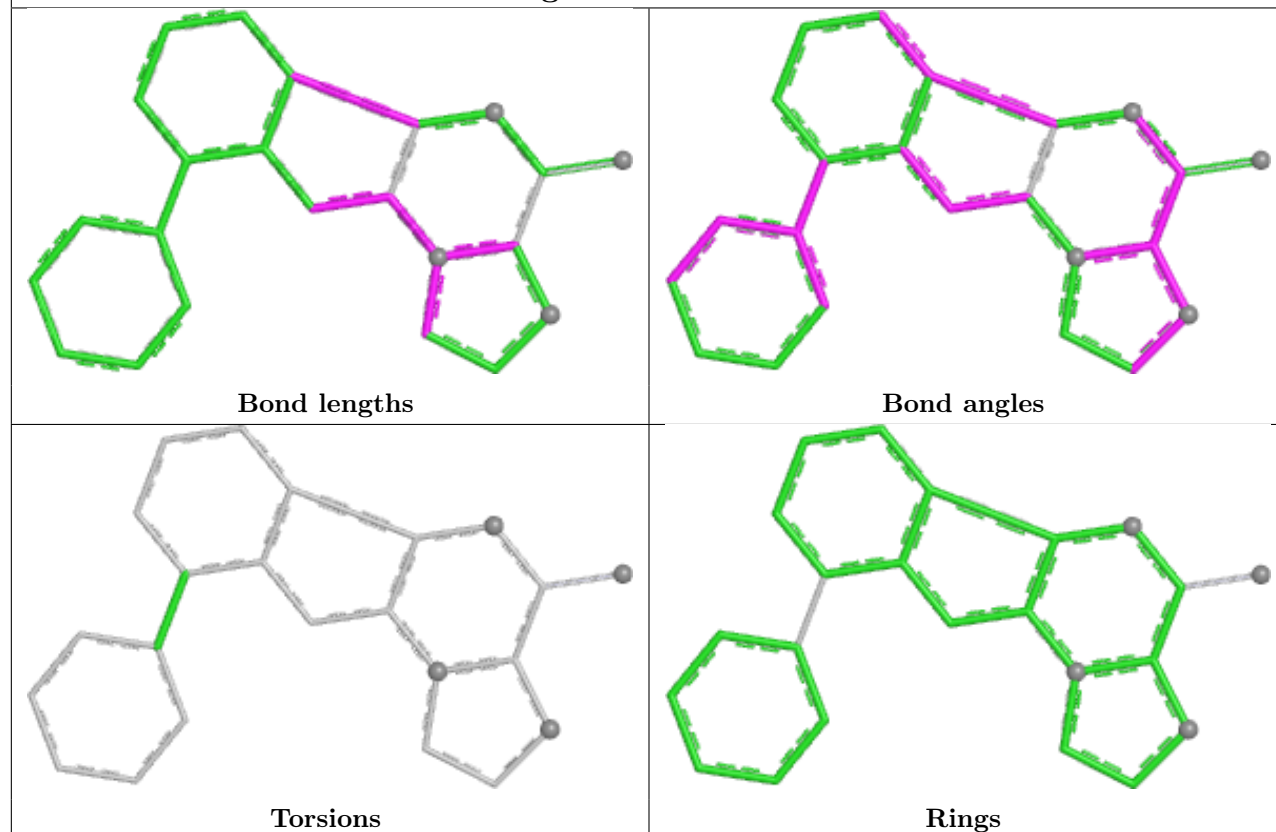
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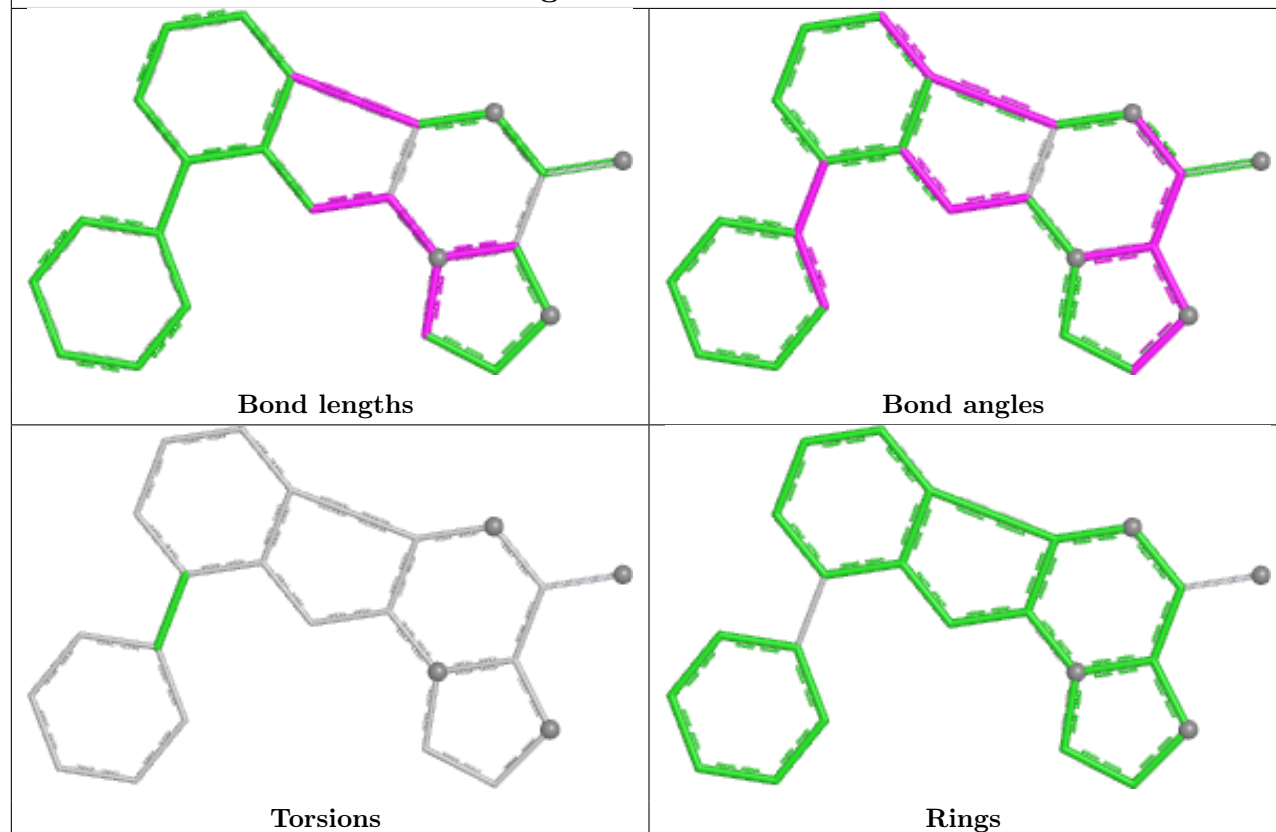
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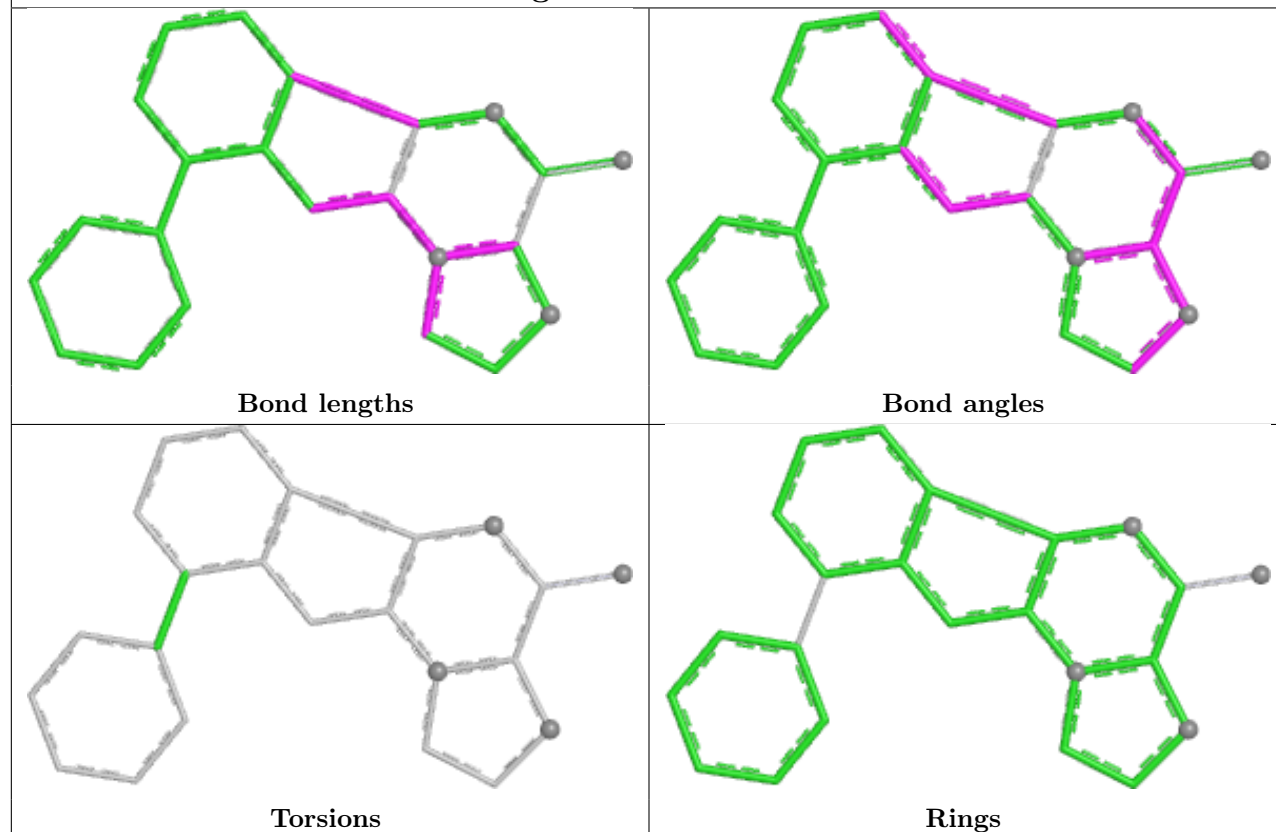
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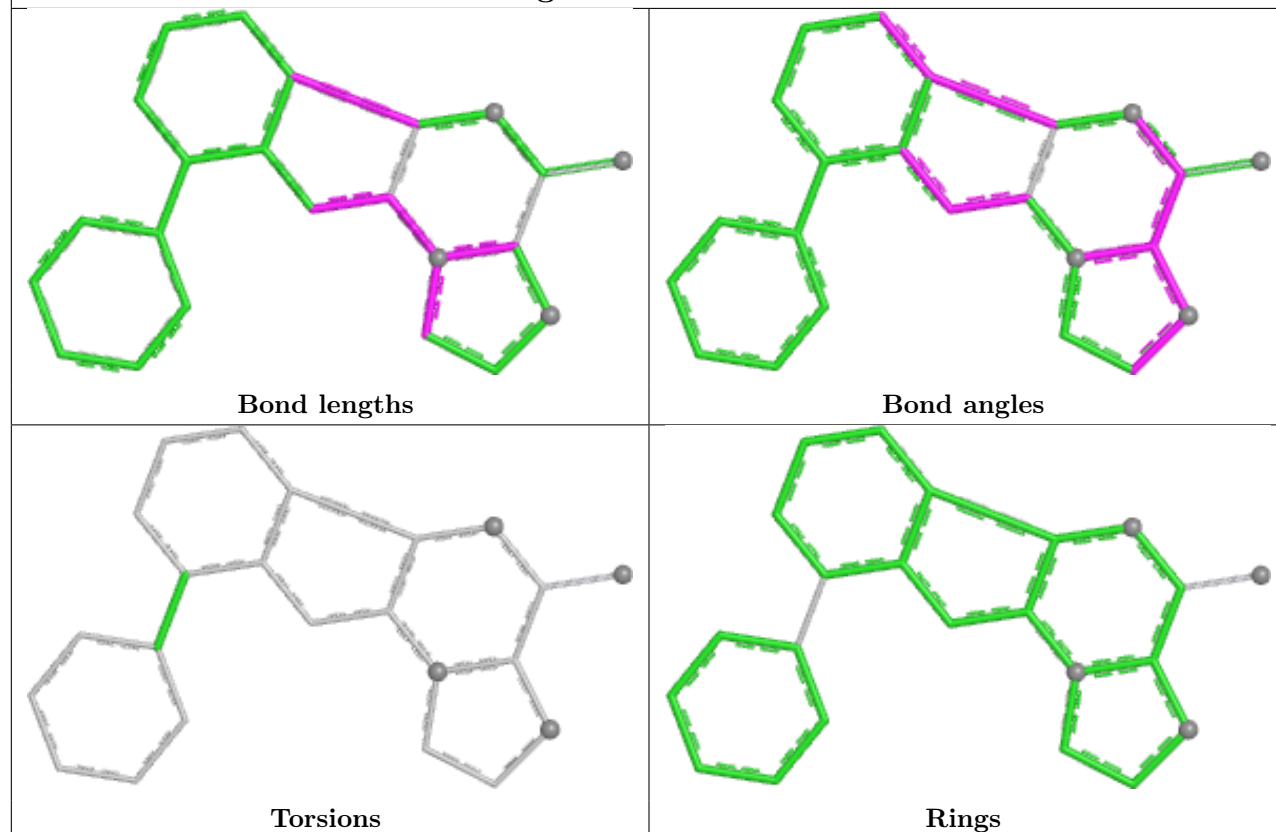
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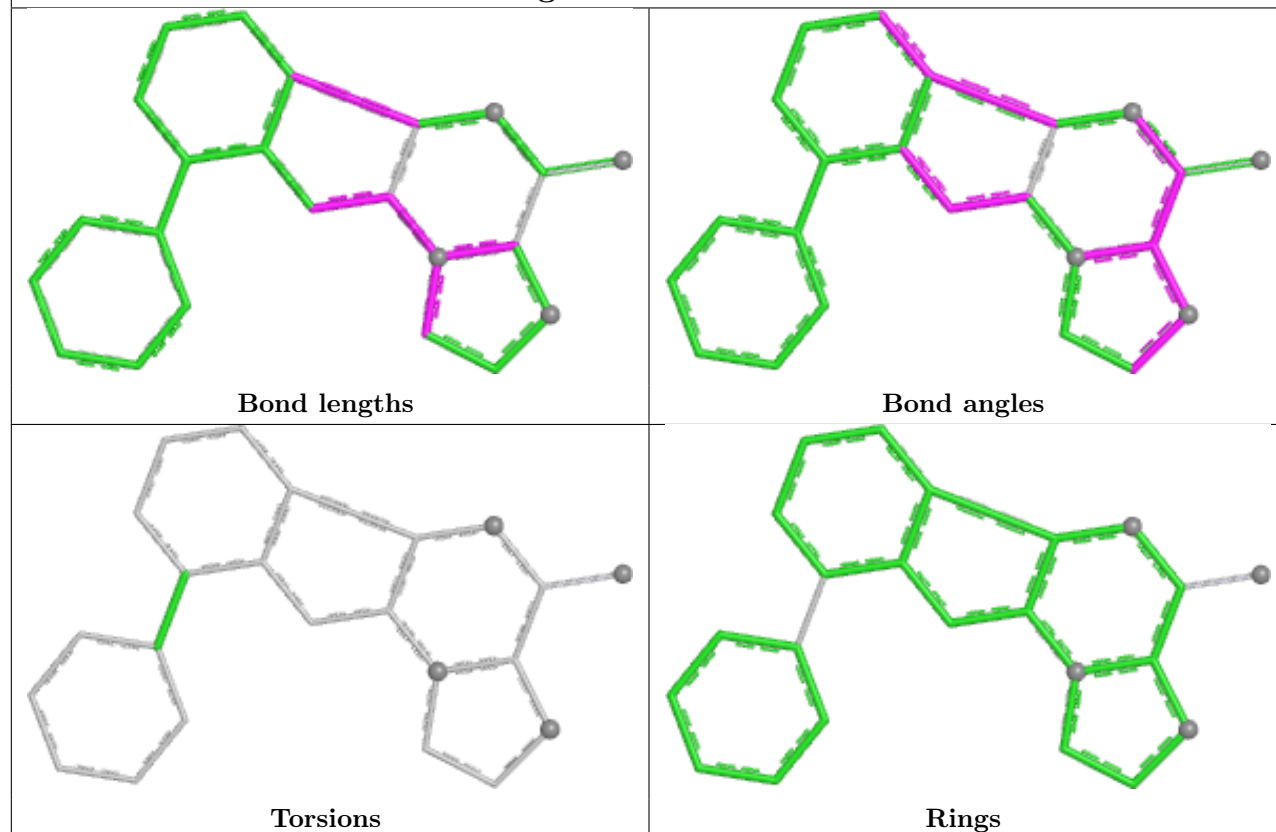
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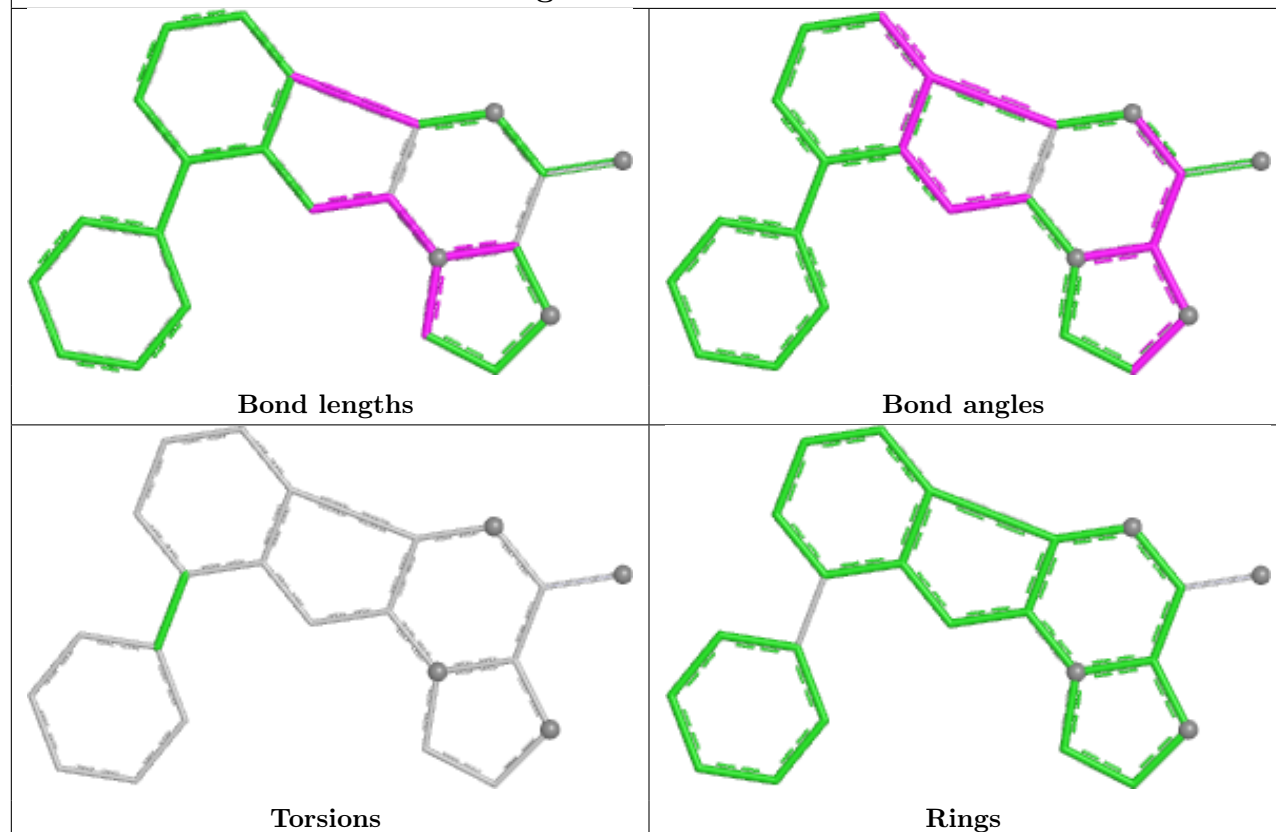
Ligand 2K9 X 900

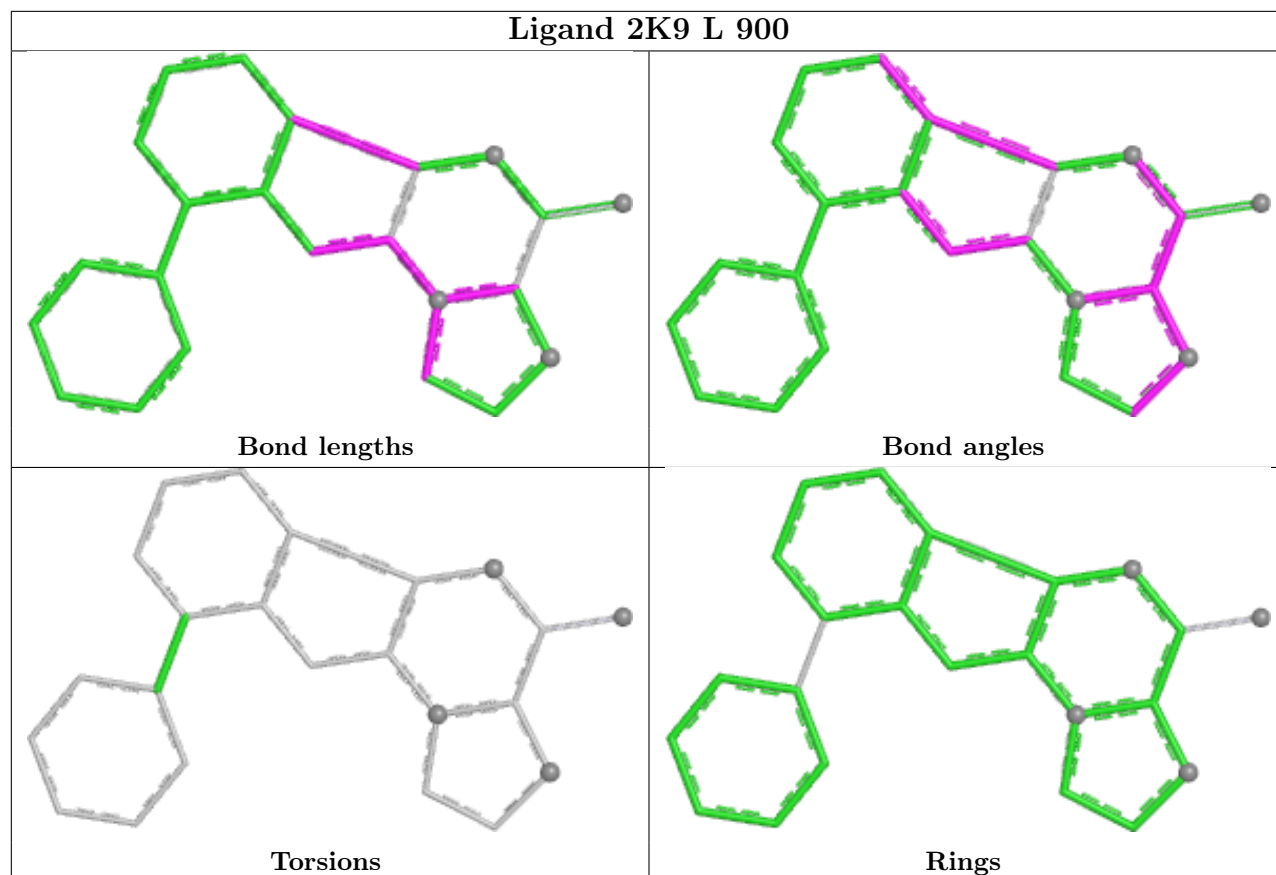


Ligand 2K9 T 900



Ligand 2K9 N 900





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	466/478 (97%)	-0.23	5 (1%) 78 60	31, 54, 85, 128	0
1	B	464/478 (97%)	-0.11	4 (0%) 81 65	33, 55, 85, 125	0
1	C	460/478 (96%)	-0.28	6 (1%) 75 56	32, 53, 83, 124	0
1	D	466/478 (97%)	-0.16	7 (1%) 72 53	31, 52, 82, 124	0
1	E	463/478 (96%)	-0.21	1 (0%) 91 86	31, 52, 82, 124	0
1	F	467/478 (97%)	-0.13	5 (1%) 78 60	31, 54, 85, 124	0
1	G	466/478 (97%)	-0.27	3 (0%) 85 73	31, 54, 84, 124	0
1	H	464/478 (97%)	-0.25	5 (1%) 78 60	32, 54, 84, 124	0
1	I	460/478 (96%)	-0.28	3 (0%) 84 70	32, 53, 82, 124	0
1	J	466/478 (97%)	-0.22	3 (0%) 85 73	31, 52, 82, 124	0
1	K	463/478 (96%)	-0.22	4 (0%) 81 65	31, 53, 82, 124	0
1	L	467/478 (97%)	-0.20	5 (1%) 78 60	32, 53, 84, 124	0
1	M	466/478 (97%)	-0.25	4 (0%) 81 65	33, 54, 85, 124	0
1	N	464/478 (97%)	-0.31	3 (0%) 85 73	32, 53, 83, 124	0
1	O	460/478 (96%)	-0.30	3 (0%) 84 70	32, 54, 83, 124	0
1	P	466/478 (97%)	-0.22	3 (0%) 85 73	32, 54, 83, 124	0
1	Q	463/478 (96%)	-0.10	2 (0%) 88 79	34, 55, 83, 125	0
1	R	467/478 (97%)	-0.25	3 (0%) 85 73	32, 53, 84, 124	0
1	S	466/478 (97%)	-0.27	4 (0%) 81 65	33, 54, 84, 124	0
1	T	464/478 (97%)	-0.32	5 (1%) 78 60	32, 54, 83, 124	0
1	U	460/478 (96%)	-0.28	5 (1%) 78 60	32, 53, 83, 124	0
1	V	466/478 (97%)	-0.25	3 (0%) 85 73	31, 53, 82, 124	0
1	W	463/478 (96%)	-0.27	1 (0%) 91 86	33, 54, 82, 124	0
1	X	467/478 (97%)	-0.22	5 (1%) 78 60	31, 53, 84, 124	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	11144/11472 (97%)	-0.23	92 (0%) 82 68	31, 54, 84, 128	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	176	VAL	4.2
1	A	176	VAL	3.7
1	B	51	GLY	3.5
1	M	176	VAL	3.4
1	N	51	GLY	3.4
1	N	176	VAL	3.3
1	O	51	GLY	3.3
1	R	51	GLY	3.3
1	T	51	GLY	3.1
1	X	330	TYR	3.1
1	D	51	GLY	3.1
1	G	51	GLY	3.1
1	Q	401	LEU	3.0
1	S	176	VAL	3.0
1	O	176	VAL	3.0
1	U	176	VAL	3.0
1	P	176	VAL	2.9
1	B	404	LEU	2.9
1	Q	176	VAL	2.9
1	M	51	GLY	2.8
1	C	176	VAL	2.8
1	J	51	GLY	2.8
1	W	330	TYR	2.8
1	I	176	VAL	2.8
1	T	176	VAL	2.8
1	I	51	GLY	2.7
1	U	51	GLY	2.7
1	H	176	VAL	2.7
1	D	212	GLY	2.7
1	X	176	VAL	2.7
1	K	176	VAL	2.6
1	A	404	LEU	2.6
1	F	404	LEU	2.5
1	R	330	TYR	2.5
1	X	401	LEU	2.5
1	F	330	TYR	2.5
1	O	180	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	330	TYR	2.5
1	L	330	TYR	2.5
1	V	180	GLY	2.5
1	F	176	VAL	2.5
1	K	401	LEU	2.5
1	L	404	LEU	2.5
1	P	330	TYR	2.5
1	H	330	TYR	2.4
1	M	330	TYR	2.4
1	H	474	VAL	2.4
1	B	330	TYR	2.4
1	E	330	TYR	2.4
1	F	181	GLY	2.4
1	S	330	TYR	2.4
1	J	330	TYR	2.4
1	K	404	LEU	2.4
1	T	62	GLU	2.4
1	B	176	VAL	2.4
1	V	-2	THR	2.3
1	N	291	TYR	2.3
1	U	330	TYR	2.3
1	C	404	LEU	2.3
1	M	404	LEU	2.3
1	C	330	TYR	2.3
1	P	51	GLY	2.2
1	X	51	GLY	2.2
1	A	401	LEU	2.2
1	J	176	VAL	2.2
1	L	176	VAL	2.2
1	C	401	LEU	2.2
1	F	51	GLY	2.2
1	L	51	GLY	2.2
1	T	330	TYR	2.2
1	G	401	LEU	2.2
1	U	404	LEU	2.1
1	S	405	PRO	2.1
1	R	401	LEU	2.1
1	D	182	TYR	2.1
1	D	180	GLY	2.1
1	U	180	GLY	2.1
1	V	407	GLU	2.1
1	C	3	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	404	LEU	2.1
1	D	330	TYR	2.1
1	K	330	TYR	2.1
1	S	404	LEU	2.0
1	L	180	GLY	2.0
1	A	406	PRO	2.0
1	I	404	LEU	2.0
1	X	404	LEU	2.0
1	T	291	TYR	2.0
1	C	4	ASP	2.0
1	D	400	ASP	2.0
1	H	401	LEU	2.0
1	H	404	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	2K9	O	900	23/23	0.89	0.14	82,85,88,88	0
2	2K9	Q	900	23/23	0.91	0.15	113,114,114,114	0
2	2K9	H	900	23/23	0.92	0.12	90,90,91,92	0
2	2K9	M	900	23/23	0.92	0.13	85,86,87,88	0
2	2K9	B	900	23/23	0.92	0.13	100,102,103,104	0
2	2K9	P	900	23/23	0.92	0.11	64,65,66,67	0
2	2K9	F	900	23/23	0.92	0.12	64,67,67,68	0
2	2K9	U	900	23/23	0.92	0.12	69,73,75,77	0
2	2K9	S	900	23/23	0.93	0.10	67,69,71,72	0
2	2K9	T	900	23/23	0.93	0.10	75,75,76,76	0

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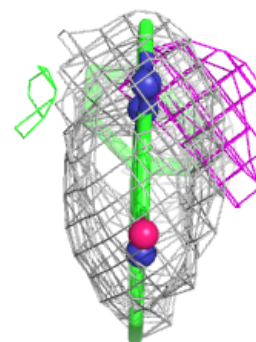
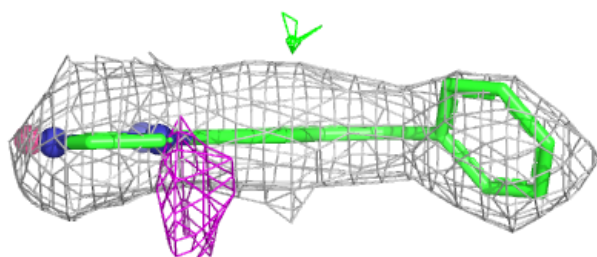
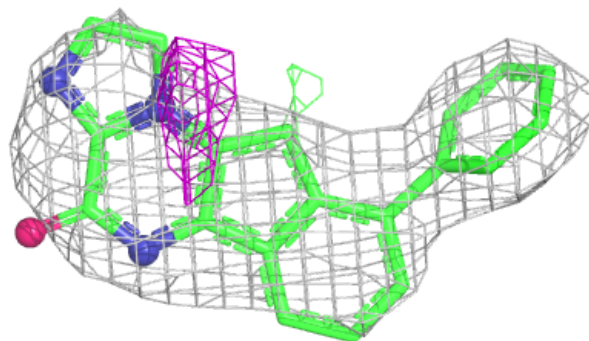
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	2K9	A	900	23/23	0.93	0.09	58,60,62,62	0
2	2K9	J	900	23/23	0.94	0.09	56,58,60,60	0
2	2K9	L	900	23/23	0.94	0.09	50,51,52,53	0
2	2K9	G	900	23/23	0.94	0.08	54,54,56,57	0
2	2K9	N	900	23/23	0.94	0.09	58,60,61,62	0
2	2K9	I	900	23/23	0.94	0.09	54,55,57,57	0
2	2K9	W	900	23/23	0.94	0.11	76,77,77,78	0
2	2K9	D	900	23/23	0.95	0.07	47,51,53,54	0
2	2K9	C	900	23/23	0.95	0.08	47,48,49,50	0
2	2K9	K	900	23/23	0.95	0.08	46,48,49,50	0
2	2K9	R	900	23/23	0.95	0.07	57,58,59,59	0
2	2K9	V	900	23/23	0.96	0.08	39,43,45,47	0
2	2K9	X	900	23/23	0.96	0.08	60,61,61,62	0
2	2K9	E	900	23/23	0.97	0.06	43,44,46,46	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.

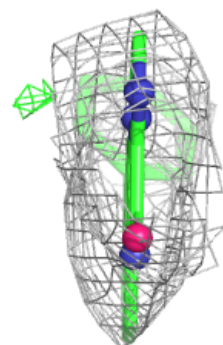
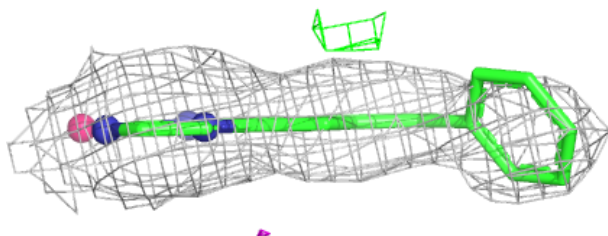
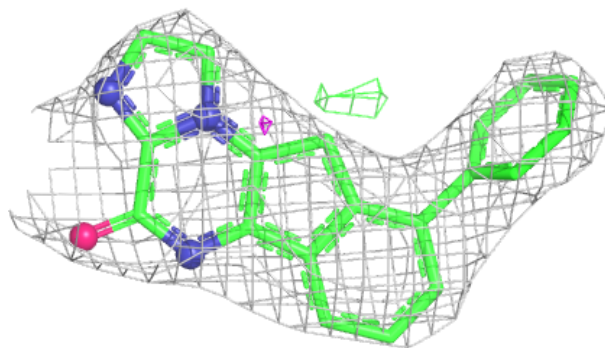
Electron density around 2K9 O 900:

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

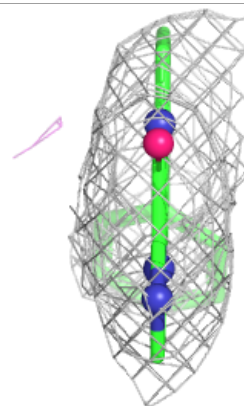
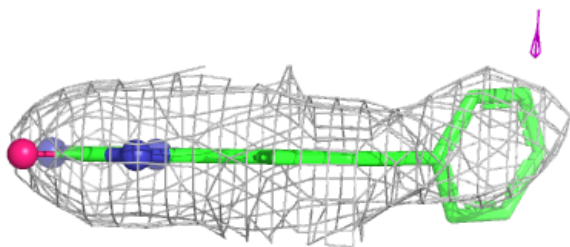
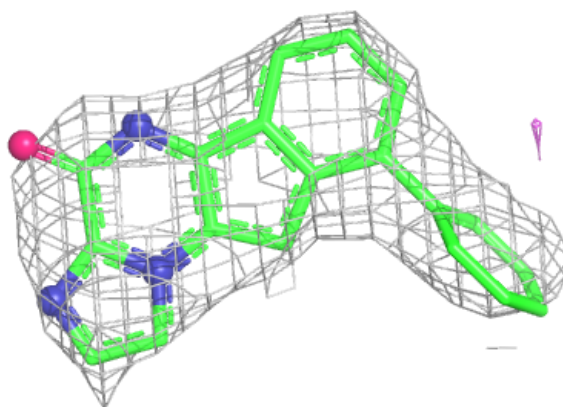


Electron density around 2K9 Q 900:

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and green (positive)

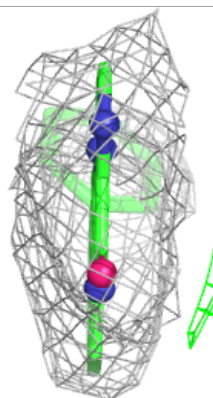
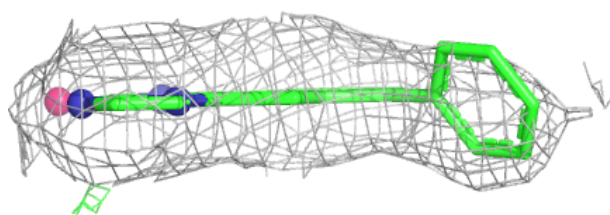
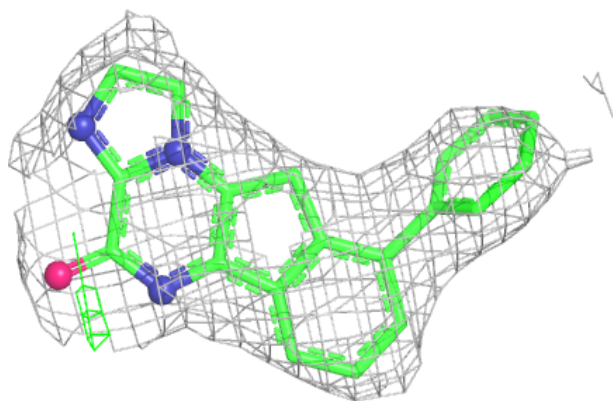
**Electron density around 2K9 H 900:**

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and green (positive)

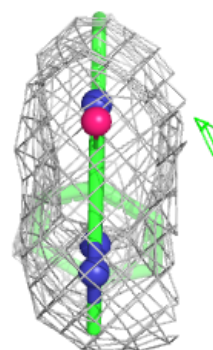
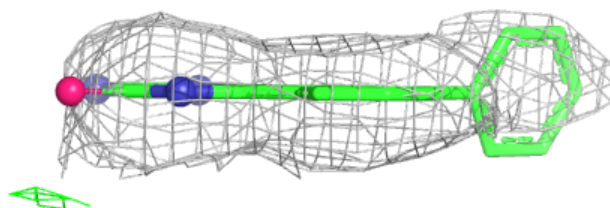
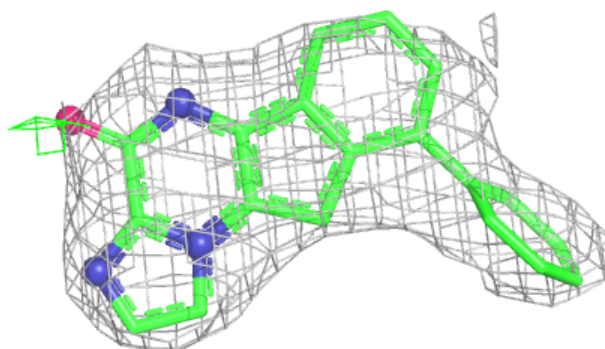


Electron density around 2K9 M 900:

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and green (positive)

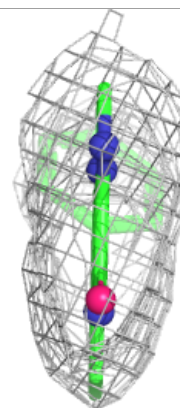
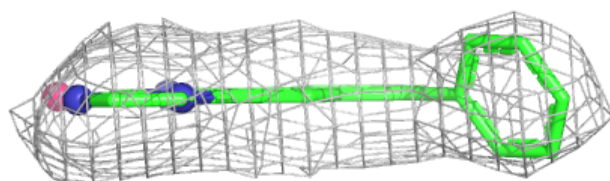
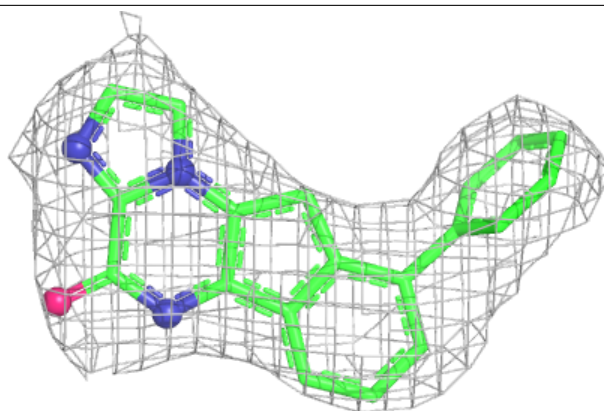
**Electron density around 2K9 B 900:**

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and green (positive)

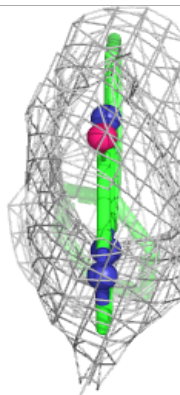
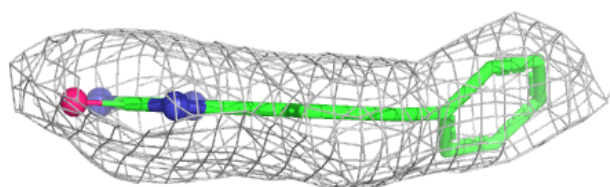
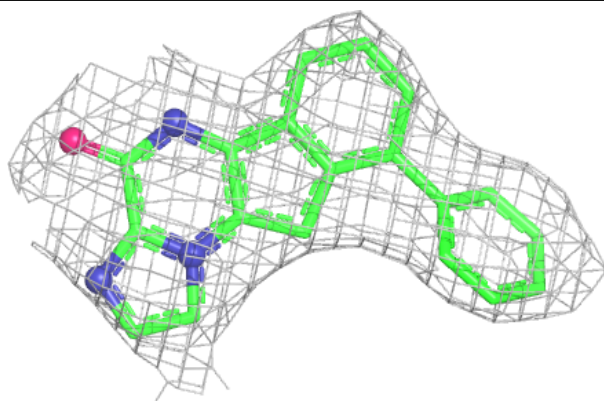


Electron density around 2K9 P 900:

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

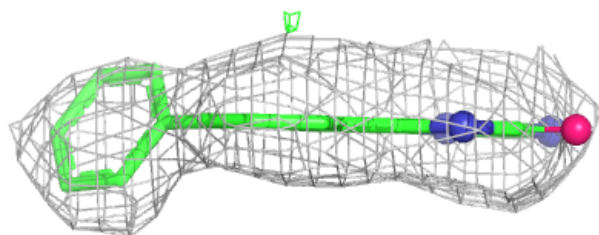
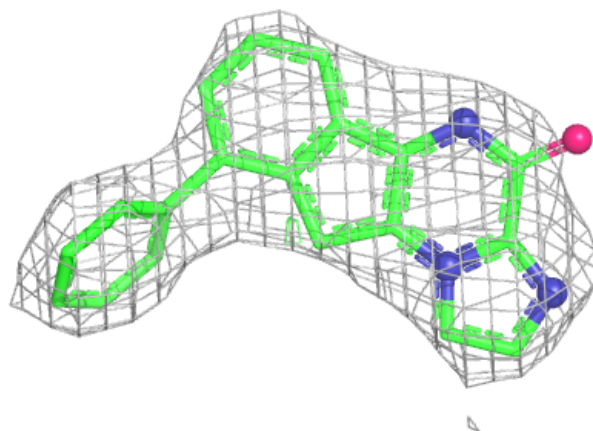
**Electron density around 2K9 F 900:**

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



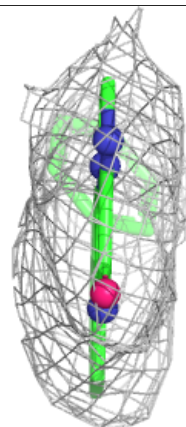
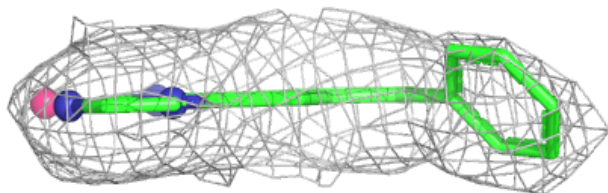
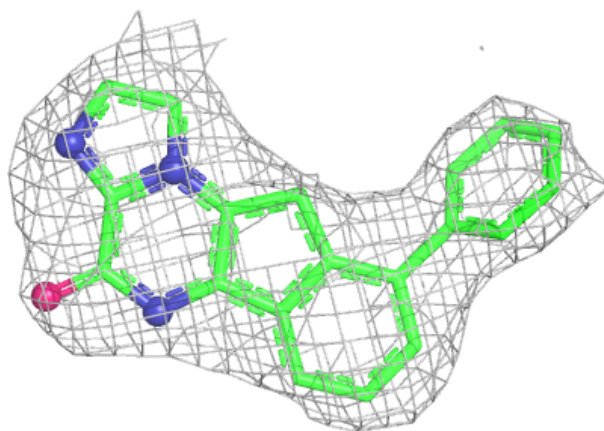
Electron density around 2K9 U 900:

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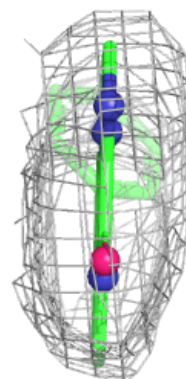
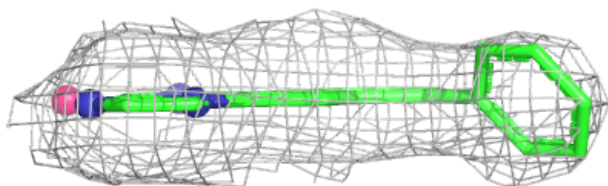
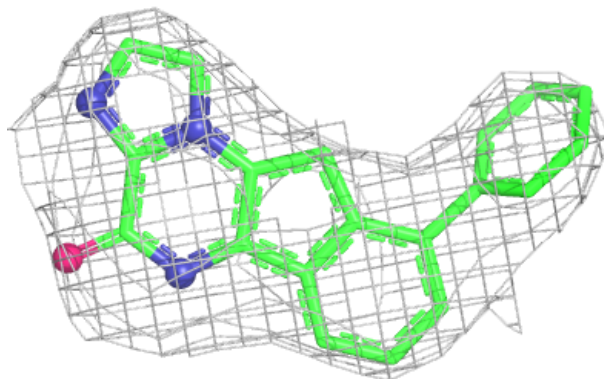


Electron density around 2K9 S 900:

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and green (positive)

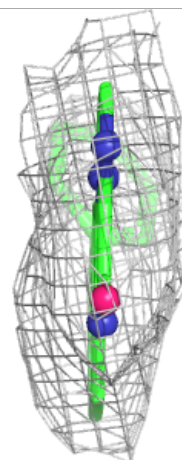
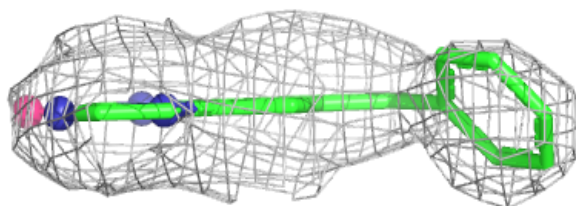
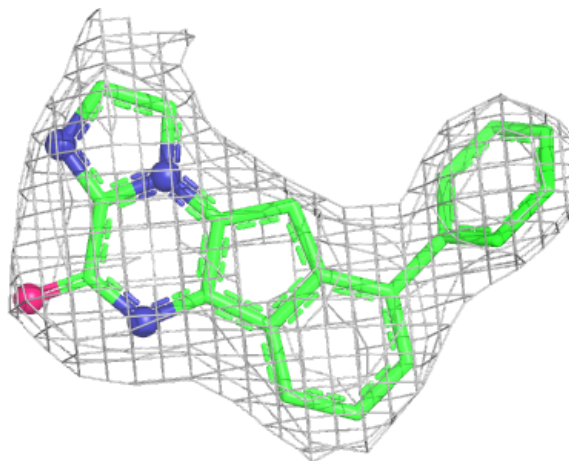
**Electron density around 2K9 T 900:**

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and green (positive)



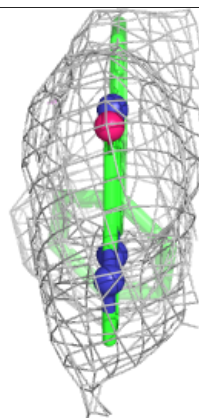
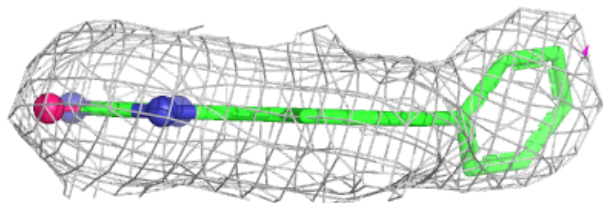
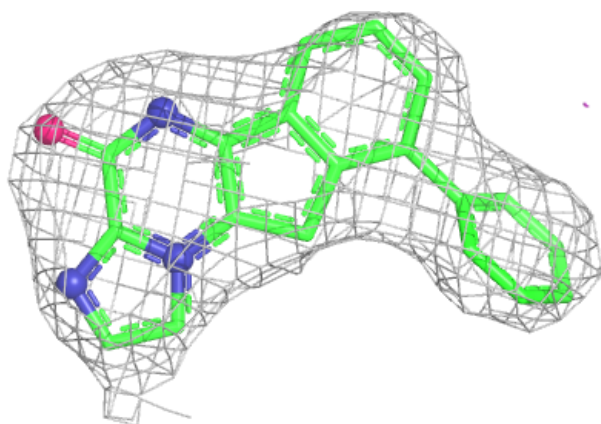
Electron density around 2K9 A 900:

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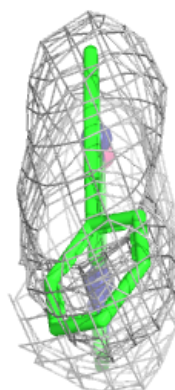
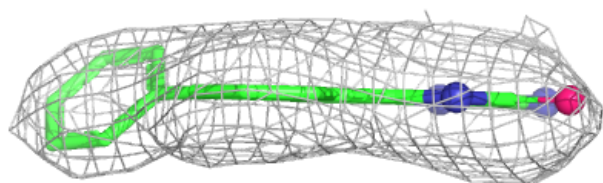
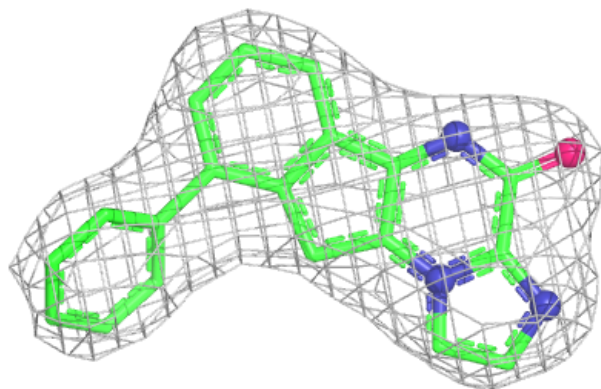


Electron density around 2K9 J 900:

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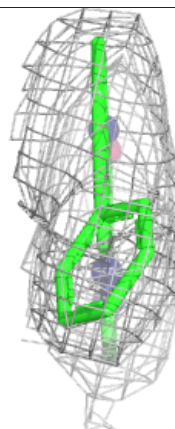
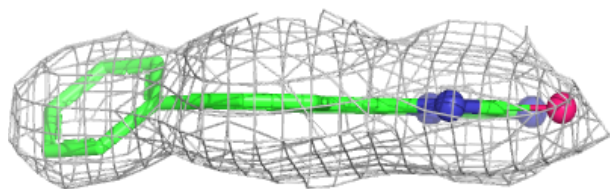
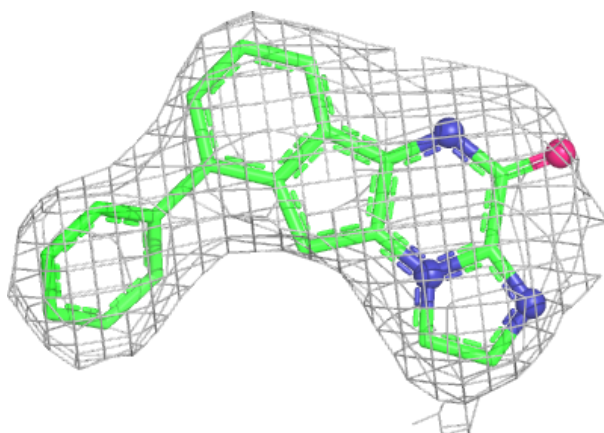
**Electron density around 2K9 L 900:**

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and green (positive)

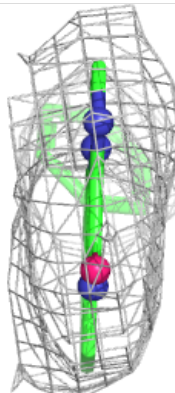
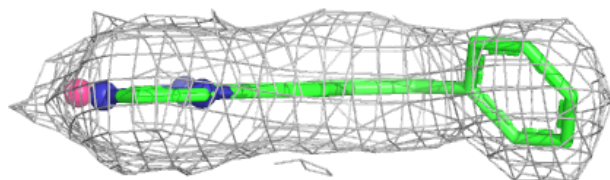
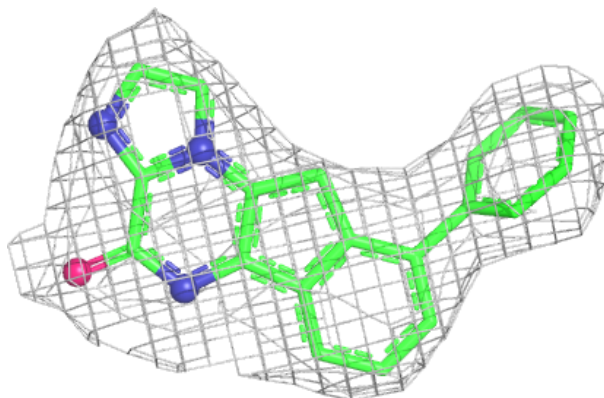


Electron density around 2K9 G 900:

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

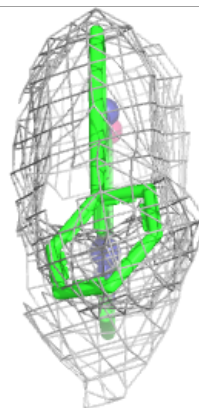
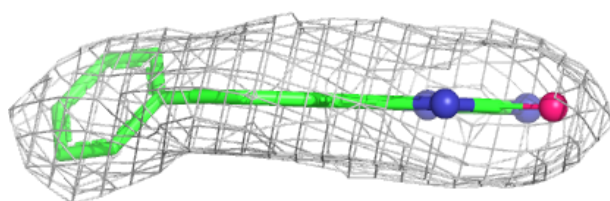
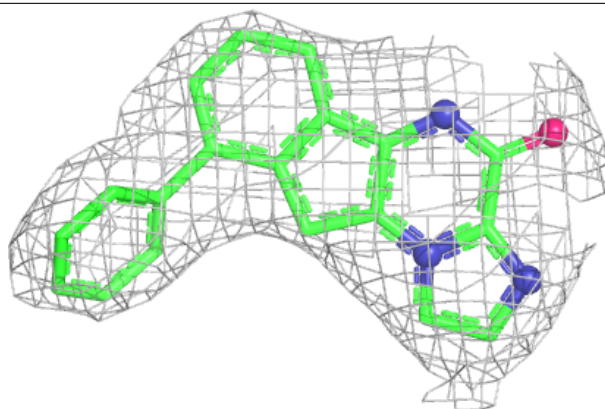
**Electron density around 2K9 N 900:**

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

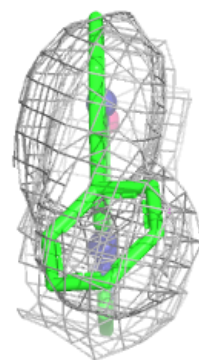
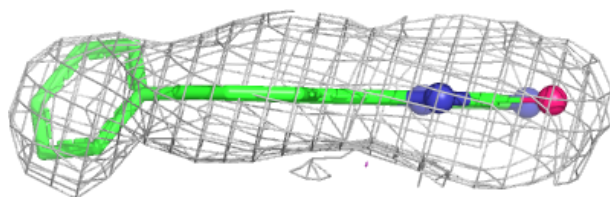
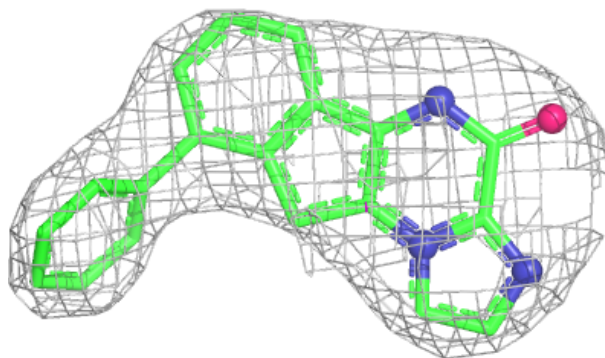


Electron density around 2K9 I 900:

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

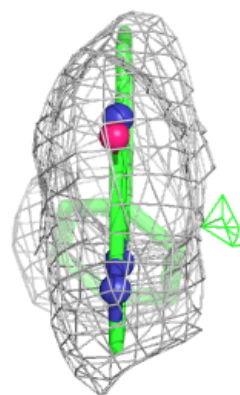
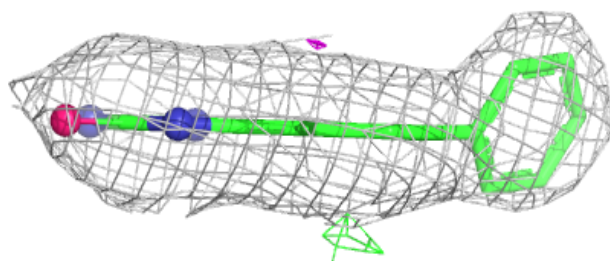
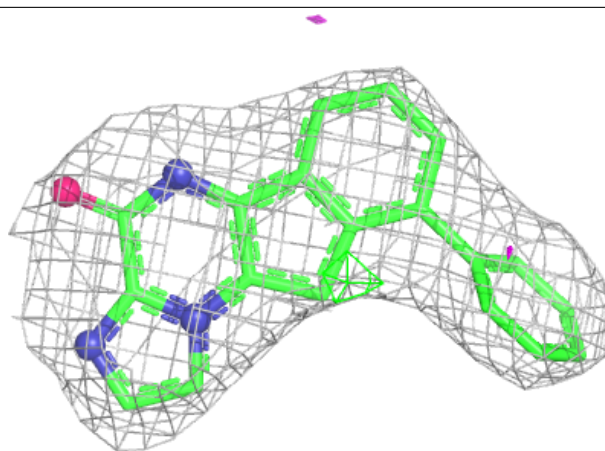
**Electron density around 2K9 W 900:**

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

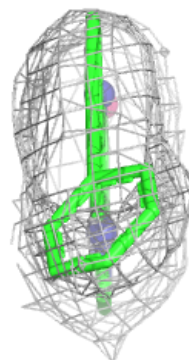
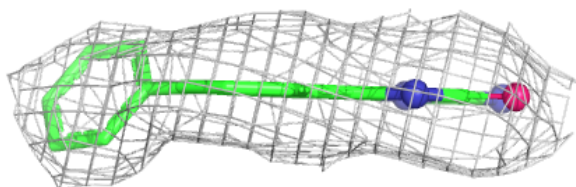
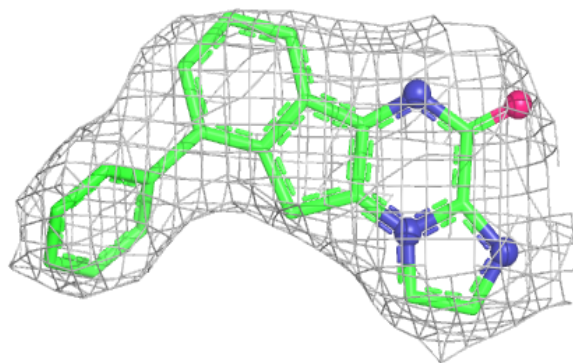


Electron density around 2K9 D 900:

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

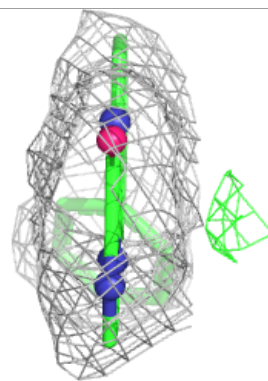
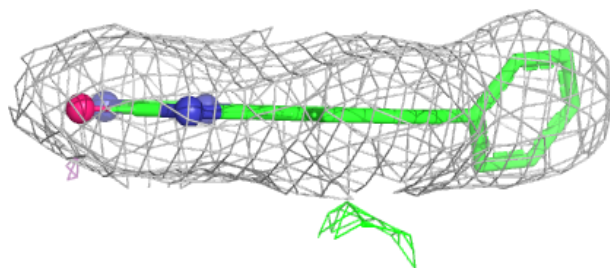
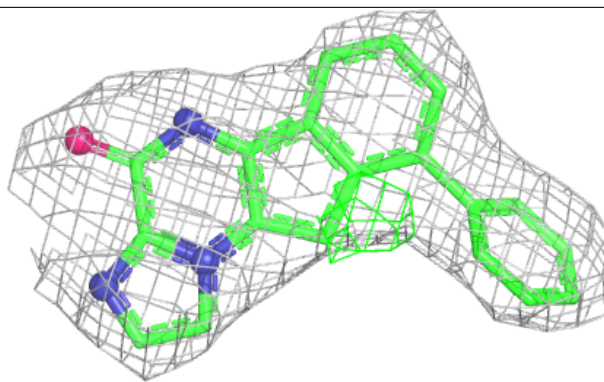
**Electron density around 2K9 C 900:**

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

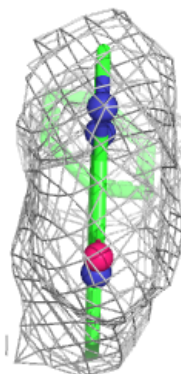
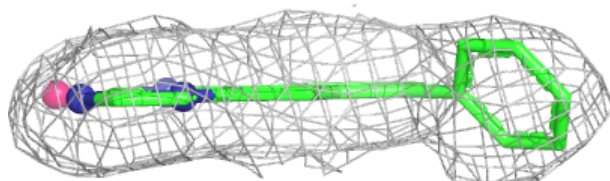
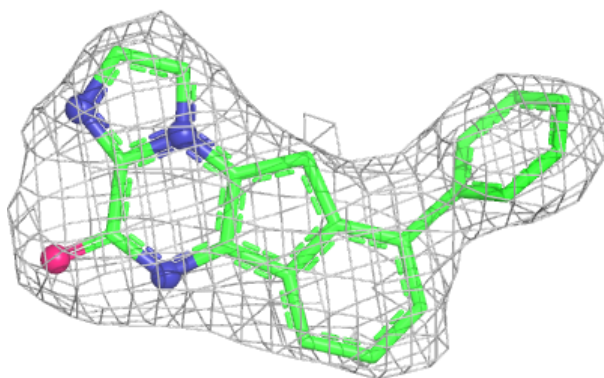


Electron density around 2K9 K 900:

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

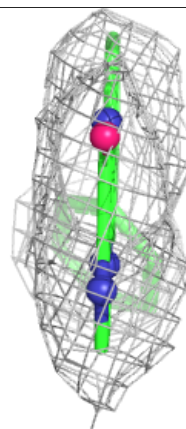
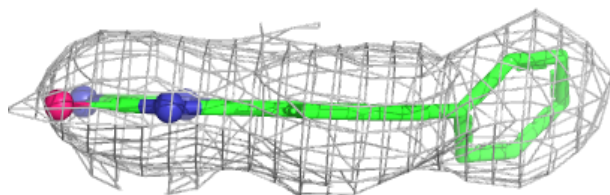
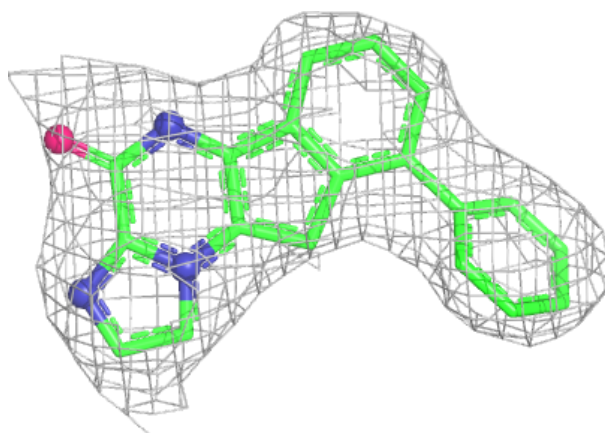
**Electron density around 2K9 R 900:**

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

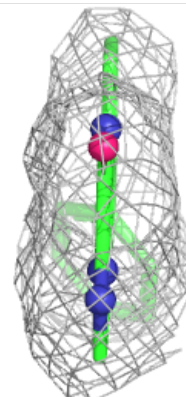
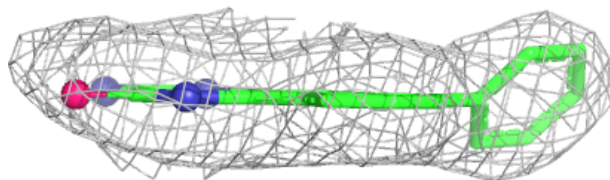
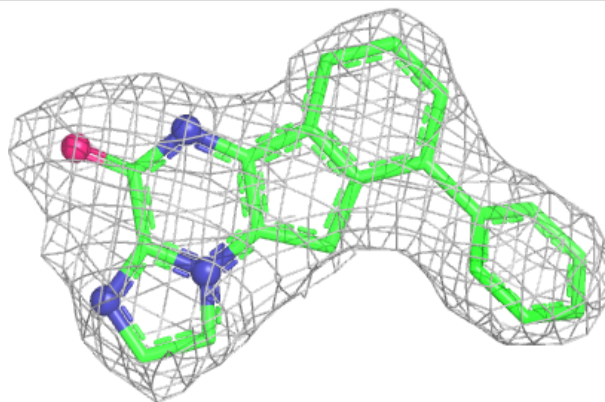


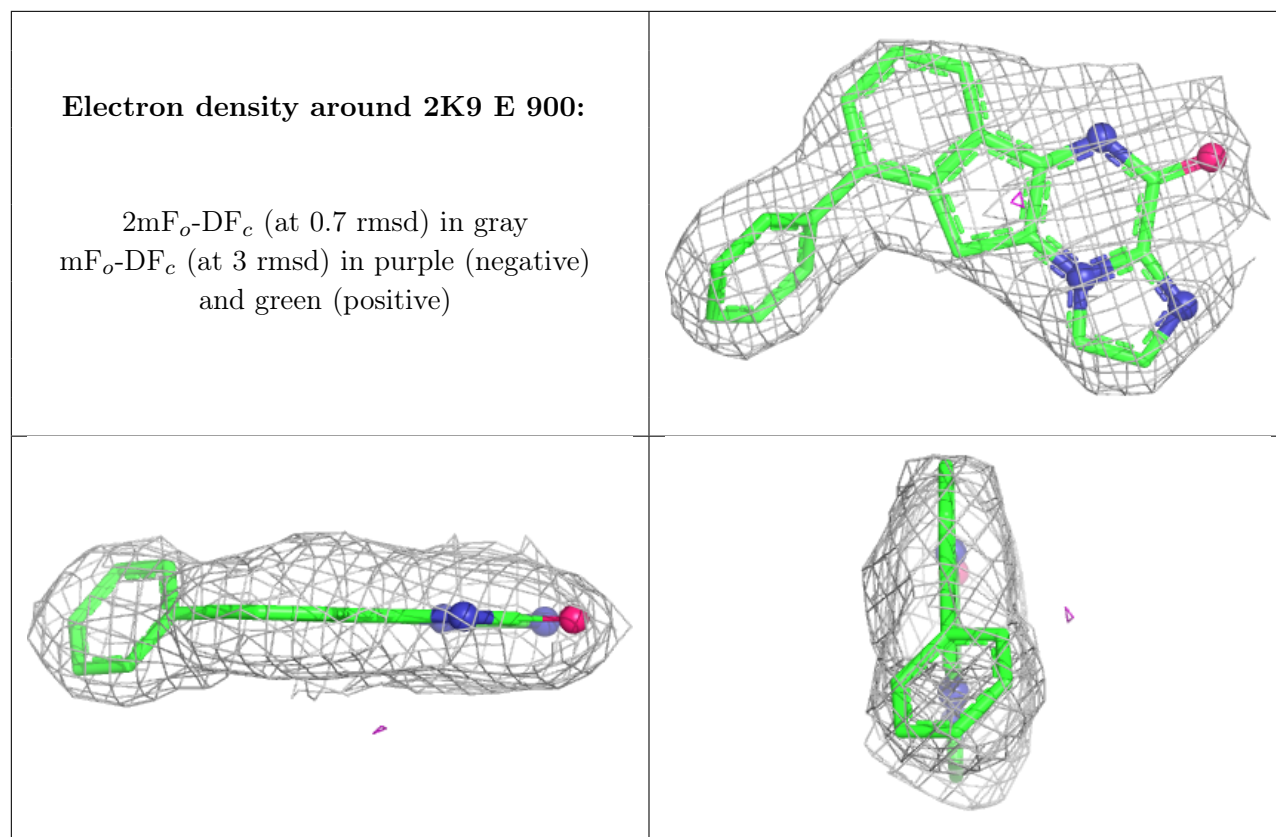
Electron density around 2K9 V 900:

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

**Electron density around 2K9 X 900:**

$2mF_o - DF_c$ (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.