



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 08:02 AM EDT

PDB ID : 4XYC
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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)

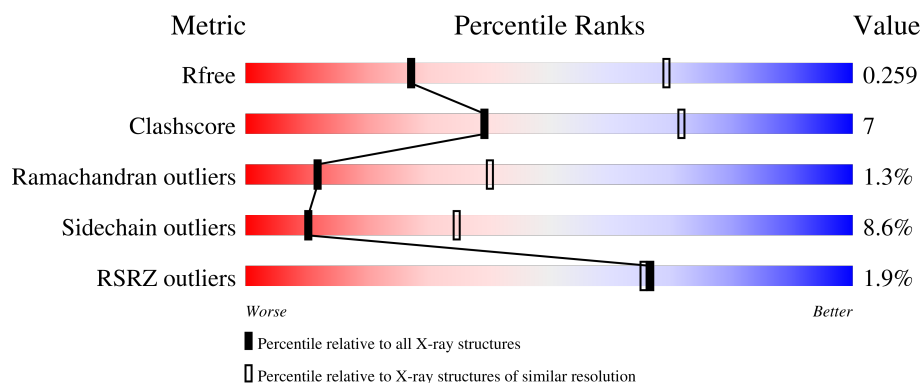
1 Overall quality at a glance

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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	<div> <div>4%</div> <div>78%</div> <div>18%</div> <div>..</div> </div>
1	B	478	<div> <div>3%</div> <div>70%</div> <div>26%</div> <div>..</div> </div>
1	C	478	<div> <div>%</div> <div>73%</div> <div>19%</div> <div>..</div> </div>

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

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Mol	Chain	Length	Quality of chain
1	D	478	
1	E	478	
1	F	478	
1	G	478	
1	H	478	
1	I	478	
1	J	478	
1	K	478	
1	L	478	
1	M	478	
1	N	478	
1	O	478	
1	P	478	
1	Q	478	
1	R	478	
1	S	478	
1	T	478	
1	U	478	
1	V	478	
1	W	478	
1	X	478	

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.

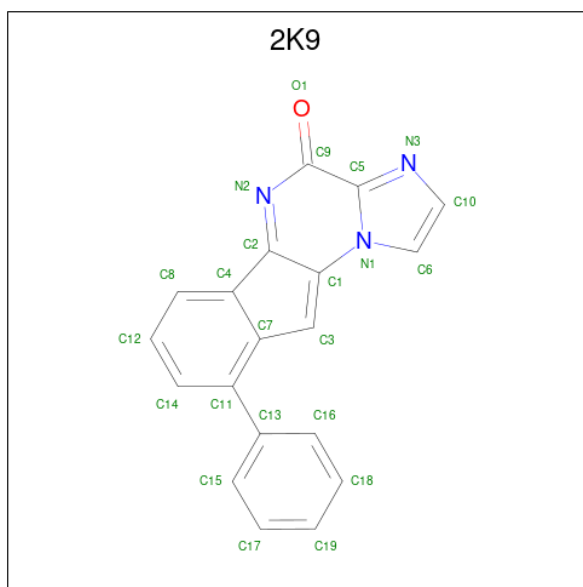
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	466	Total	C	N	O	S	0	0	0
			3693	2354	618	709	12			
1	B	464	Total	C	N	O	S	0	0	0
			3674	2342	613	707	12			
1	C	460	Total	C	N	O	S	0	0	0
			3645	2325	609	699	12			
1	D	466	Total	C	N	O	S	0	0	0
			3690	2352	616	710	12			
1	E	463	Total	C	N	O	S	0	0	0
			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 (three-letter code: 2K9) (formula: C₁₉H₁₁N₃O).



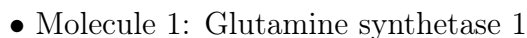
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			23	19	3	1		
2	B	1	Total	C	N	O	0	0
			23	19	3	1		
2	C	1	Total	C	N	O	0	0
			23	19	3	1		

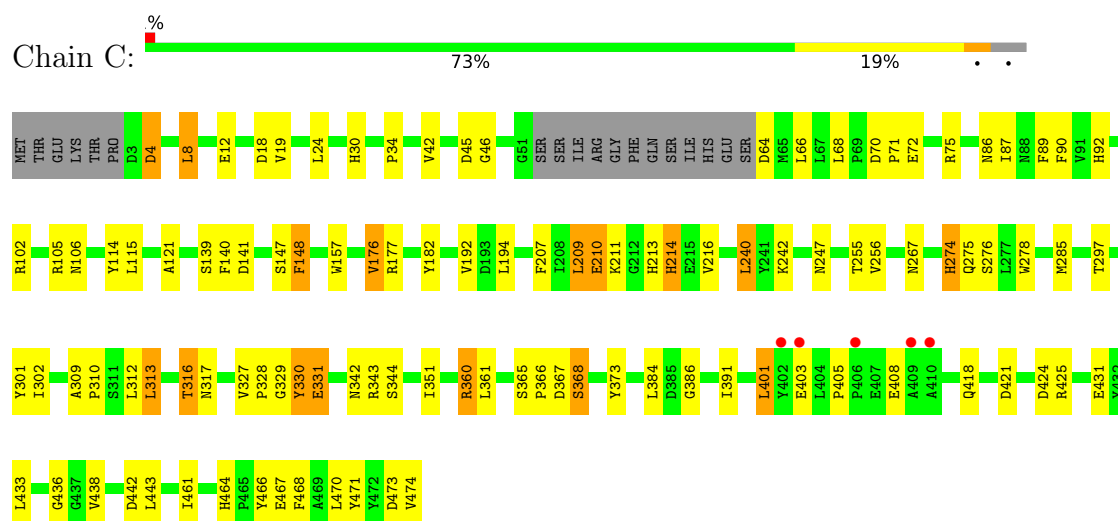
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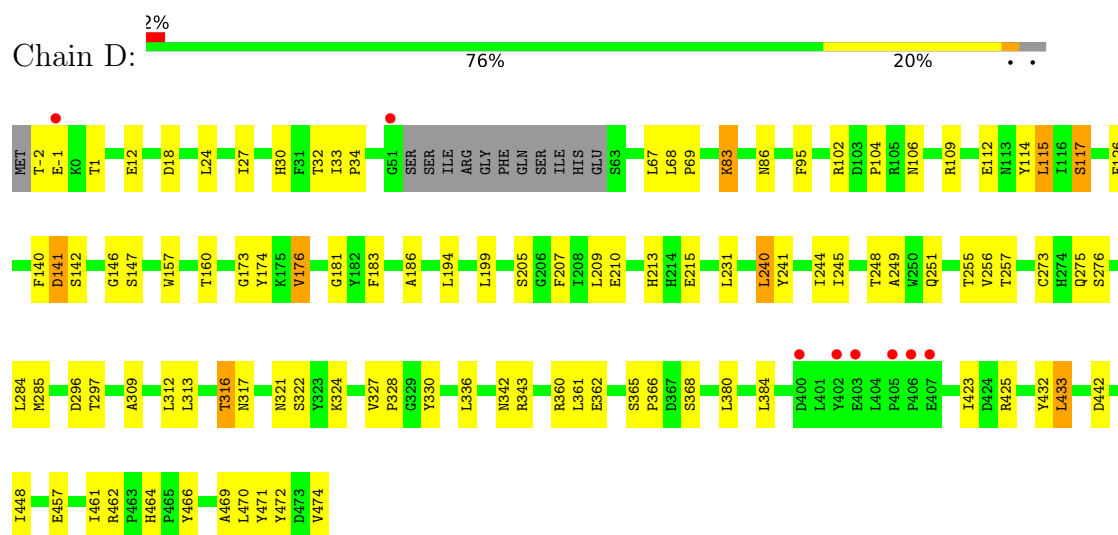
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total 23	C 19	N 3	O 1	0	0
2	E	1	Total 23	C 19	N 3	O 1	0	0
2	F	1	Total 23	C 19	N 3	O 1	0	0
2	G	1	Total 23	C 19	N 3	O 1	0	0
2	H	1	Total 23	C 19	N 3	O 1	0	0
2	I	1	Total 23	C 19	N 3	O 1	0	0
2	J	1	Total 23	C 19	N 3	O 1	0	0
2	K	1	Total 23	C 19	N 3	O 1	0	0
2	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

- Molecule 1: Glutamine synthetase 1

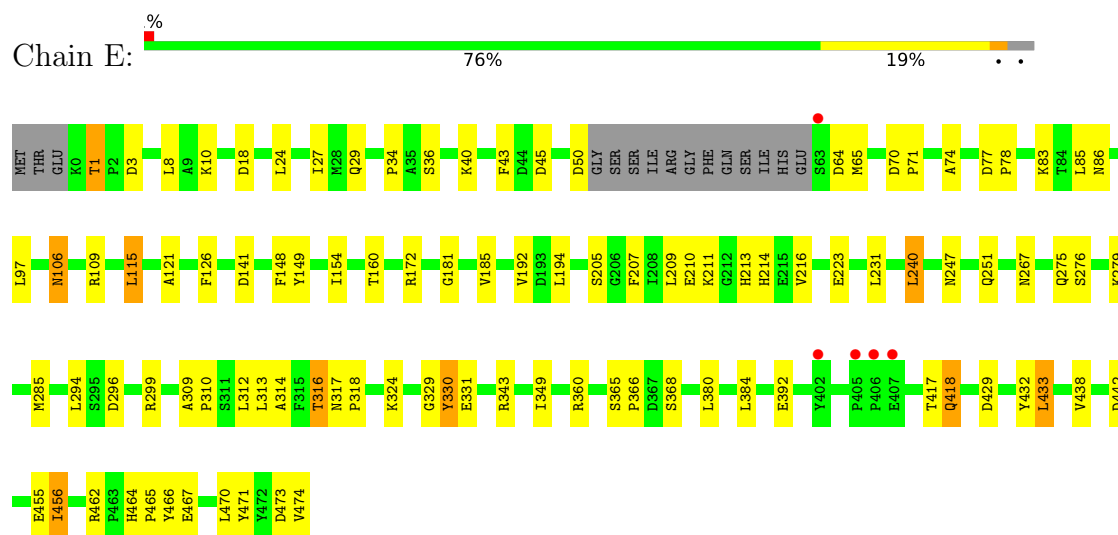




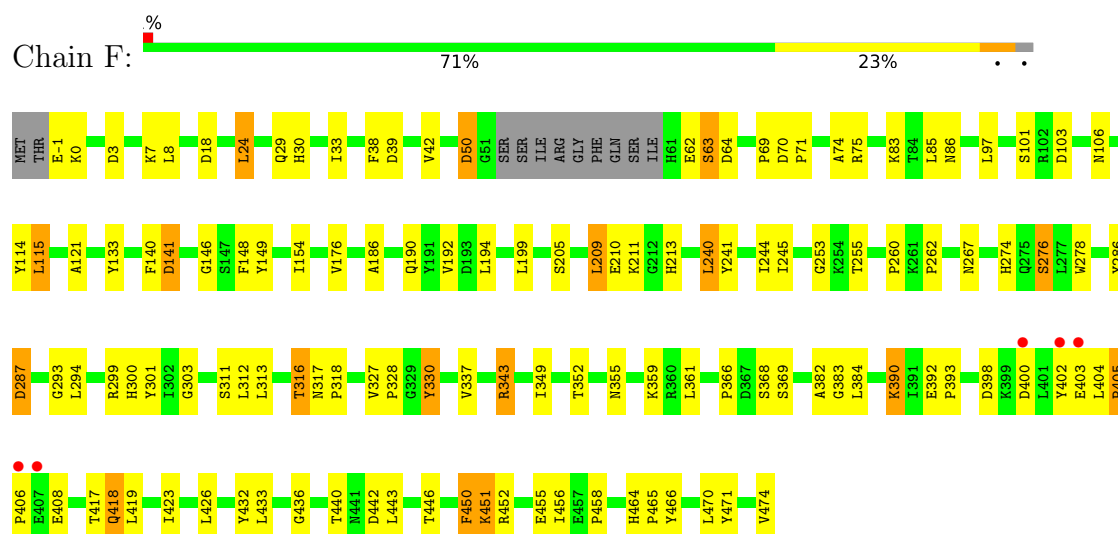
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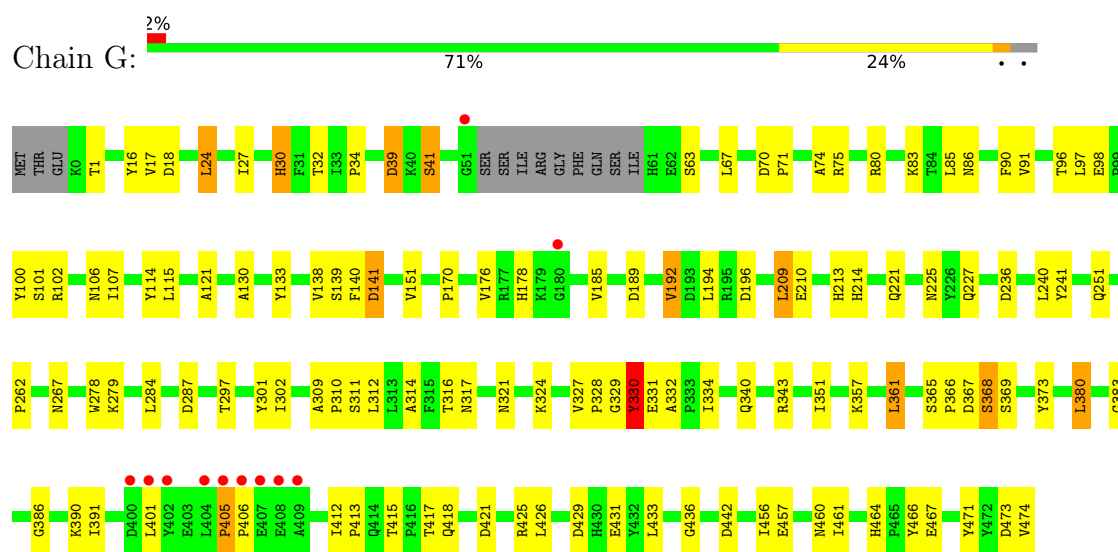
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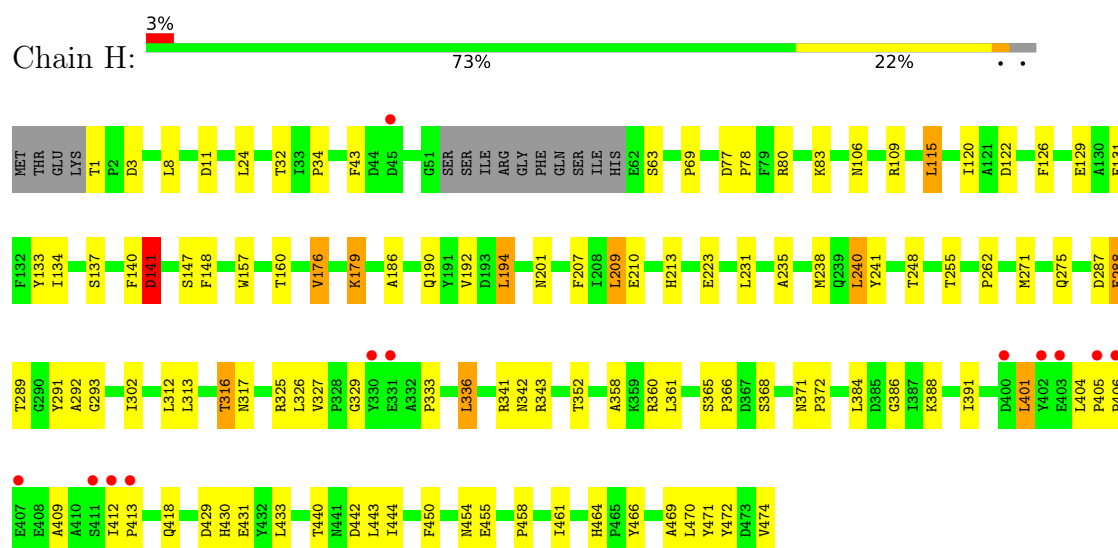
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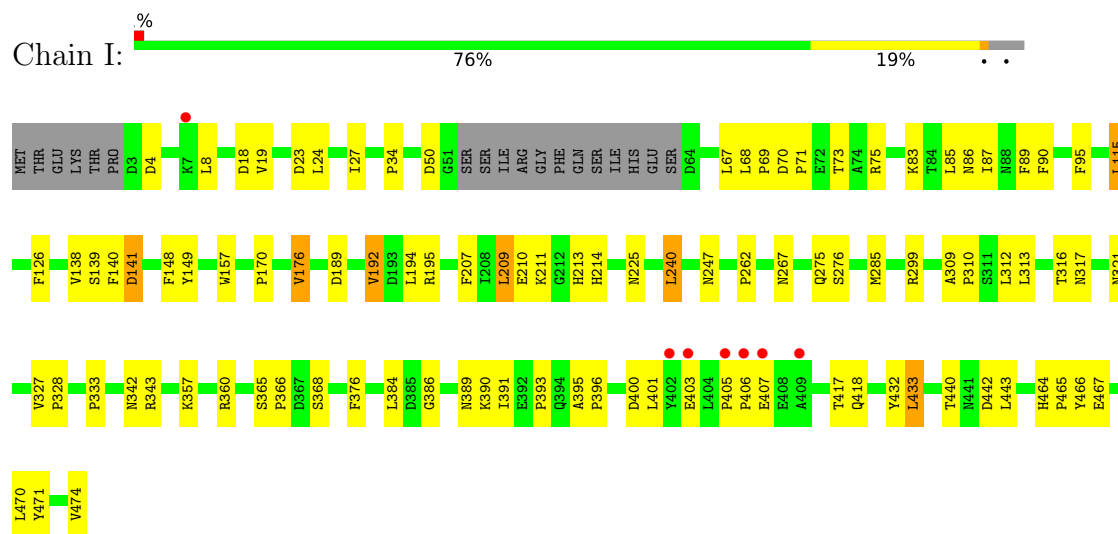
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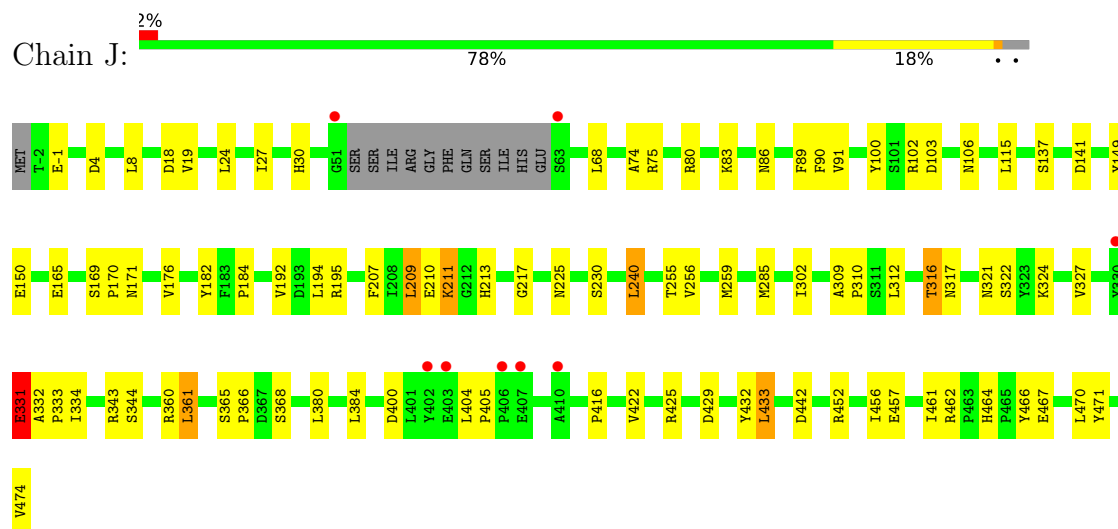
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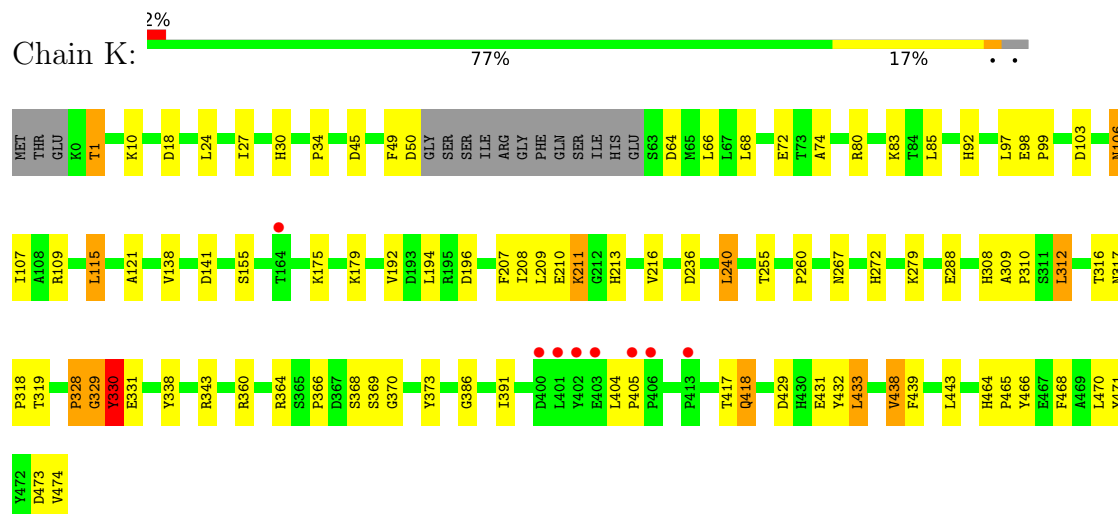
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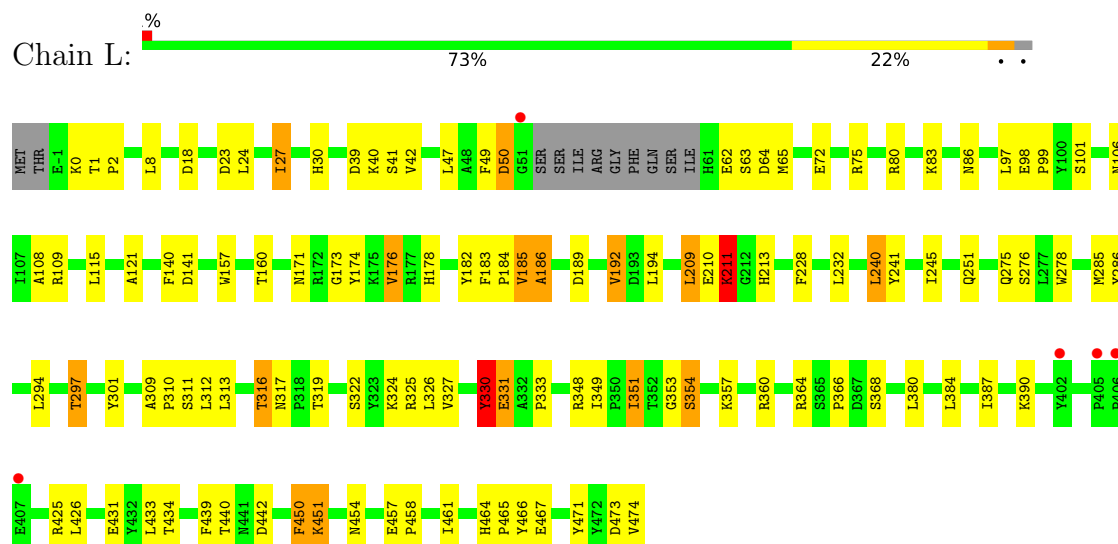
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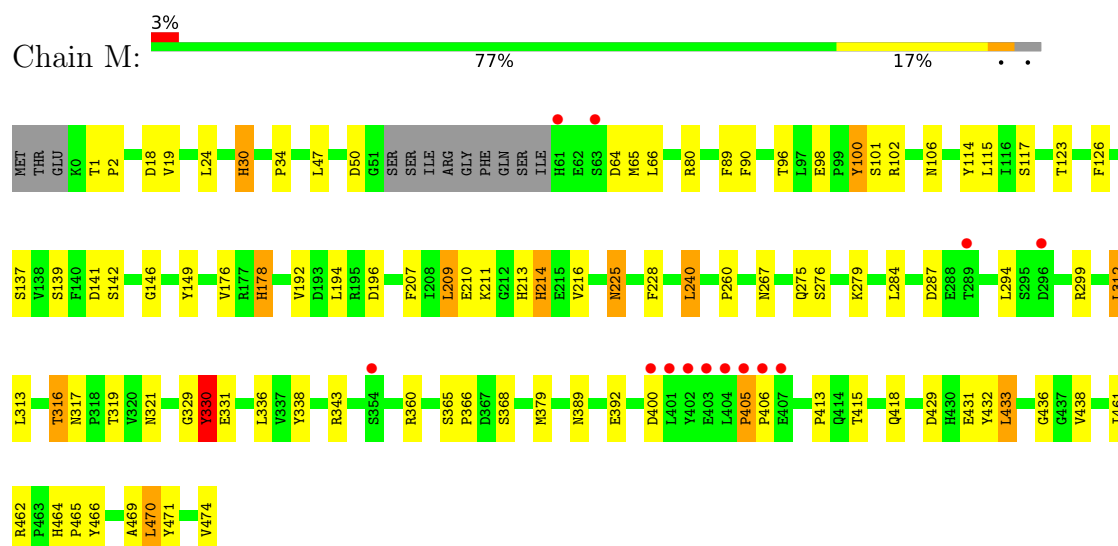
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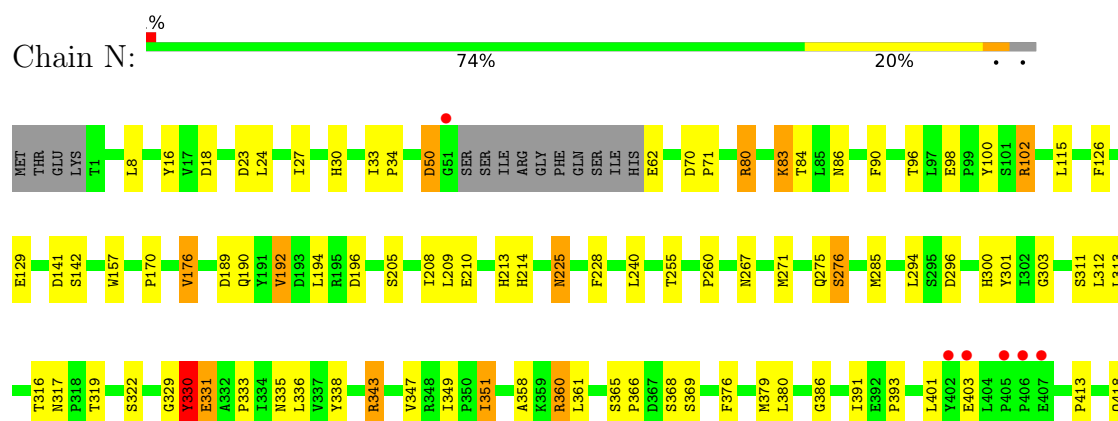
• Molecule 1: Glutamine synthetase 1



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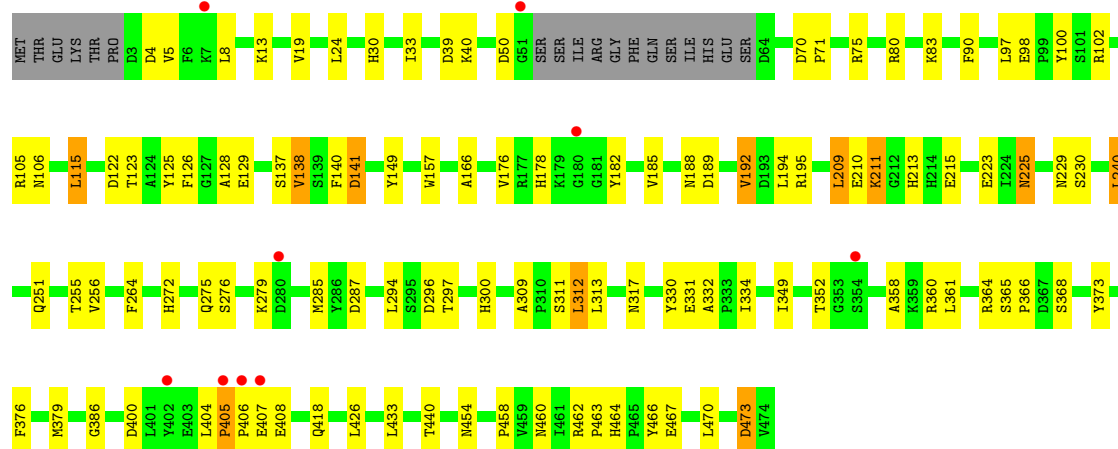
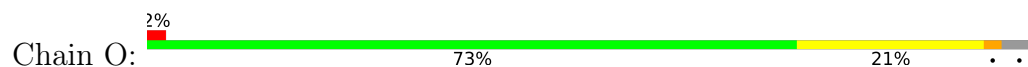


• Molecule 1: Glutamine synthetase 1

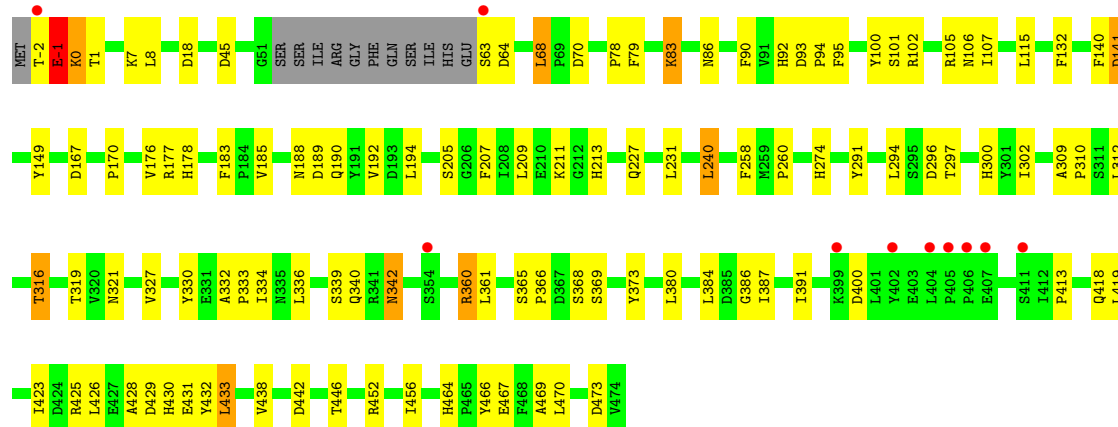
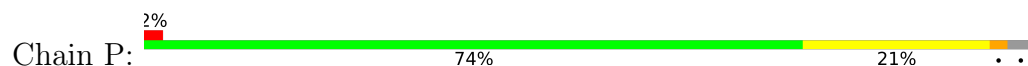




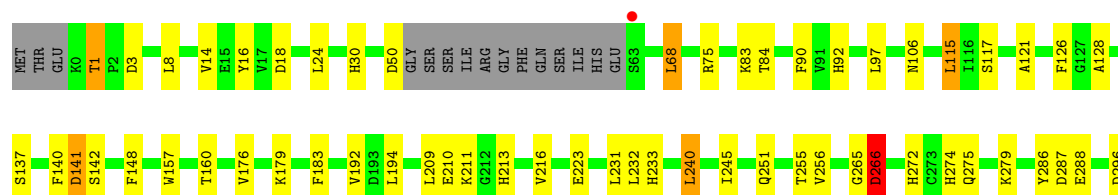
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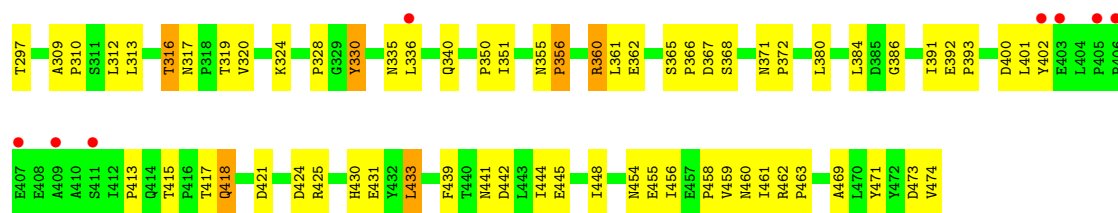


• Molecule 1: Glutamine synthetase 1

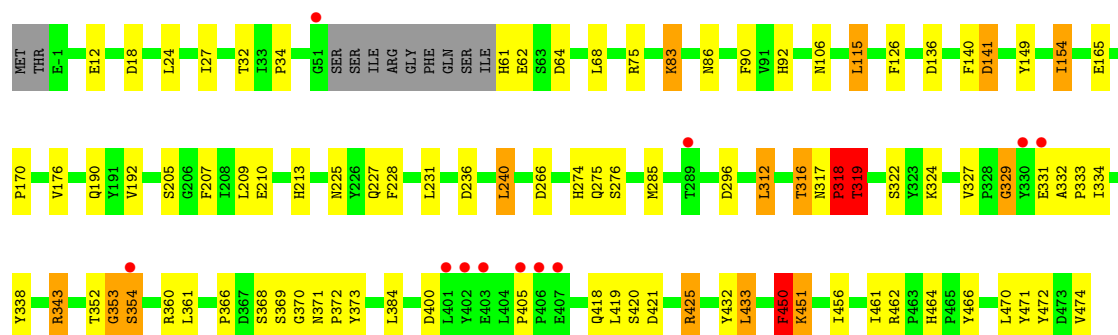
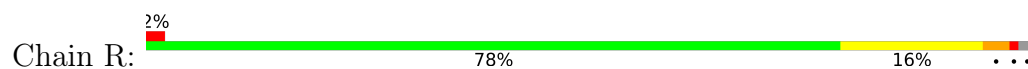


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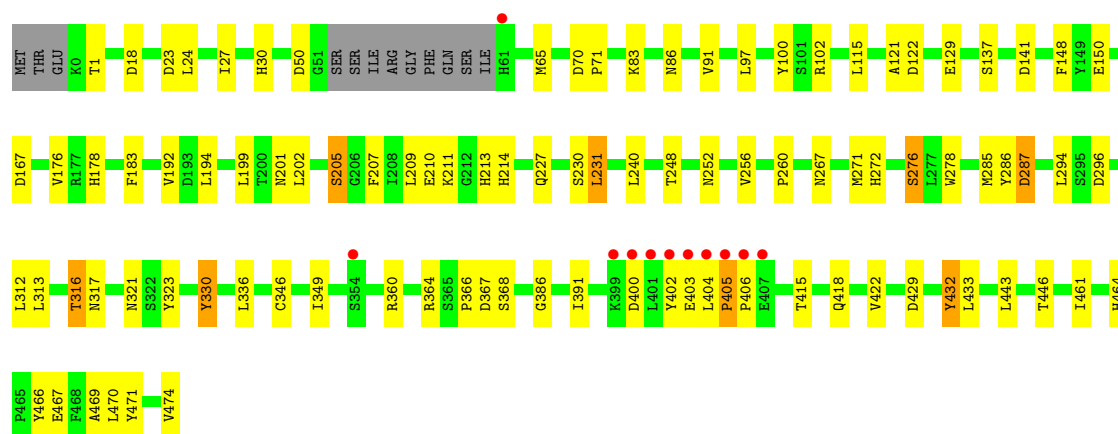
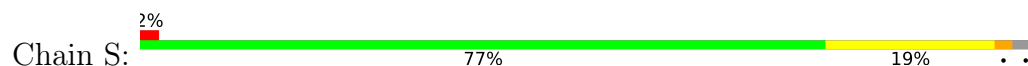




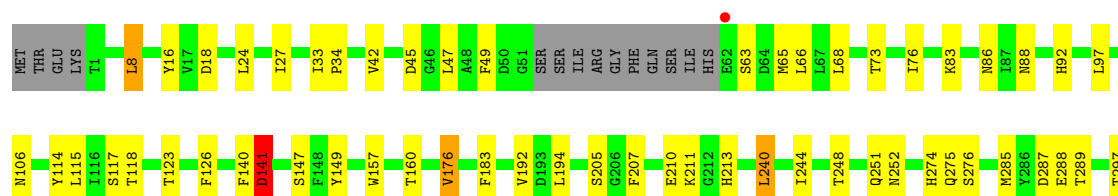
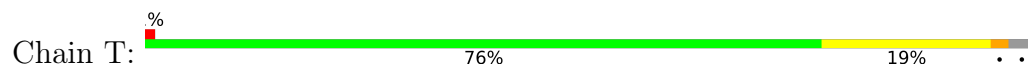
• Molecule 1: Glutamine synthetase 1

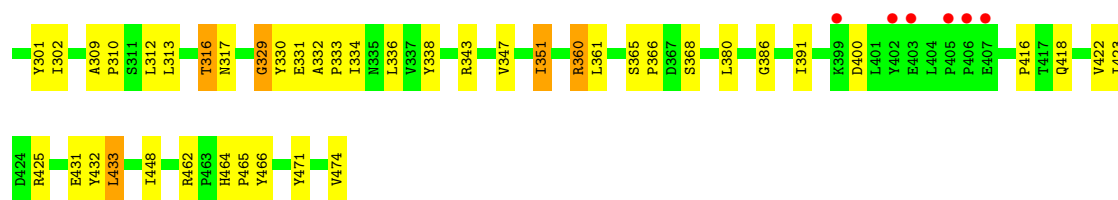


• Molecule 1: Glutamine synthetase 1

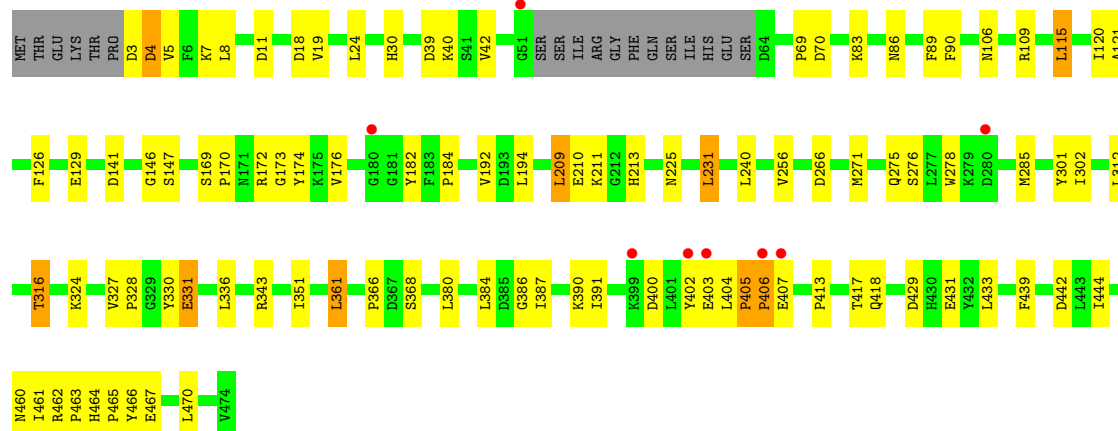
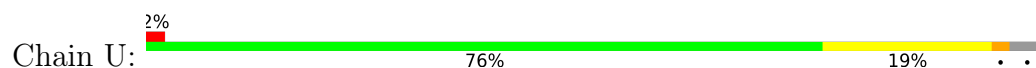


• Molecule 1: Glutamine synthetase 1

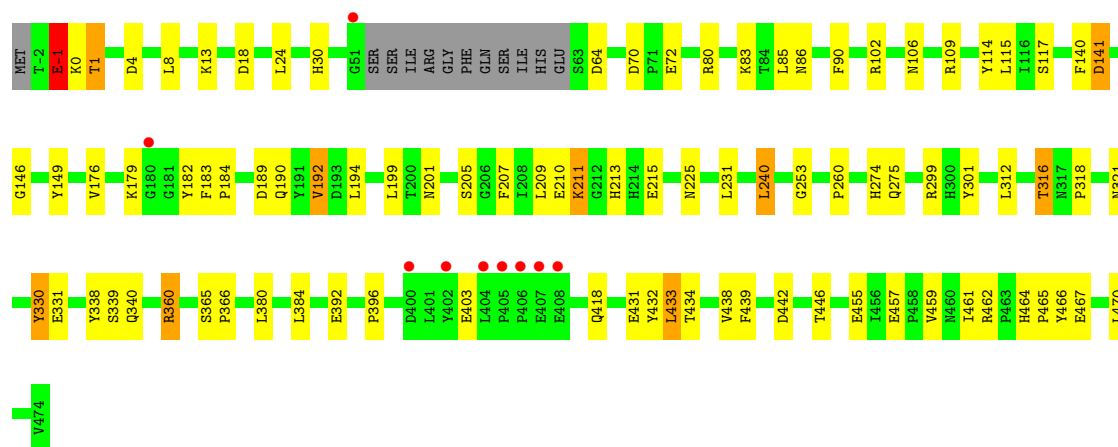
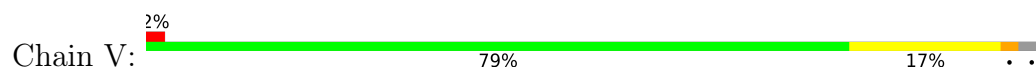




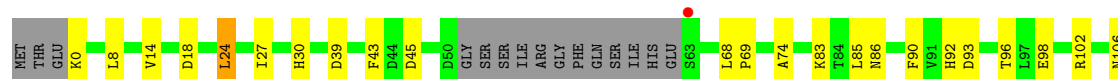
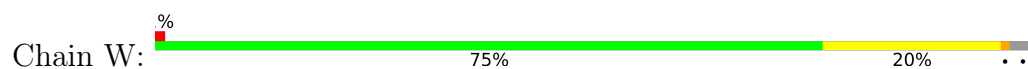
• Molecule 1: Glutamine synthetase 1

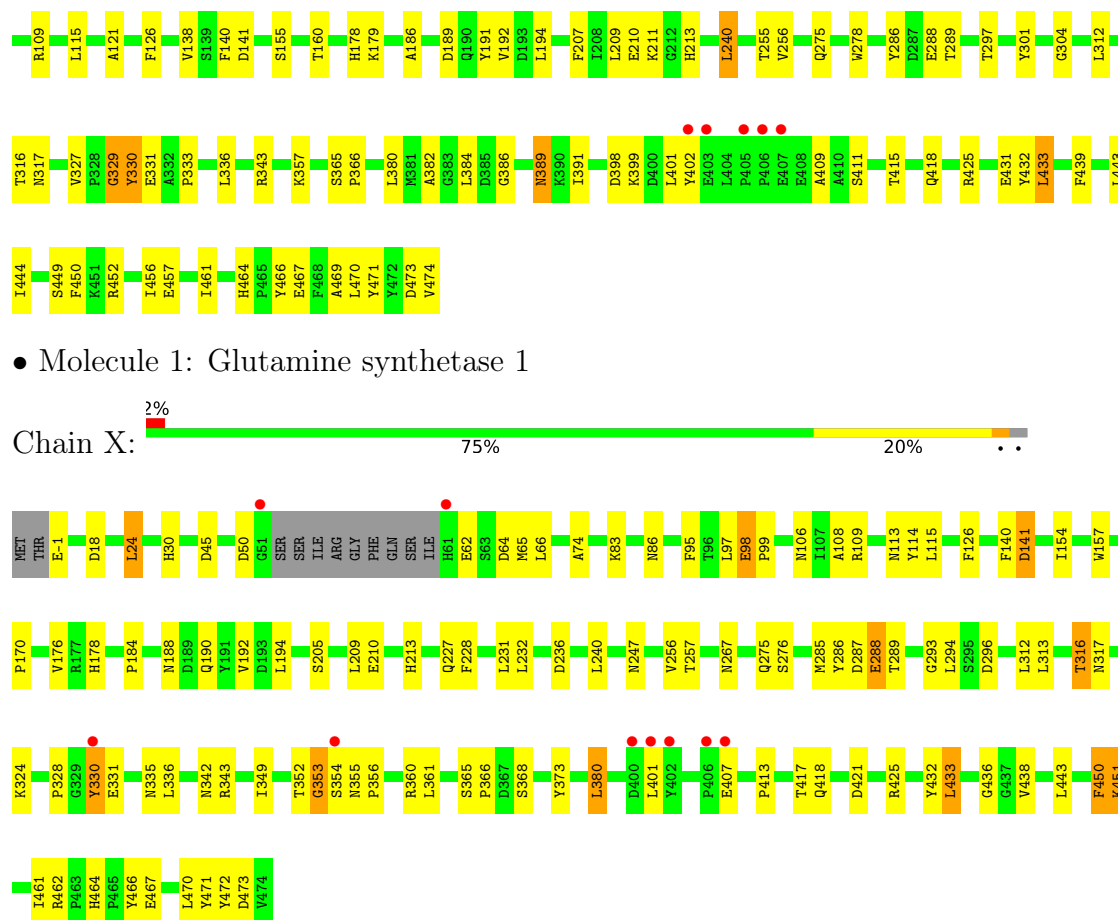


• Molecule 1: Glutamine synthetase 1



• Molecule 1: Glutamine synthetase 1





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 49.62 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-3.30) 99.9 (49.62-3.30)	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 , 0.259	Depositor DCC
R_{free} test set	11105 reflections (5.02%)	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 , 22.9	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	0.48	0/3797	0.59	0/5161
1	B	0.59	0/3777	0.62	0/5135
1	C	0.50	0/3747	0.62	0/5093
1	D	0.47	0/3793	0.61	0/5156
1	E	0.47	0/3773	0.62	0/5129
1	F	0.52	0/3806	0.63	1/5173 (0.0%)
1	G	0.49	0/3797	0.61	1/5161 (0.0%)
1	H	0.52	0/3777	0.63	0/5135
1	I	0.49	0/3747	0.61	1/5093 (0.0%)
1	J	0.46	0/3793	0.62	1/5156 (0.0%)
1	K	0.47	0/3773	0.61	0/5129
1	L	0.49	0/3806	0.65	1/5173 (0.0%)
1	M	0.53	0/3797	0.61	1/5161 (0.0%)
1	N	0.50	0/3777	0.61	1/5135 (0.0%)
1	O	0.51	0/3747	0.62	1/5093 (0.0%)
1	P	0.51	0/3793	0.62	0/5156
1	Q	0.57	0/3773	0.63	1/5129 (0.0%)
1	R	0.48	0/3806	0.65	5/5173 (0.1%)
1	S	0.47	0/3797	0.61	0/5161
1	T	0.51	0/3777	0.60	1/5135 (0.0%)
1	U	0.50	0/3747	0.62	0/5093
1	V	0.48	0/3793	0.61	0/5156
1	W	0.49	0/3773	0.61	0/5129
1	X	0.46	0/3806	0.63	2/5173 (0.0%)
All	All	0.50	0/90772	0.62	17/123388 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	1
1	R	0	1
All	All	0	2

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	318	PRO	N-CA-C	7.49	131.58	112.10
1	R	318	PRO	C-N-CA	7.06	139.35	121.70
1	R	318	PRO	CA-C-N	5.83	130.02	117.20
1	X	380	LEU	CA-CB-CG	5.83	128.70	115.30
1	N	380	LEU	CA-CB-CG	5.74	128.50	115.30
1	O	115	LEU	CA-CB-CG	5.67	128.33	115.30
1	Q	380	LEU	CA-CB-CG	5.64	128.27	115.30
1	X	450	PHE	C-N-CA	5.52	135.49	121.70
1	T	380	LEU	CA-CB-CG	5.48	127.91	115.30
1	J	209	LEU	CA-CB-CG	5.46	127.86	115.30
1	I	209	LEU	CA-CB-CG	5.44	127.81	115.30
1	L	450	PHE	C-N-CA	5.43	135.28	121.70
1	R	319	THR	N-CA-CB	5.39	120.54	110.30
1	G	380	LEU	CA-CB-CG	5.31	127.50	115.30
1	R	450	PHE	C-N-CA	5.25	134.83	121.70
1	M	115	LEU	CA-CB-CG	5.06	126.94	115.30
1	F	450	PHE	C-N-CA	5.04	134.31	121.70

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

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	53	0
1	B	3674	0	3503	81	0
1	C	3645	0	3475	61	0
1	D	3690	0	3523	58	0
1	E	3670	0	3507	59	0
1	F	3702	0	3529	78	0
1	G	3693	0	3523	73	0
1	H	3674	0	3503	62	0
1	I	3645	0	3475	56	0
1	J	3690	0	3523	50	0
1	K	3670	0	3507	46	0
1	L	3702	0	3529	69	0
1	M	3693	0	3523	61	0
1	N	3674	0	3503	63	0
1	O	3645	0	3475	59	0
1	P	3690	0	3523	55	0
1	Q	3670	0	3507	64	0
1	R	3702	0	3529	62	0
1	S	3693	0	3523	47	0
1	T	3674	0	3503	58	0
1	U	3645	0	3475	50	0
1	V	3690	0	3523	49	0
1	W	3670	0	3507	56	0
1	X	3702	0	3529	58	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1283	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 7.

All (1283) 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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:330:TYR:O	1:A:331:GLU:HB2	1.99	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:HIS:CD2	1:A:466:TYR:H	2.16	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:405:PRO:C	1:I:407:GLU:H	2.07	0.56
1:R:213:HIS:HA	1:R:225:ASN:ND2	2.20	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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: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:W:409:ALA:C	1:W:411:SER:H	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:W:24:LEU:HD21	1:W:443:LEU:HD11	1.90	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: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:B:291:TYR:C	1:B:293:GLY:H	2.13	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: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: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: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
1:C:121:ALA:HB1	1:C:278:TRP:O	2.11	0.50
1:F:50:ASP:OD2	1:F:50:ASP:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:T:329:GLY:C	1:T:331:GLU:H	2.14	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: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
1:A:207:PHE:HE1	1:A:240:LEU:HD13	1.76	0.50
1:E:18:ASP:CB	1:E:86:ASN:HD22	2.23	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:I:405:PRO:C	1:I:407:GLU:N	2.65	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
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:N:376:PHE:HA	1:N:379:MET:HE3	1.95	0.49
1:V:339:SER:OG	1:V:340:GLN:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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: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:O:189:ASP:CG	1:O:195:ARG:HH12	2.16	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:G:236:ASP:OD1	1:G:373:TYR:OH	2.24	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: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:K:329:GLY:C	1:K:331:GLU:H	2.17	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
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:C:473:ASP:HB2	1:O:178:HIS:CE1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:I:140:PHE:O	1:I:141:ASP:HB3	2.16	0.46
1:M:329:GLY:C	1:M:331:GLU:H	2.19	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O:376:PHE:HA	1:O:379:MET:HE3	1.98	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:N:329:GLY:C	1:N:331:GLU:H	2.20	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
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:K:45:ASP:O	1:K:66:LEU:HD11	2.16	0.45
1:C:86:ASN:C	1:C:87:ILE:HG13	2.37	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:C:148:PHE:CD1	1:C:148:PHE:C	2.90	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:W:155:SER:HG	1:W:191:TYR:HE1	1.63	0.45
1:A:18:ASP:OD2	1:A:30:HIS:HD2	2.00	0.45
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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:M:287:ASP:C	1:M:287:ASP:OD1	2.55	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:H:291:TYR:C	1:H:293:GLY:H	2.21	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:E:455:GLU:O	1:E:456:ILE:C	2.56	0.44
1:H:210:GLU:H	1:H:213:HIS:CD2	2.32	0.44
1:N:96:THR:OG1	1:N:98:GLU:HB2	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:W:121:ALA:HB1	1:W:278:TRP:O	2.18	0.44
1:W:329:GLY:C	1:W:331:GLU:H	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:49:PHE:HD1	1:L:65:MET:HE2	1.83	0.43
1:M:389:ASN:N	1:M:389:ASN:HD22	2.16	0.43
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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:464:HIS:HD2	1:O:466:TYR:N	2.09	0.43
1:Q:160:THR:OG1	1:R:140:PHE:CE1	2.72	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: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:U:3:ASP:C	1:U:5:VAL:H	2.22	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: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: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: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
1:H:430:HIS:CD2	1:H:444:ILE:HG21	2.53	0.42
1:I:189:ASP:CG	1:I:195:ARG:HH12	2.22	0.42
1:J:100:TYR:CE2	1:J:102:ARG:HB2	2.54	0.42
1:M:276:SER:CB	2:M:900:2K9:H11	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:Q:455:GLU:C	1:Q:458:PRO:HD2	2.40	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: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:X:471:TYR:O	1:X:472:TYR:C	2.56	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:207:PHE:CE1	1:M:240:LEU:HD13	2.54	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: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: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:R:316:THR:C	1:R:318:PRO:HD3	2.40	0.42
1:U:404:LEU:O	1:U:405:PRO:C	2.58	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: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
1:B:74:ALA:HB1	1:B:85:LEU:HD11	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
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: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: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:327:VAL:CG2	1:D:328:PRO:HD2	2.50	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:L:454:ASN:C	1:L:458:PRO:HG2	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:SER:N	1:B:366:PRO:CD	2.83	0.41
1:H:455:GLU:O	1:H:458:PRO:HD2	2.20	0.41
1:I:138:VAL:HG22	1:I:139:SER:N	2.36	0.41
1:N:338:TYR:HA	1:N:347:VAL:O	2.21	0.41
1:S:405:PRO:HA	1:S:406:PRO:HD3	1.85	0.41
1:X:256:VAL:CG1	1:X:257:THR:N	2.83	0.41
1:A:172:ARG:NH2	1:B:253:GLY:HA2	2.36	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: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
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:V:210:GLU:O	1:V:211:LYS:C	2.58	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:F:293:GLY:HA3	1:F:359:LYS:HZ1	1.86	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:S:230:SER:O	1:S:231:LEU:C	2.58	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:F:455:GLU:C	1:F:458:PRO:HD2	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:329:GLY:C	1:G:331:GLU:H	2.23	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: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: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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:367:ASP:C	1:G:369:SER:H	2.24	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:J:259:MET:HE3	1:J:259:MET:HB2	2.01	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:138:VAL:HG11	1:R:472:TYR:CZ	2.56	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
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: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:R:329:GLY:C	1:R:331:GLU:H	2.24	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	462/478 (97%)	432 (94%)	25 (5%)	5 (1%)	14 45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	460/478 (96%)	414 (90%)	40 (9%)	6 (1%)	12	40
1	C	456/478 (95%)	408 (90%)	44 (10%)	4 (1%)	17	48
1	D	462/478 (97%)	430 (93%)	30 (6%)	2 (0%)	34	66
1	E	459/478 (96%)	421 (92%)	32 (7%)	6 (1%)	12	40
1	F	463/478 (97%)	419 (90%)	38 (8%)	6 (1%)	12	40
1	G	462/478 (97%)	426 (92%)	28 (6%)	8 (2%)	9	35
1	H	460/478 (96%)	424 (92%)	30 (6%)	6 (1%)	12	40
1	I	456/478 (95%)	421 (92%)	30 (7%)	5 (1%)	14	45
1	J	462/478 (97%)	432 (94%)	26 (6%)	4 (1%)	17	48
1	K	459/478 (96%)	418 (91%)	34 (7%)	7 (2%)	10	38
1	L	463/478 (97%)	424 (92%)	29 (6%)	10 (2%)	6	30
1	M	462/478 (97%)	425 (92%)	32 (7%)	5 (1%)	14	45
1	N	460/478 (96%)	422 (92%)	34 (7%)	4 (1%)	17	48
1	O	456/478 (95%)	421 (92%)	29 (6%)	6 (1%)	12	40
1	P	462/478 (97%)	418 (90%)	35 (8%)	9 (2%)	8	34
1	Q	459/478 (96%)	420 (92%)	31 (7%)	8 (2%)	9	35
1	R	463/478 (97%)	422 (91%)	32 (7%)	9 (2%)	8	34
1	S	462/478 (97%)	424 (92%)	32 (7%)	6 (1%)	12	40
1	T	460/478 (96%)	420 (91%)	34 (7%)	6 (1%)	12	40
1	U	456/478 (95%)	425 (93%)	27 (6%)	4 (1%)	17	48
1	V	462/478 (97%)	429 (93%)	26 (6%)	7 (2%)	10	38
1	W	459/478 (96%)	426 (93%)	29 (6%)	4 (1%)	17	48
1	X	463/478 (97%)	428 (92%)	28 (6%)	7 (2%)	10	38
All	All	11048/11472 (96%)	10149 (92%)	755 (7%)	144 (1%)	12	40

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	16	46
1	B	392/405 (97%)	360 (92%)	32 (8%)	11	36
1	C	388/405 (96%)	349 (90%)	39 (10%)	7	27
1	D	394/405 (97%)	361 (92%)	33 (8%)	11	35
1	E	392/405 (97%)	359 (92%)	33 (8%)	11	35
1	F	395/405 (98%)	351 (89%)	44 (11%)	6	23
1	G	394/405 (97%)	361 (92%)	33 (8%)	11	35
1	H	392/405 (97%)	358 (91%)	34 (9%)	10	34
1	I	388/405 (96%)	363 (94%)	25 (6%)	17	46
1	J	394/405 (97%)	363 (92%)	31 (8%)	12	37
1	K	392/405 (97%)	356 (91%)	36 (9%)	9	31
1	L	395/405 (98%)	363 (92%)	32 (8%)	11	36
1	M	394/405 (97%)	360 (91%)	34 (9%)	10	35
1	N	392/405 (97%)	353 (90%)	39 (10%)	8	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	388/405 (96%)	351 (90%)	37 (10%)	8	29
1	P	394/405 (97%)	359 (91%)	35 (9%)	9	32
1	Q	392/405 (97%)	357 (91%)	35 (9%)	9	32
1	R	395/405 (98%)	364 (92%)	31 (8%)	12	38
1	S	394/405 (97%)	360 (91%)	34 (9%)	10	35
1	T	392/405 (97%)	362 (92%)	30 (8%)	13	38
1	U	388/405 (96%)	350 (90%)	38 (10%)	8	29
1	V	394/405 (97%)	364 (92%)	30 (8%)	13	39
1	W	392/405 (97%)	358 (91%)	34 (9%)	10	34
1	X	395/405 (98%)	360 (91%)	35 (9%)	9	32
All	All	9420/9720 (97%)	8610 (91%)	810 (9%)	10	35

All (810) 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	240	LEU
1	A	251	GLN
1	A	297	THR
1	A	312	LEU
1	A	316	THR
1	A	330	TYR
1	A	343	ARG
1	A	360	ARG
1	A	361	LEU
1	A	368	SER
1	A	380	LEU
1	A	418	GLN

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Mol	Chain	Res	Type
1	A	433	LEU
1	A	442	ASP
1	A	470	LEU
1	B	4	ASP
1	B	8	LEU
1	B	62	GLU
1	B	63	SER
1	B	72	GLU
1	B	83	LYS
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	205	SER
1	B	240	LEU
1	B	256	VAL
1	B	288	GLU
1	B	312	LEU
1	B	316	THR
1	B	351	ILE
1	B	368	SER
1	B	380	LEU
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	457	GLU
1	B	470	LEU
1	C	4	ASP
1	C	8	LEU
1	C	24	LEU
1	C	64	ASP
1	C	139	SER
1	C	141	ASP
1	C	147	SER

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Mol	Chain	Res	Type
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
1	C	211	LYS
1	C	214	HIS
1	C	216	VAL
1	C	240	LEU
1	C	255	THR
1	C	256	VAL
1	C	267	ASN
1	C	274	HIS
1	C	297	THR
1	C	312	LEU
1	C	313	LEU
1	C	316	THR
1	C	330	TYR
1	C	343	ARG
1	C	360	ARG
1	C	367	ASP
1	C	368	SER
1	C	401	LEU
1	C	403	GLU
1	C	418	GLN
1	C	431	GLU
1	C	433	LEU
1	C	442	ASP
1	C	470	LEU
1	D	-2	THR
1	D	24	LEU
1	D	27	ILE
1	D	30	HIS
1	D	32	THR
1	D	67	LEU
1	D	83	LYS
1	D	115	LEU
1	D	117	SER
1	D	141	ASP

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Mol	Chain	Res	Type
1	D	142	SER
1	D	147	SER
1	D	176	VAL
1	D	183	PHE
1	D	194	LEU
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	342	ASN
1	D	360	ARG
1	D	361	LEU
1	D	368	SER
1	D	380	LEU
1	D	433	LEU
1	D	442	ASP
1	D	457	GLU
1	D	470	LEU
1	E	8	LEU
1	E	10	LYS
1	E	24	LEU
1	E	27	ILE
1	E	36	SER
1	E	40	LYS
1	E	45	ASP
1	E	64	ASP
1	E	65	MET
1	E	83	LYS
1	E	97	LEU
1	E	106	ASN
1	E	115	LEU
1	E	154	ILE
1	E	185	VAL
1	E	192	VAL
1	E	194	LEU
1	E	205	SER
1	E	240	LEU

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Mol	Chain	Res	Type
1	E	251	GLN
1	E	267	ASN
1	E	296	ASP
1	E	312	LEU
1	E	316	THR
1	E	330	TYR
1	E	360	ARG
1	E	368	SER
1	E	380	LEU
1	E	418	GLN
1	E	429	ASP
1	E	433	LEU
1	E	442	ASP
1	E	470	LEU
1	F	-1	GLU
1	F	0	LYS
1	F	3	ASP
1	F	7	LYS
1	F	8	LEU
1	F	24	LEU
1	F	39	ASP
1	F	50	ASP
1	F	62	GLU
1	F	64	ASP
1	F	83	LYS
1	F	97	LEU
1	F	115	LEU
1	F	141	ASP
1	F	148	PHE
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	240	LEU
1	F	255	THR
1	F	267	ASN
1	F	276	SER
1	F	312	LEU
1	F	316	THR

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Mol	Chain	Res	Type
1	F	330	TYR
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	398	ASP
1	F	400	ASP
1	F	402	TYR
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	41	SER
1	G	80	ARG
1	G	83	LYS
1	G	115	LEU
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	312	LEU
1	G	316	THR
1	G	330	TYR
1	G	343	ARG
1	G	361	LEU
1	G	368	SER

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Mol	Chain	Res	Type
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	H	8	LEU
1	H	11	ASP
1	H	32	THR
1	H	63	SER
1	H	83	LYS
1	H	115	LEU
1	H	122	ASP
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	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	401	LEU
1	H	418	GLN
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

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Mol	Chain	Res	Type
1	I	8	LEU
1	I	50	ASP
1	I	83	LYS
1	I	115	LEU
1	I	141	ASP
1	I	148	PHE
1	I	176	VAL
1	I	192	VAL
1	I	194	LEU
1	I	209	LEU
1	I	214	HIS
1	I	240	LEU
1	I	267	ASN
1	I	312	LEU
1	I	343	ARG
1	I	357	LYS
1	I	360	ARG
1	I	368	SER
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	4	ASP
1	J	8	LEU
1	J	24	LEU
1	J	27	ILE
1	J	68	LEU
1	J	80	ARG
1	J	83	LYS
1	J	141	ASP
1	J	150	GLU
1	J	176	VAL
1	J	192	VAL
1	J	194	LEU
1	J	211	LYS
1	J	230	SER
1	J	240	LEU
1	J	255	THR
1	J	256	VAL
1	J	285	MET

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Mol	Chain	Res	Type
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	400	ASP
1	J	429	ASP
1	J	433	LEU
1	J	442	ASP
1	J	470	LEU
1	K	1	THR
1	K	27	ILE
1	K	64	ASP
1	K	72	GLU
1	K	80	ARG
1	K	83	LYS
1	K	97	LEU
1	K	98	GLU
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	288	GLU
1	K	312	LEU
1	K	316	THR
1	K	330	TYR
1	K	338	TYR
1	K	343	ARG

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Mol	Chain	Res	Type
1	K	360	ARG
1	K	368	SER
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	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	141	ASP
1	L	160	THR
1	L	176	VAL
1	L	182	TYR
1	L	183	PHE
1	L	192	VAL
1	L	194	LEU
1	L	209	LEU
1	L	211	LYS
1	L	240	LEU
1	L	251	GLN
1	L	297	THR
1	L	312	LEU
1	L	316	THR
1	L	330	TYR
1	L	354	SER
1	L	360	ARG
1	L	368	SER
1	L	390	LYS
1	L	431	GLU
1	L	433	LEU
1	L	442	ASP
1	M	24	LEU
1	M	30	HIS
1	M	64	ASP

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Mol	Chain	Res	Type
1	M	65	MET
1	M	80	ARG
1	M	100	TYR
1	M	117	SER
1	M	123	THR
1	M	139	SER
1	M	141	ASP
1	M	142	SER
1	M	176	VAL
1	M	178	HIS
1	M	192	VAL
1	M	194	LEU
1	M	209	LEU
1	M	214	HIS
1	M	216	VAL
1	M	225	ASN
1	M	240	LEU
1	M	267	ASN
1	M	312	LEU
1	M	316	THR
1	M	330	TYR
1	M	338	TYR
1	M	343	ARG
1	M	360	ARG
1	M	368	SER
1	M	400	ASP
1	M	418	GLN
1	M	429	ASP
1	M	431	GLU
1	M	433	LEU
1	M	470	LEU
1	N	8	LEU
1	N	23	ASP
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	83	LYS
1	N	102	ARG
1	N	115	LEU

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Mol	Chain	Res	Type
1	N	141	ASP
1	N	142	SER
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
1	N	255	THR
1	N	267	ASN
1	N	276	SER
1	N	296	ASP
1	N	312	LEU
1	N	330	TYR
1	N	331	GLU
1	N	343	ARG
1	N	351	ILE
1	N	360	ARG
1	N	361	LEU
1	N	368	SER
1	N	403	GLU
1	N	418	GLN
1	N	431	GLU
1	N	433	LEU
1	N	449	SER
1	N	470	LEU
1	O	4	ASP
1	O	8	LEU
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	182	TYR
1	O	192	VAL
1	O	194	LEU

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Mol	Chain	Res	Type
1	O	209	LEU
1	O	211	LYS
1	O	215	GLU
1	O	225	ASN
1	O	240	LEU
1	O	251	GLN
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	400	ASP
1	O	407	GLU
1	O	418	GLN
1	O	433	LEU
1	O	440	THR
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	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	167	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

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Mol	Chain	Res	Type
1	P	205	SER
1	P	240	LEU
1	P	296	ASP
1	P	297	THR
1	P	312	LEU
1	P	316	THR
1	P	342	ASN
1	P	360	ARG
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	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	148	PHE
1	Q	179	LYS
1	Q	183	PHE
1	Q	192	VAL
1	Q	194	LEU
1	Q	240	LEU
1	Q	251	GLN
1	Q	255	THR
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

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Mol	Chain	Res	Type
1	Q	367	ASP
1	Q	368	SER
1	Q	400	ASP
1	Q	418	GLN
1	Q	424	ASP
1	Q	431	GLU
1	Q	433	LEU
1	Q	441	ASN
1	Q	442	ASP
1	R	24	LEU
1	R	27	ILE
1	R	32	THR
1	R	61	HIS
1	R	62	GLU
1	R	64	ASP
1	R	83	LYS
1	R	115	LEU
1	R	141	ASP
1	R	154	ILE
1	R	176	VAL
1	R	190	GLN
1	R	192	VAL
1	R	205	SER
1	R	240	LEU
1	R	266	ASP
1	R	296	ASP
1	R	312	LEU
1	R	316	THR
1	R	338	TYR
1	R	343	ARG
1	R	354	SER
1	R	360	ARG
1	R	361	LEU
1	R	368	SER
1	R	400	ASP
1	R	418	GLN
1	R	420	SER
1	R	425	ARG
1	R	433	LEU
1	R	470	LEU
1	S	24	LEU
1	S	83	LYS

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Mol	Chain	Res	Type
1	S	97	LEU
1	S	115	LEU
1	S	122	ASP
1	S	141	ASP
1	S	148	PHE
1	S	150	GLU
1	S	167	ASP
1	S	176	VAL
1	S	183	PHE
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	276	SER
1	S	296	ASP
1	S	312	LEU
1	S	316	THR
1	S	330	TYR
1	S	360	ARG
1	S	367	ASP
1	S	368	SER
1	S	400	ASP
1	S	402	TYR
1	S	403	GLU
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	24	LEU
1	T	27	ILE
1	T	83	LYS
1	T	97	LEU
1	T	115	LEU
1	T	117	SER
1	T	123	THR
1	T	141	ASP
1	T	147	SER

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Mol	Chain	Res	Type
1	T	160	THR
1	T	176	VAL
1	T	183	PHE
1	T	192	VAL
1	T	194	LEU
1	T	205	SER
1	T	240	LEU
1	T	251	GLN
1	T	297	THR
1	T	312	LEU
1	T	316	THR
1	T	343	ARG
1	T	351	ILE
1	T	360	ARG
1	T	368	SER
1	T	400	ASP
1	T	418	GLN
1	T	425	ARG
1	T	431	GLU
1	T	433	LEU
1	U	4	ASP
1	U	8	LEU
1	U	24	LEU
1	U	39	ASP
1	U	40	LYS
1	U	83	LYS
1	U	115	LEU
1	U	141	ASP
1	U	147	SER
1	U	176	VAL
1	U	192	VAL
1	U	194	LEU
1	U	209	LEU
1	U	211	LYS
1	U	231	LEU
1	U	240	LEU
1	U	256	VAL
1	U	266	ASP
1	U	312	LEU
1	U	316	THR
1	U	330	TYR
1	U	331	GLU

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Mol	Chain	Res	Type
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	402	TYR
1	U	403	GLU
1	U	407	GLU
1	U	418	GLN
1	U	429	ASP
1	U	431	GLU
1	U	433	LEU
1	U	442	ASP
1	U	470	LEU
1	V	-1	GLU
1	V	0	LYS
1	V	13	LYS
1	V	24	LEU
1	V	64	ASP
1	V	80	ARG
1	V	83	LYS
1	V	85	LEU
1	V	141	ASP
1	V	149	TYR
1	V	176	VAL
1	V	182	TYR
1	V	183	PHE
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	312	LEU
1	V	316	THR
1	V	330	TYR
1	V	360	ARG
1	V	380	LEU
1	V	403	GLU
1	V	418	GLN

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Mol	Chain	Res	Type
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	39	ASP
1	W	45	ASP
1	W	83	LYS
1	W	115	LEU
1	W	141	ASP
1	W	160	THR
1	W	179	LYS
1	W	192	VAL
1	W	194	LEU
1	W	240	LEU
1	W	255	THR
1	W	256	VAL
1	W	289	THR
1	W	297	THR
1	W	312	LEU
1	W	316	THR
1	W	330	TYR
1	W	343	ARG
1	W	357	LYS
1	W	389	ASN
1	W	398	ASP
1	W	399	LYS
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	24	LEU
1	X	50	ASP
1	X	62	GLU

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Mol	Chain	Res	Type
1	X	64	ASP
1	X	65	MET
1	X	83	LYS
1	X	95	PHE
1	X	97	LEU
1	X	98	GLU
1	X	113	ASN
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	267	ASN
1	X	296	ASP
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	433	LEU
1	X	470	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (288) 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	213	HIS
1	A	225	ASN
1	A	275	GLN

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Mol	Chain	Res	Type
1	A	342	ASN
1	A	418	GLN
1	A	464	HIS
1	B	30	HIS
1	B	86	ASN
1	B	106	ASN
1	B	178	HIS
1	B	190	GLN
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	106	ASN
1	C	113	ASN
1	C	213	HIS
1	C	221	GLN
1	C	247	ASN
1	C	267	ASN
1	C	274	HIS
1	C	275	GLN
1	C	342	ASN
1	C	464	HIS
1	D	30	HIS
1	D	86	ASN
1	D	106	ASN
1	D	113	ASN
1	D	190	GLN
1	D	213	HIS
1	D	275	GLN
1	D	307	HIS
1	D	317	ASN
1	D	464	HIS
1	E	30	HIS
1	E	86	ASN
1	E	113	ASN

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Mol	Chain	Res	Type
1	E	190	GLN
1	E	213	HIS
1	E	247	ASN
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	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	225	ASN
1	G	247	ASN
1	G	267	ASN
1	G	275	GLN
1	G	307	HIS
1	G	418	GLN
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	188	ASN
1	H	190	GLN
1	H	201	ASN
1	H	213	HIS
1	H	251	GLN

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Mol	Chain	Res	Type
1	H	275	GLN
1	H	317	ASN
1	H	342	ASN
1	H	418	GLN
1	H	464	HIS
1	I	30	HIS
1	I	86	ASN
1	I	92	HIS
1	I	106	ASN
1	I	113	ASN
1	I	213	HIS
1	I	225	ASN
1	I	227	GLN
1	I	247	ASN
1	I	272	HIS
1	I	275	GLN
1	I	317	ASN
1	I	335	ASN
1	I	342	ASN
1	I	389	ASN
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	225	ASN
1	J	275	GLN
1	J	307	HIS
1	J	464	HIS
1	K	30	HIS
1	K	86	ASN
1	K	92	HIS
1	K	106	ASN
1	K	113	ASN
1	K	178	HIS
1	K	188	ASN
1	K	190	GLN
1	K	213	HIS
1	K	247	ASN
1	K	272	HIS

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Mol	Chain	Res	Type
1	K	275	GLN
1	K	342	ASN
1	K	464	HIS
1	L	30	HIS
1	L	86	ASN
1	L	106	ASN
1	L	113	ASN
1	L	178	HIS
1	L	221	GLN
1	L	267	ASN
1	L	275	GLN
1	L	418	GLN
1	L	464	HIS
1	M	30	HIS
1	M	86	ASN
1	M	106	ASN
1	M	113	ASN
1	M	190	GLN
1	M	213	HIS
1	M	225	ASN
1	M	247	ASN
1	M	272	HIS
1	M	275	GLN
1	M	389	ASN
1	M	464	HIS
1	N	86	ASN
1	N	106	ASN
1	N	113	ASN
1	N	213	HIS
1	N	275	GLN
1	N	335	ASN
1	N	342	ASN
1	N	389	ASN
1	N	418	GLN
1	N	464	HIS
1	O	30	HIS
1	O	86	ASN
1	O	106	ASN
1	O	113	ASN
1	O	178	HIS
1	O	213	HIS
1	O	251	GLN

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Mol	Chain	Res	Type
1	O	272	HIS
1	O	275	GLN
1	O	317	ASN
1	O	342	ASN
1	O	418	GLN
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	267	ASN
1	P	275	GLN
1	P	394	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	225	ASN
1	Q	247	ASN
1	Q	335	ASN
1	Q	340	GLN
1	Q	342	ASN
1	Q	418	GLN
1	Q	464	HIS
1	R	30	HIS
1	R	86	ASN
1	R	92	HIS
1	R	106	ASN
1	R	190	GLN
1	R	213	HIS
1	R	225	ASN
1	R	233	HIS
1	R	275	GLN
1	R	300	HIS
1	R	335	ASN
1	R	342	ASN
1	R	414	GLN
1	R	464	HIS

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Mol	Chain	Res	Type
1	S	30	HIS
1	S	86	ASN
1	S	113	ASN
1	S	178	HIS
1	S	190	GLN
1	S	213	HIS
1	S	225	ASN
1	S	272	HIS
1	S	275	GLN
1	S	342	ASN
1	S	460	ASN
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	213	HIS
1	T	225	ASN
1	T	233	HIS
1	T	247	ASN
1	T	275	GLN
1	T	317	ASN
1	T	418	GLN
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	225	ASN
1	U	275	GLN
1	U	307	HIS
1	U	418	GLN
1	U	464	HIS
1	V	30	HIS
1	V	86	ASN
1	V	106	ASN
1	V	113	ASN
1	V	190	GLN

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Mol	Chain	Res	Type
1	V	213	HIS
1	V	225	ASN
1	V	247	ASN
1	V	272	HIS
1	V	275	GLN
1	V	342	ASN
1	V	418	GLN
1	V	464	HIS
1	W	30	HIS
1	W	86	ASN
1	W	106	ASN
1	W	113	ASN
1	W	190	GLN
1	W	213	HIS
1	W	275	GLN
1	W	389	ASN
1	W	464	HIS
1	X	30	HIS
1	X	86	ASN
1	X	106	ASN
1	X	178	HIS
1	X	190	GLN
1	X	213	HIS
1	X	221	GLN
1	X	247	ASN
1	X	275	GLN
1	X	300	HIS
1	X	317	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 monosaccharides 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	C	900	-	25,27,27	2.09	4 (16%)	26,40,40	2.40	7 (26%)
2	2K9	K	900	-	25,27,27	2.03	3 (12%)	26,40,40	2.13	4 (15%)
2	2K9	M	900	-	25,27,27	2.04	4 (16%)	26,40,40	2.28	6 (23%)
2	2K9	V	900	-	25,27,27	2.00	4 (16%)	26,40,40	2.36	5 (19%)
2	2K9	A	900	-	25,27,27	1.89	3 (12%)	26,40,40	2.32	5 (19%)
2	2K9	G	900	-	25,27,27	2.01	4 (16%)	26,40,40	2.33	5 (19%)
2	2K9	L	900	-	25,27,27	2.01	3 (12%)	26,40,40	2.16	3 (11%)
2	2K9	I	900	-	25,27,27	2.04	4 (16%)	26,40,40	2.34	4 (15%)
2	2K9	E	900	-	25,27,27	2.02	3 (12%)	26,40,40	2.24	4 (15%)
2	2K9	N	900	-	25,27,27	2.09	4 (16%)	26,40,40	2.39	5 (19%)
2	2K9	S	900	-	25,27,27	1.99	4 (16%)	26,40,40	2.30	4 (15%)
2	2K9	P	900	-	25,27,27	2.11	4 (16%)	26,40,40	2.30	5 (19%)
2	2K9	R	900	-	25,27,27	2.02	4 (16%)	26,40,40	2.25	3 (11%)
2	2K9	U	900	-	25,27,27	2.10	4 (16%)	26,40,40	2.33	5 (19%)
2	2K9	D	900	-	25,27,27	1.99	4 (16%)	26,40,40	2.31	5 (19%)
2	2K9	X	900	-	25,27,27	2.03	4 (16%)	26,40,40	2.26	4 (15%)
2	2K9	F	900	-	25,27,27	1.99	3 (12%)	26,40,40	2.30	5 (19%)
2	2K9	W	900	-	25,27,27	2.08	3 (12%)	26,40,40	2.20	4 (15%)
2	2K9	O	900	-	25,27,27	1.96	3 (12%)	26,40,40	2.23	4 (15%)
2	2K9	B	900	-	25,27,27	2.06	4 (16%)	26,40,40	2.21	3 (11%)
2	2K9	H	900	-	25,27,27	1.99	4 (16%)	26,40,40	2.31	5 (19%)
2	2K9	Q	900	-	25,27,27	2.04	3 (12%)	26,40,40	2.17	3 (11%)
2	2K9	T	900	-	25,27,27	2.00	4 (16%)	26,40,40	2.30	4 (15%)
2	2K9	J	900	-	25,27,27	1.95	4 (16%)	26,40,40	2.29	4 (15%)

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	C	900	-	-	0/4/12/12	0/4/5/5
2	2K9	K	900	-	-	0/4/12/12	0/4/5/5
2	2K9	M	900	-	-	0/4/12/12	0/4/5/5
2	2K9	V	900	-	-	0/4/12/12	0/4/5/5
2	2K9	A	900	-	-	0/4/12/12	0/4/5/5
2	2K9	G	900	-	-	0/4/12/12	0/4/5/5
2	2K9	L	900	-	-	0/4/12/12	0/4/5/5
2	2K9	I	900	-	-	0/4/12/12	0/4/5/5
2	2K9	E	900	-	-	0/4/12/12	0/4/5/5
2	2K9	N	900	-	-	0/4/12/12	0/4/5/5
2	2K9	S	900	-	-	0/4/12/12	0/4/5/5
2	2K9	P	900	-	-	0/4/12/12	0/4/5/5
2	2K9	R	900	-	-	0/4/12/12	0/4/5/5
2	2K9	U	900	-	-	0/4/12/12	0/4/5/5
2	2K9	D	900	-	-	0/4/12/12	0/4/5/5
2	2K9	X	900	-	-	0/4/12/12	0/4/5/5
2	2K9	F	900	-	-	0/4/12/12	0/4/5/5
2	2K9	W	900	-	-	0/4/12/12	0/4/5/5
2	2K9	O	900	-	-	0/4/12/12	0/4/5/5
2	2K9	B	900	-	-	3/4/12/12	0/4/5/5
2	2K9	H	900	-	-	1/4/12/12	0/4/5/5
2	2K9	Q	900	-	-	0/4/12/12	0/4/5/5
2	2K9	T	900	-	-	0/4/12/12	0/4/5/5
2	2K9	J	900	-	-	0/4/12/12	0/4/5/5

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	900	2K9	C3-C1	6.72	1.48	1.37
2	C	900	2K9	C3-C1	6.60	1.47	1.37
2	W	900	2K9	C3-C1	6.50	1.47	1.37
2	Q	900	2K9	C3-C1	6.49	1.47	1.37
2	U	900	2K9	C3-C1	6.45	1.47	1.37
2	T	900	2K9	C3-C1	6.45	1.47	1.37
2	V	900	2K9	C3-C1	6.43	1.47	1.37
2	N	900	2K9	C3-C1	6.39	1.47	1.37
2	R	900	2K9	C3-C1	6.38	1.47	1.37
2	J	900	2K9	C3-C1	6.38	1.47	1.37
2	M	900	2K9	C3-C1	6.36	1.47	1.37
2	S	900	2K9	C3-C1	6.32	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	900	2K9	C3-C1	6.31	1.47	1.37
2	B	900	2K9	C3-C1	6.27	1.47	1.37
2	L	900	2K9	C3-C1	6.26	1.47	1.37
2	K	900	2K9	C3-C1	6.23	1.47	1.37
2	D	900	2K9	C3-C1	6.17	1.47	1.37
2	X	900	2K9	C3-C1	6.15	1.47	1.37
2	O	900	2K9	C3-C1	6.15	1.47	1.37
2	W	900	2K9	C6-N1	-6.08	1.33	1.38
2	K	900	2K9	C6-N1	-6.06	1.33	1.38
2	G	900	2K9	C3-C1	6.00	1.46	1.37
2	I	900	2K9	C3-C1	5.97	1.46	1.37
2	E	900	2K9	C3-C1	5.96	1.46	1.37
2	B	900	2K9	C6-N1	-5.88	1.33	1.38
2	Q	900	2K9	C6-N1	-5.85	1.33	1.38
2	E	900	2K9	C6-N1	-5.83	1.33	1.38
2	X	900	2K9	C6-N1	-5.83	1.33	1.38
2	L	900	2K9	C6-N1	-5.78	1.33	1.38
2	U	900	2K9	C6-N1	-5.73	1.33	1.38
2	H	900	2K9	C3-C1	5.73	1.46	1.37
2	I	900	2K9	C6-N1	-5.69	1.33	1.38
2	H	900	2K9	C6-N1	-5.69	1.33	1.38
2	N	900	2K9	C6-N1	-5.64	1.33	1.38
2	F	900	2K9	C6-N1	-5.63	1.33	1.38
2	A	900	2K9	C3-C1	5.59	1.46	1.37
2	G	900	2K9	C6-N1	-5.58	1.33	1.38
2	R	900	2K9	C6-N1	-5.57	1.33	1.38
2	D	900	2K9	C6-N1	-5.48	1.33	1.38
2	C	900	2K9	C6-N1	-5.46	1.33	1.38
2	M	900	2K9	C6-N1	-5.39	1.33	1.38
2	P	900	2K9	C6-N1	-5.37	1.33	1.38
2	A	900	2K9	C6-N1	-5.13	1.34	1.38
2	O	900	2K9	C6-N1	-5.05	1.34	1.38
2	J	900	2K9	C6-N1	-4.97	1.34	1.38
2	T	900	2K9	C6-N1	-4.97	1.34	1.38
2	S	900	2K9	C6-N1	-4.91	1.34	1.38
2	V	900	2K9	C6-N1	-4.72	1.34	1.38
2	C	900	2K9	C4-C2	-4.13	1.37	1.45
2	O	900	2K9	C4-C2	-4.00	1.37	1.45
2	H	900	2K9	C4-C2	-3.92	1.37	1.45
2	I	900	2K9	C4-C2	-3.85	1.37	1.45
2	E	900	2K9	C4-C2	-3.83	1.37	1.45
2	P	900	2K9	C4-C2	-3.80	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	U	900	2K9	C4-C2	-3.72	1.38	1.45
2	J	900	2K9	C4-C2	-3.71	1.38	1.45
2	N	900	2K9	C4-C2	-3.69	1.38	1.45
2	D	900	2K9	C4-C2	-3.64	1.38	1.45
2	G	900	2K9	C4-C2	-3.63	1.38	1.45
2	B	900	2K9	C4-C2	-3.61	1.38	1.45
2	M	900	2K9	C4-C2	-3.53	1.38	1.45
2	R	900	2K9	C4-C2	-3.53	1.38	1.45
2	V	900	2K9	C4-C2	-3.52	1.38	1.45
2	T	900	2K9	C4-C2	-3.51	1.38	1.45
2	S	900	2K9	C4-C2	-3.49	1.38	1.45
2	A	900	2K9	C4-C2	-3.47	1.38	1.45
2	W	900	2K9	C4-C2	-3.40	1.38	1.45
2	L	900	2K9	C4-C2	-3.24	1.39	1.45
2	Q	900	2K9	C4-C2	-3.11	1.39	1.45
2	K	900	2K9	C4-C2	-3.01	1.39	1.45
2	F	900	2K9	C4-C2	-2.98	1.39	1.45
2	X	900	2K9	C4-C2	-2.94	1.39	1.45
2	V	900	2K9	C5-C9	2.79	1.52	1.47
2	P	900	2K9	C5-C9	2.61	1.51	1.47
2	S	900	2K9	C5-C9	2.53	1.51	1.47
2	N	900	2K9	C5-C9	2.51	1.51	1.47
2	I	900	2K9	C5-C9	2.48	1.51	1.47
2	X	900	2K9	C5-C9	2.45	1.51	1.47
2	T	900	2K9	C5-C9	2.41	1.51	1.47
2	U	900	2K9	C5-C9	2.37	1.51	1.47
2	M	900	2K9	C5-C9	2.35	1.51	1.47
2	C	900	2K9	C9-N2	-2.26	1.34	1.39
2	D	900	2K9	C9-N2	-2.10	1.34	1.39
2	J	900	2K9	C9-N2	-2.08	1.34	1.39
2	H	900	2K9	C9-N2	-2.06	1.34	1.39
2	R	900	2K9	C5-C9	2.06	1.50	1.47
2	B	900	2K9	C9-N2	-2.01	1.34	1.39
2	G	900	2K9	C5-C9	2.01	1.50	1.47

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	900	2K9	C9-C5-N3	9.92	135.19	119.92
2	T	900	2K9	C9-C5-N3	9.90	135.15	119.92
2	N	900	2K9	C9-C5-N3	9.85	135.09	119.92
2	H	900	2K9	C9-C5-N3	9.81	135.02	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	900	2K9	C9-C5-N3	9.79	134.98	119.92
2	A	900	2K9	C9-C5-N3	9.78	134.97	119.92
2	P	900	2K9	C9-C5-N3	9.71	134.87	119.92
2	X	900	2K9	C9-C5-N3	9.69	134.84	119.92
2	I	900	2K9	C9-C5-N3	9.68	134.82	119.92
2	G	900	2K9	C9-C5-N3	9.64	134.76	119.92
2	M	900	2K9	C9-C5-N3	9.62	134.73	119.92
2	B	900	2K9	C9-C5-N3	9.56	134.64	119.92
2	U	900	2K9	C9-C5-N3	9.54	134.60	119.92
2	R	900	2K9	C9-C5-N3	9.50	134.53	119.92
2	E	900	2K9	C9-C5-N3	9.48	134.51	119.92
2	J	900	2K9	C9-C5-N3	9.36	134.33	119.92
2	D	900	2K9	C9-C5-N3	9.36	134.32	119.92
2	W	900	2K9	C9-C5-N3	9.27	134.18	119.92
2	C	900	2K9	C9-C5-N3	9.22	134.11	119.92
2	L	900	2K9	C9-C5-N3	9.21	134.10	119.92
2	O	900	2K9	C9-C5-N3	9.18	134.05	119.92
2	Q	900	2K9	C9-C5-N3	9.14	133.99	119.92
2	F	900	2K9	C9-C5-N3	9.08	133.89	119.92
2	K	900	2K9	C9-C5-N3	8.90	133.62	119.92
2	C	900	2K9	C8-C4-C2	-3.59	126.66	133.86
2	C	900	2K9	C16-C13-C11	-3.40	115.40	120.91
2	D	900	2K9	C16-C13-C11	-3.39	115.42	120.91
2	N	900	2K9	N3-C5-N1	-3.35	103.67	114.71
2	N	900	2K9	C8-C4-C2	-3.32	127.21	133.86
2	X	900	2K9	N3-C5-N1	-3.31	103.80	114.71
2	V	900	2K9	N3-C5-N1	-3.30	103.84	114.71
2	O	900	2K9	C8-C4-C2	-3.20	127.45	133.86
2	R	900	2K9	N3-C5-N1	-3.20	104.17	114.71
2	U	900	2K9	C8-C4-C2	-3.19	127.47	133.86
2	I	900	2K9	N3-C5-N1	-3.18	104.22	114.71
2	T	900	2K9	N3-C5-N1	-3.18	104.25	114.71
2	M	900	2K9	N3-C5-N1	-3.17	104.26	114.71
2	G	900	2K9	N3-C5-N1	-3.17	104.26	114.71
2	H	900	2K9	N3-C5-N1	-3.14	104.35	114.71
2	A	900	2K9	N3-C5-N1	-3.11	104.45	114.71
2	E	900	2K9	N3-C5-N1	-3.11	104.46	114.71
2	U	900	2K9	N3-C5-N1	-3.10	104.49	114.71
2	B	900	2K9	N3-C5-N1	-3.09	104.53	114.71
2	S	900	2K9	N3-C5-N1	-3.08	104.55	114.71
2	P	900	2K9	N3-C5-N1	-3.06	104.62	114.71
2	F	900	2K9	N3-C5-N1	-3.04	104.68	114.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	900	2K9	C16-C13-C11	-3.03	116.00	120.91
2	G	900	2K9	C8-C4-C2	-3.01	127.83	133.86
2	W	900	2K9	N3-C5-N1	-2.99	104.85	114.71
2	P	900	2K9	C8-C4-C2	-2.98	127.89	133.86
2	Q	900	2K9	N3-C5-N1	-2.97	104.93	114.71
2	R	900	2K9	C8-C4-C2	-2.96	127.94	133.86
2	D	900	2K9	N3-C5-N1	-2.94	105.03	114.71
2	J	900	2K9	N3-C5-N1	-2.93	105.04	114.71
2	I	900	2K9	C8-C4-C2	-2.92	128.01	133.86
2	V	900	2K9	C8-C4-C2	-2.92	128.01	133.86
2	W	900	2K9	C8-C4-C2	-2.92	128.02	133.86
2	O	900	2K9	N3-C5-N1	-2.87	105.25	114.71
2	L	900	2K9	N3-C5-N1	-2.84	105.35	114.71
2	K	900	2K9	N3-C5-N1	-2.83	105.39	114.71
2	F	900	2K9	C8-C4-C2	-2.82	128.22	133.86
2	D	900	2K9	C8-C4-C2	-2.81	128.24	133.86
2	M	900	2K9	C8-C4-C2	-2.81	128.24	133.86
2	T	900	2K9	C8-C4-C2	-2.80	128.26	133.86
2	C	900	2K9	N3-C5-N1	-2.79	105.52	114.71
2	B	900	2K9	C8-C4-C2	-2.77	128.32	133.86
2	E	900	2K9	C8-C4-C2	-2.73	128.40	133.86
2	J	900	2K9	C8-C4-C2	-2.72	128.41	133.86
2	F	900	2K9	C15-C13-C11	2.68	125.25	120.91
2	Q	900	2K9	C8-C4-C2	-2.67	128.51	133.86
2	S	900	2K9	C8-C4-C2	-2.67	128.52	133.86
2	F	900	2K9	C16-C13-C11	-2.66	116.60	120.91
2	H	900	2K9	C8-C4-C2	-2.64	128.57	133.86
2	I	900	2K9	C16-C13-C11	-2.62	116.66	120.91
2	C	900	2K9	C8-C4-C7	2.59	123.65	120.10
2	K	900	2K9	C16-C13-C11	-2.58	116.73	120.91
2	O	900	2K9	C8-C4-C7	2.54	123.59	120.10
2	L	900	2K9	C8-C4-C2	-2.52	128.81	133.86
2	U	900	2K9	C8-C4-C7	2.52	123.56	120.10
2	X	900	2K9	C8-C4-C2	-2.48	128.89	133.86
2	K	900	2K9	C8-C4-C2	-2.46	128.93	133.86
2	N	900	2K9	C8-C4-C7	2.38	123.37	120.10
2	A	900	2K9	C8-C4-C2	-2.35	129.16	133.86
2	N	900	2K9	C10-N3-C5	2.31	109.66	104.01
2	G	900	2K9	C8-C4-C7	2.28	123.23	120.10
2	H	900	2K9	C8-C4-C7	2.28	123.23	120.10
2	V	900	2K9	C8-C4-C7	2.25	123.18	120.10
2	M	900	2K9	C16-C13-C11	-2.22	117.32	120.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	900	2K9	C16-C13-C11	-2.20	117.34	120.91
2	V	900	2K9	C10-N3-C5	2.18	109.36	104.01
2	A	900	2K9	C11-C7-C3	-2.17	125.59	133.48
2	U	900	2K9	C16-C13-C11	-2.15	117.42	120.91
2	P	900	2K9	C8-C4-C7	2.12	123.01	120.10
2	T	900	2K9	C10-N3-C5	2.11	109.17	104.01
2	X	900	2K9	C10-N3-C5	2.10	109.14	104.01
2	E	900	2K9	C8-C4-C7	2.08	122.96	120.10
2	H	900	2K9	C10-N3-C5	2.06	109.05	104.01
2	C	900	2K9	C7-C11-C13	2.06	124.83	122.07
2	M	900	2K9	C10-N3-C5	2.04	109.01	104.01
2	W	900	2K9	C16-C13-C11	-2.04	117.61	120.91
2	P	900	2K9	C10-N3-C5	2.04	109.00	104.01
2	C	900	2K9	C15-C13-C11	2.03	124.20	120.91
2	G	900	2K9	C11-C7-C3	-2.03	126.09	133.48
2	D	900	2K9	C15-C13-C11	2.02	124.19	120.91
2	A	900	2K9	C10-N3-C5	2.01	108.94	104.01
2	M	900	2K9	C8-C4-C7	2.01	122.86	120.10

There are no chirality outliers.

All (4) 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
2	B	900	2K9	C14-C11-C13-C16

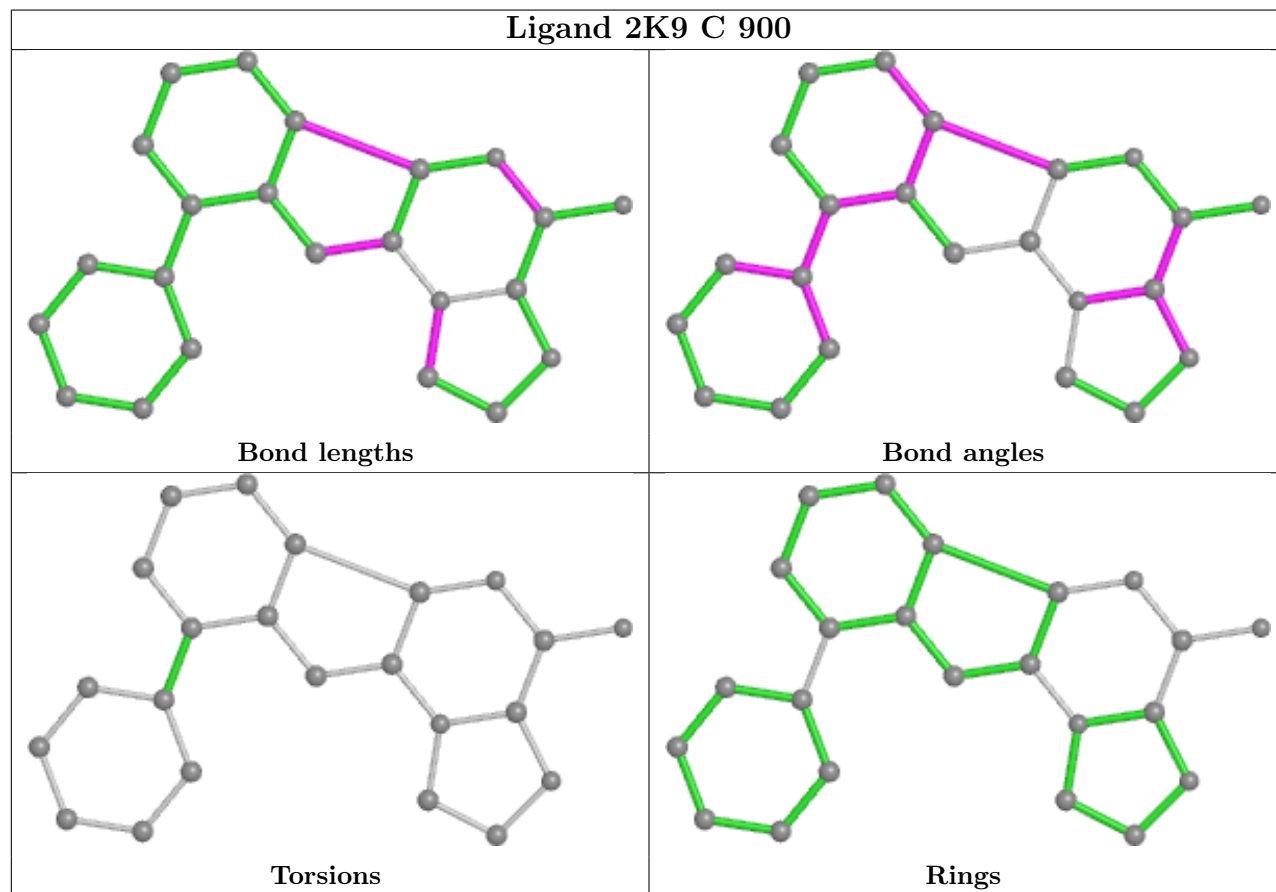
There are no ring outliers.

6 monomers are involved in 8 short contacts:

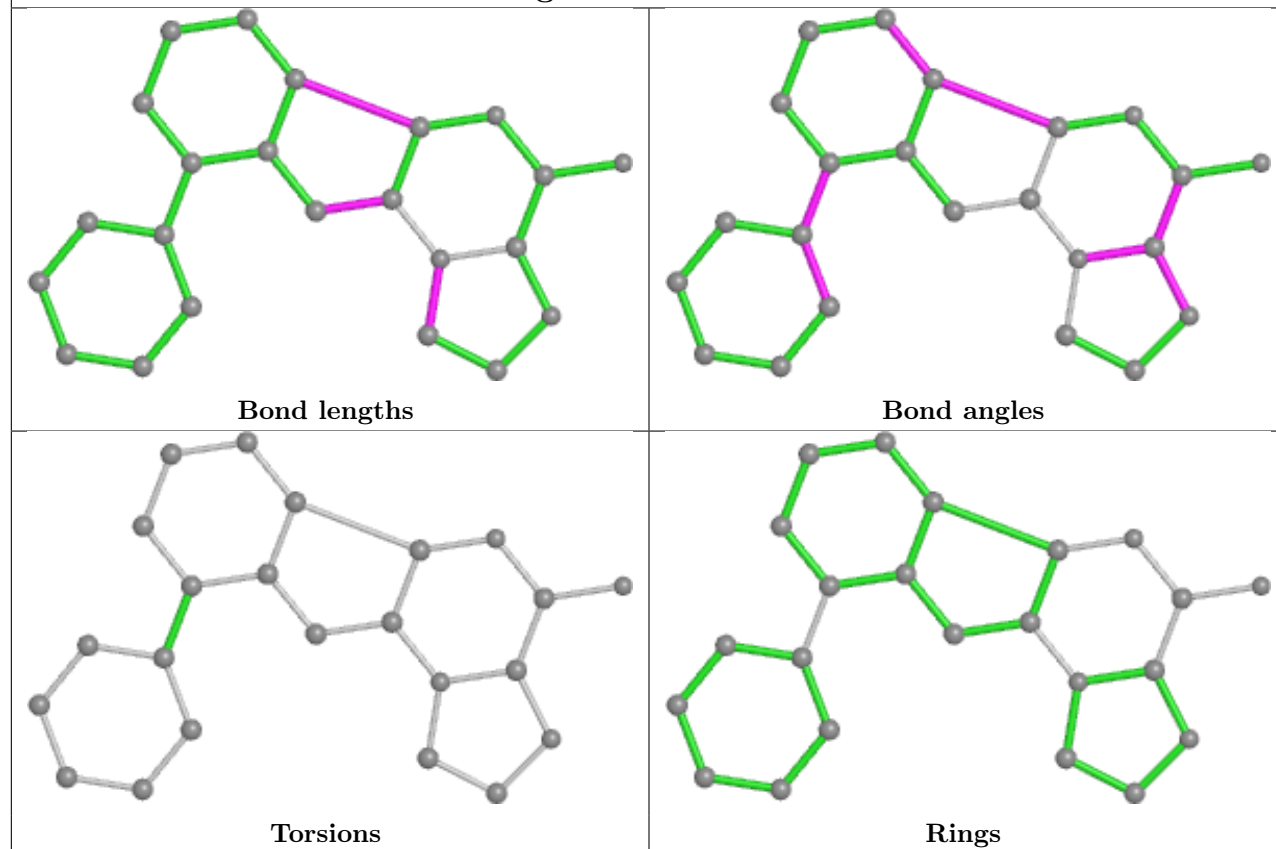
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	900	2K9	2	0
2	N	900	2K9	1	0
2	P	900	2K9	1	0
2	R	900	2K9	1	0
2	F	900	2K9	2	0
2	B	900	2K9	1	0

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

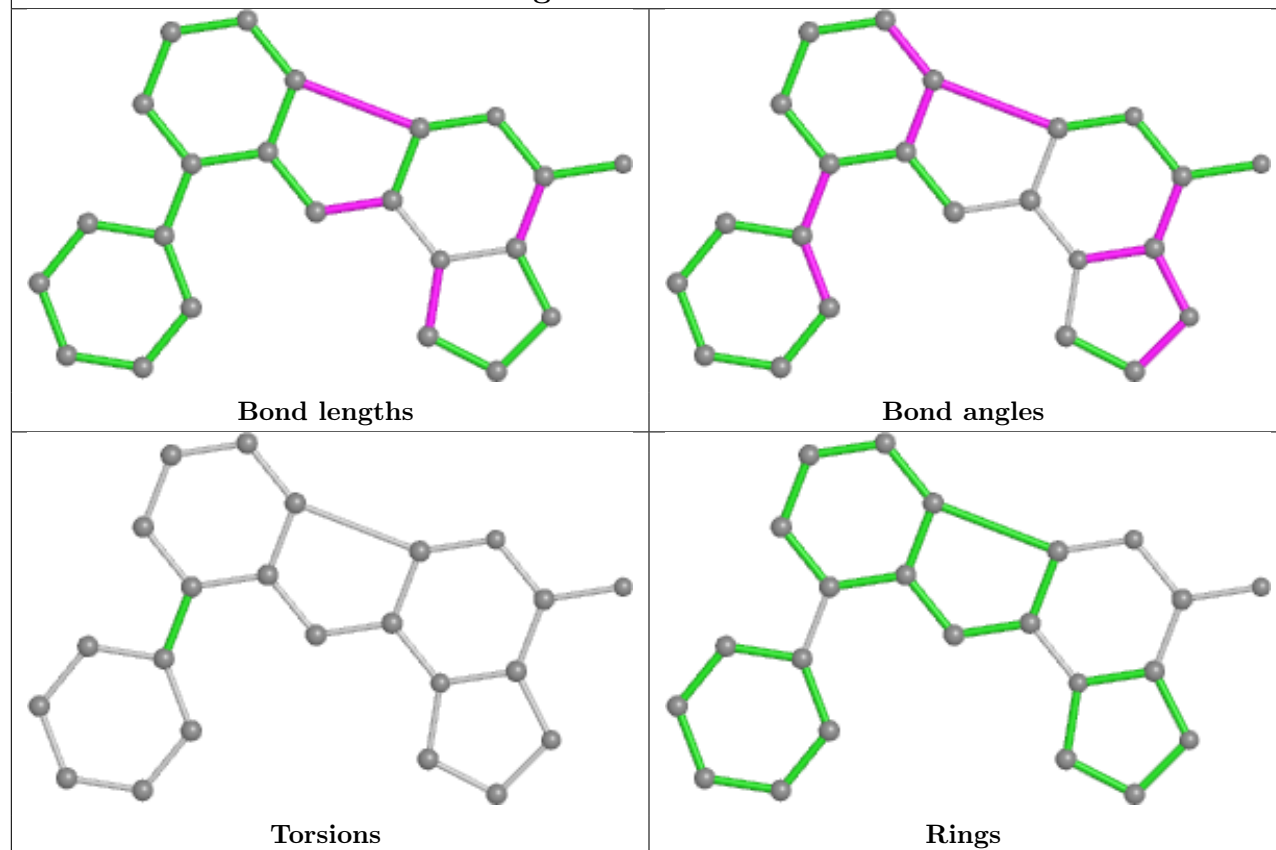
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.



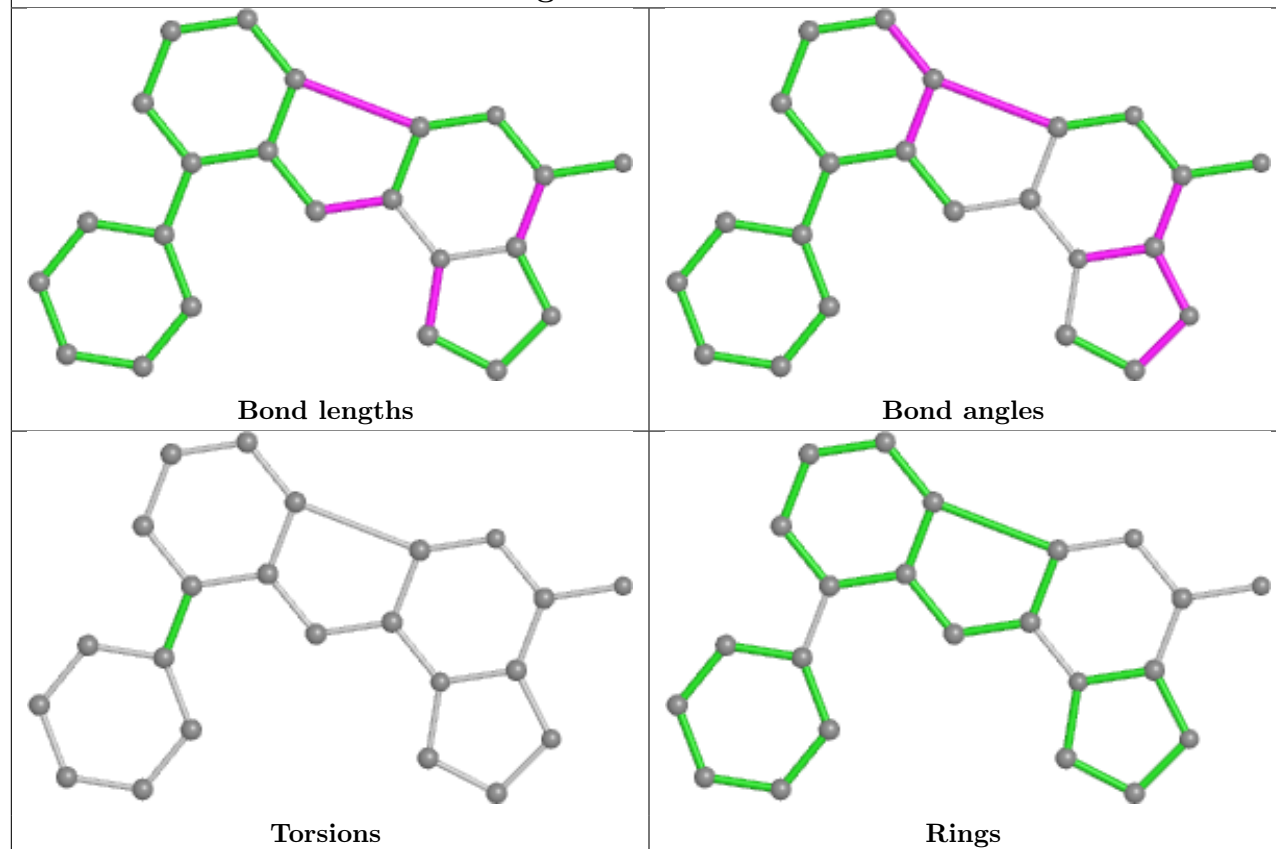
Ligand 2K9 K 900



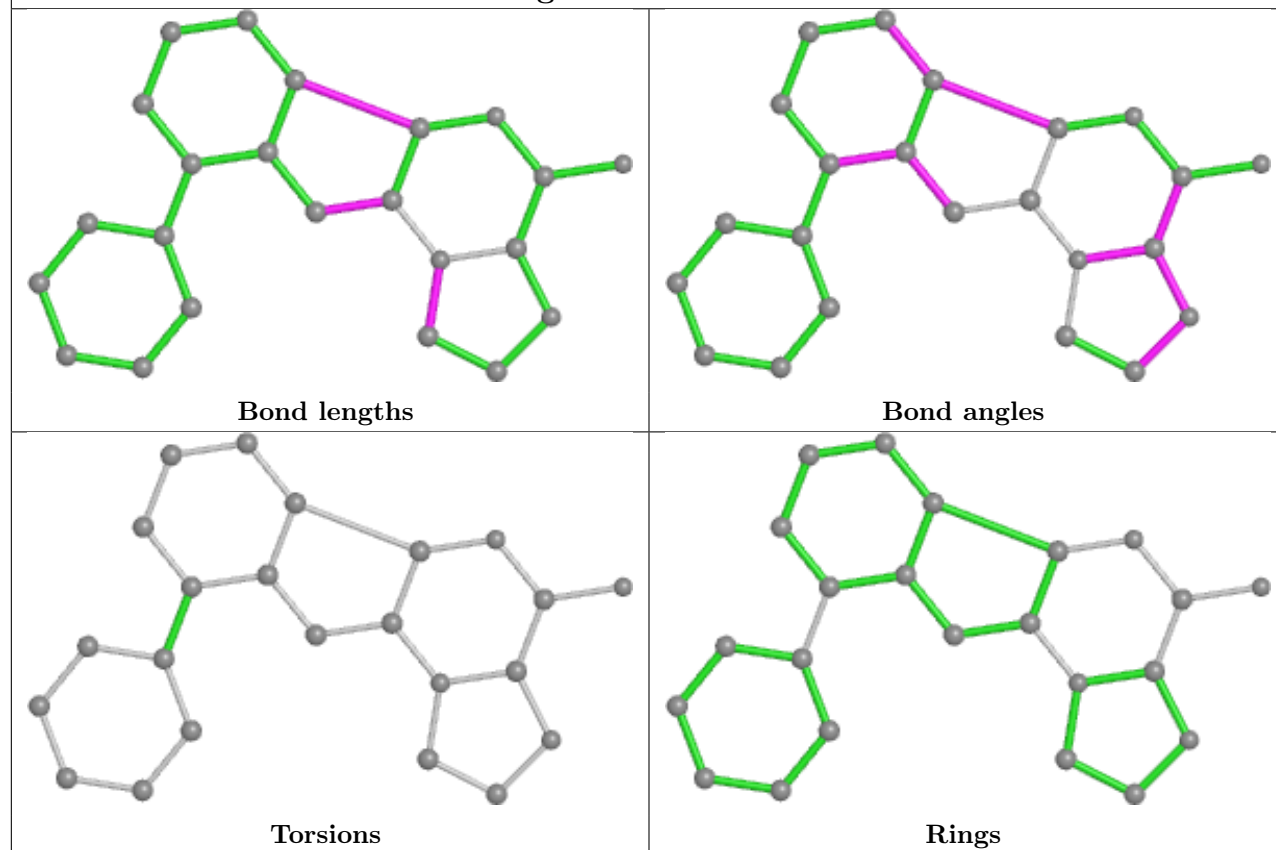
Ligand 2K9 M 900



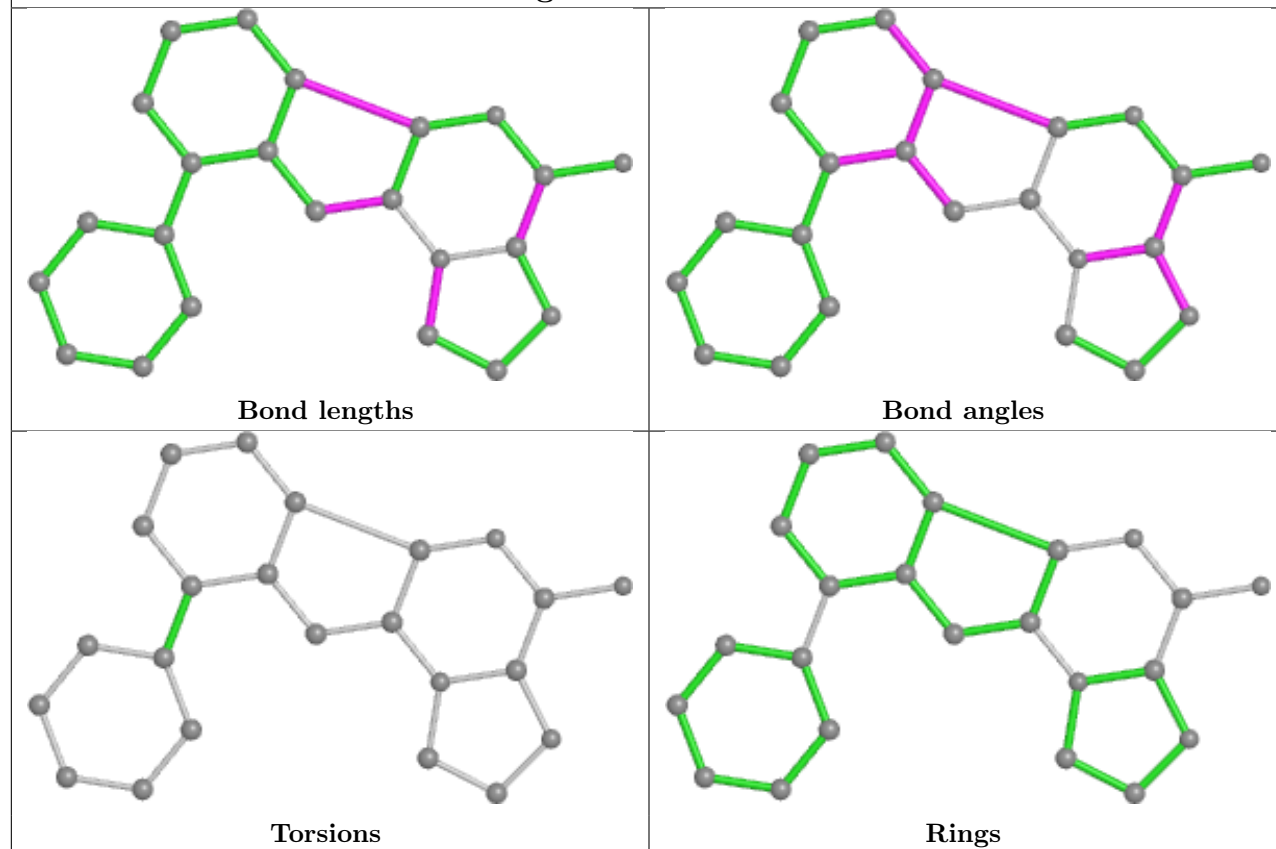
Ligand 2K9 V 900



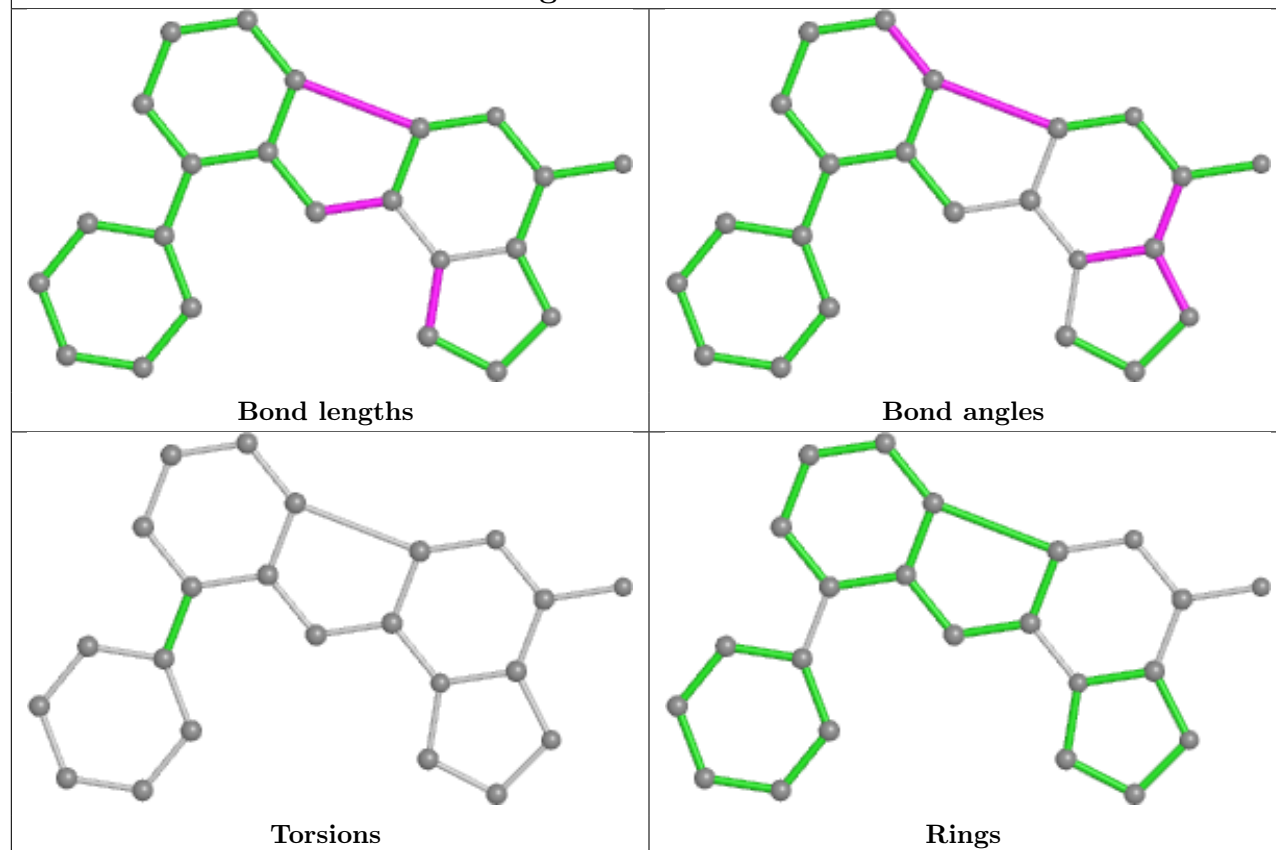
Ligand 2K9 A 900



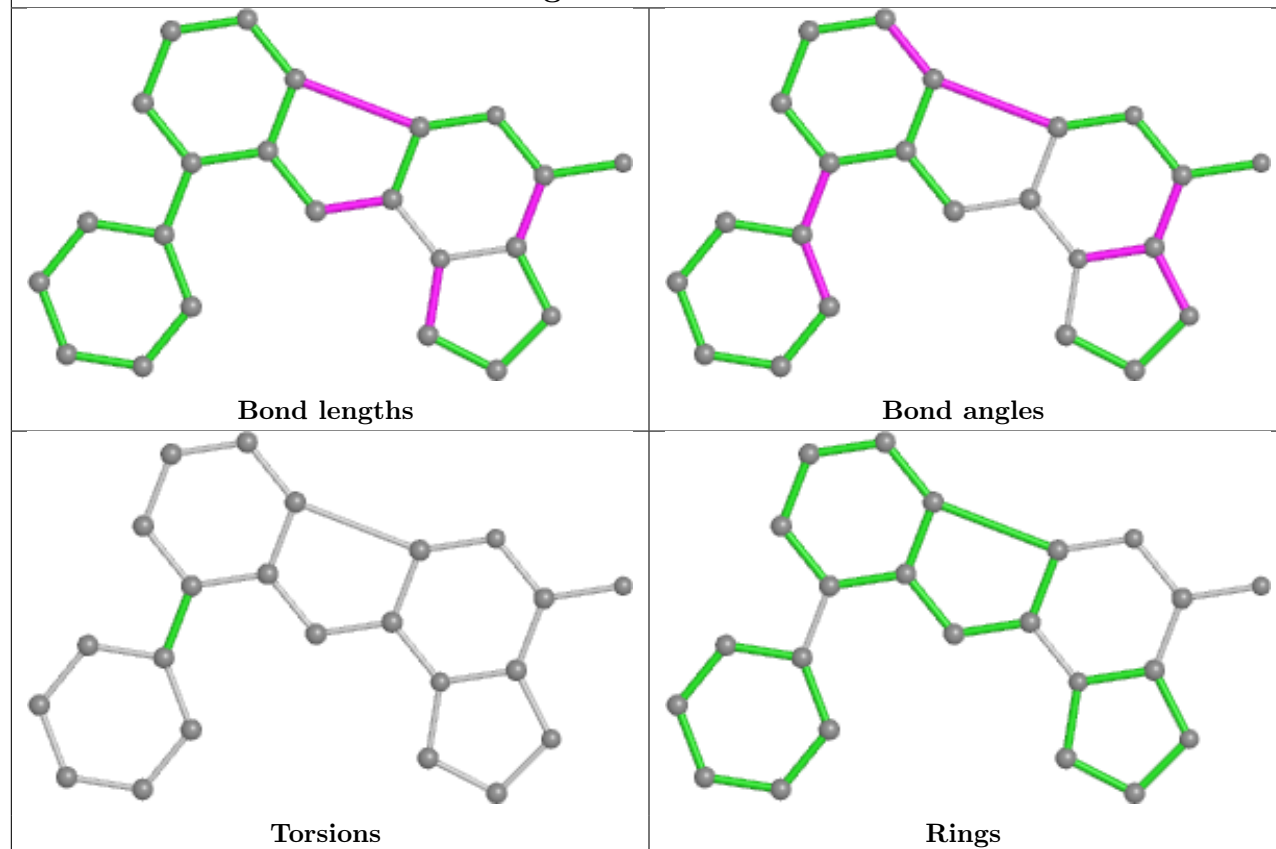
Ligand 2K9 G 900



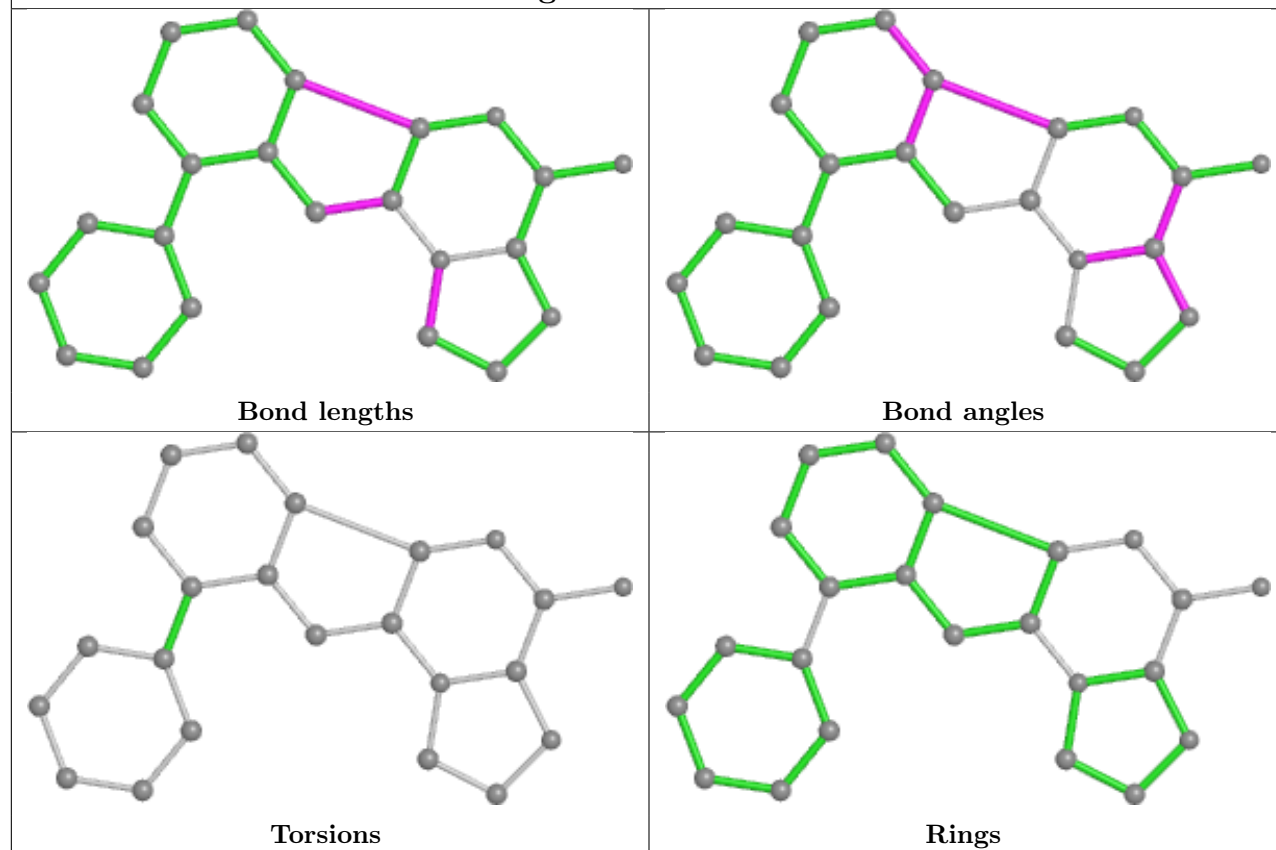
Ligand 2K9 L 900



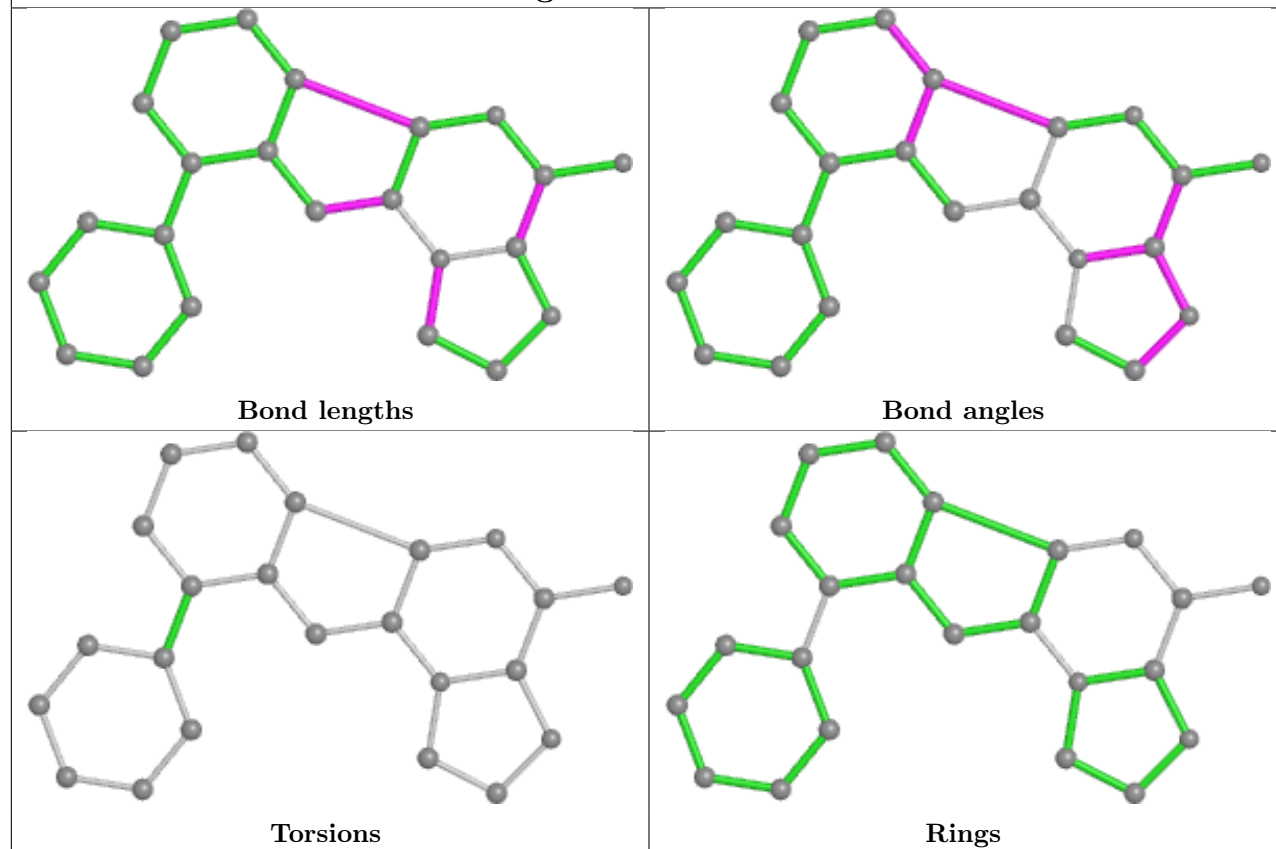
Ligand 2K9 I 900



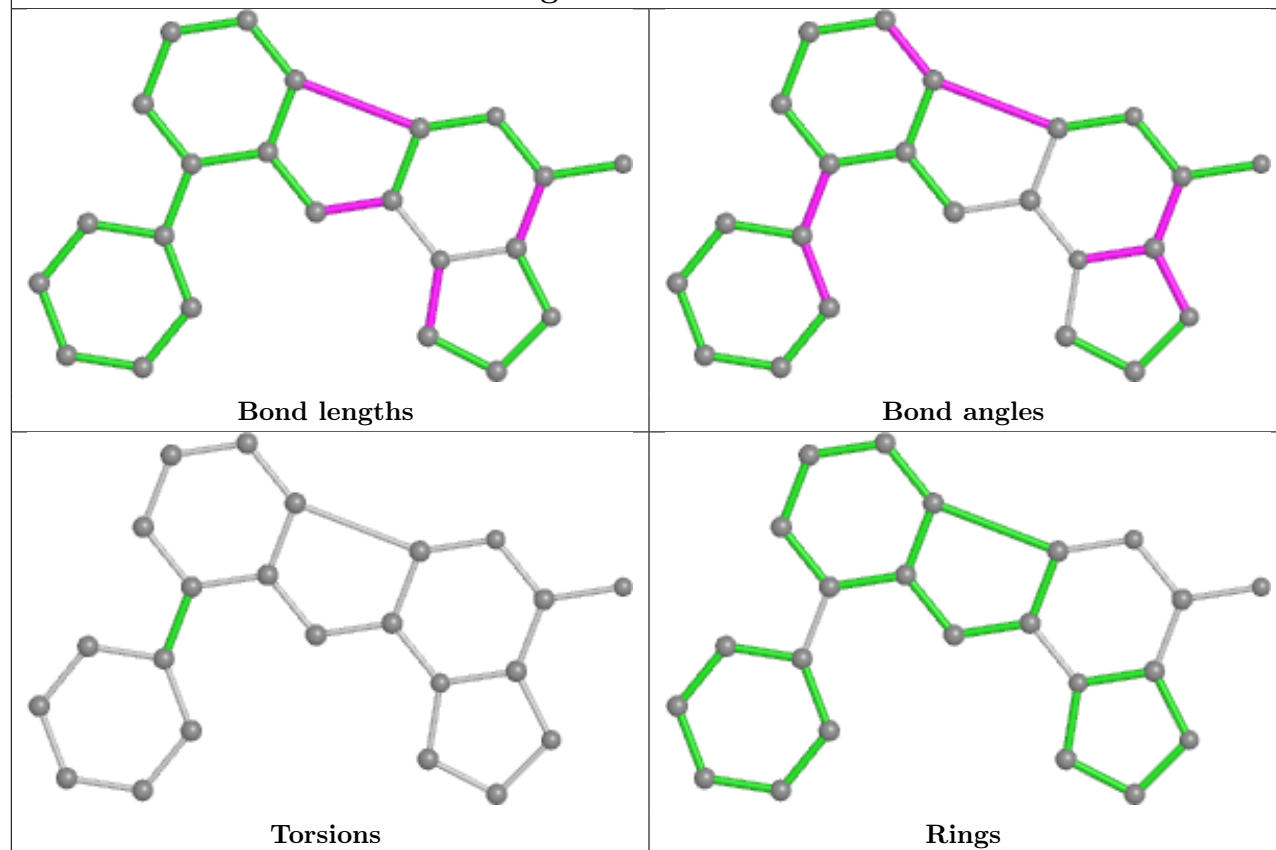
Ligand 2K9 E 900



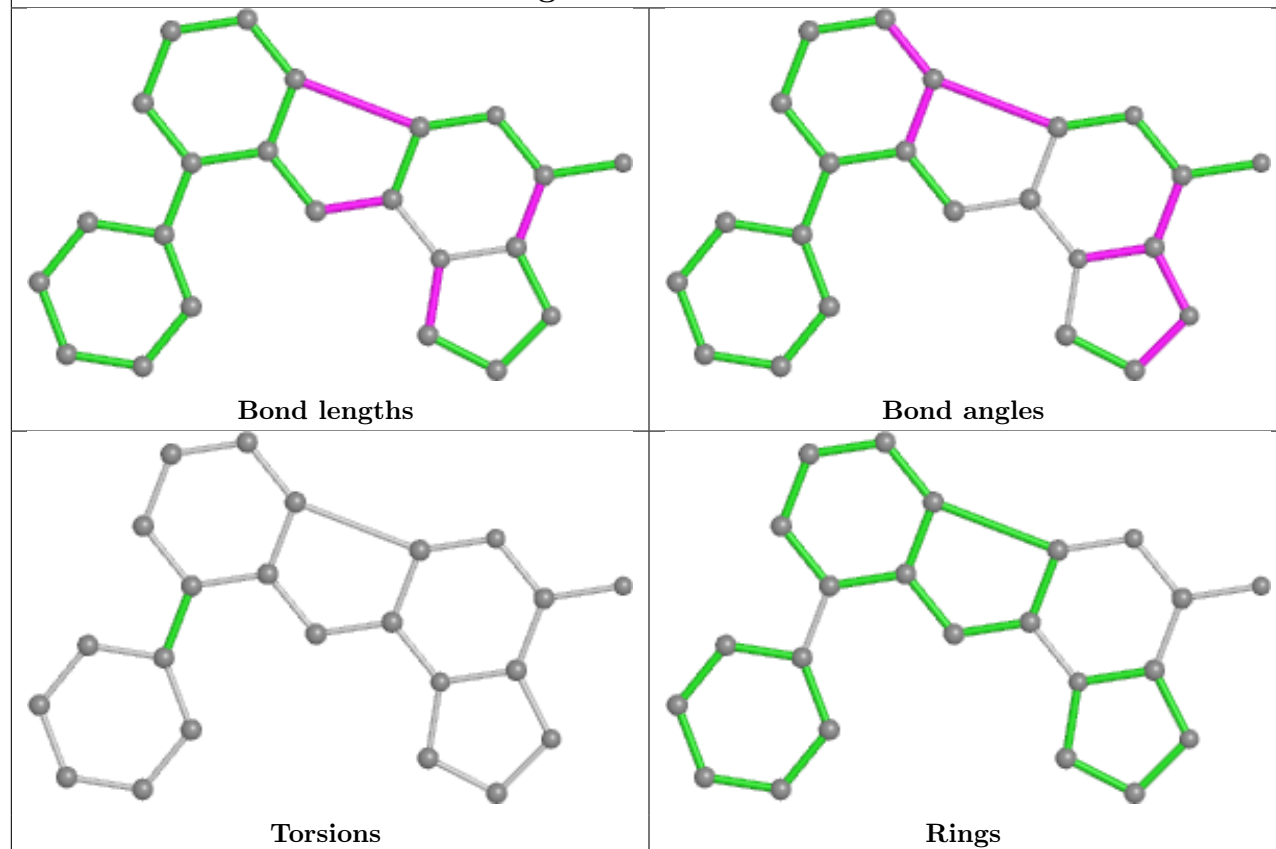
Ligand 2K9 N 900



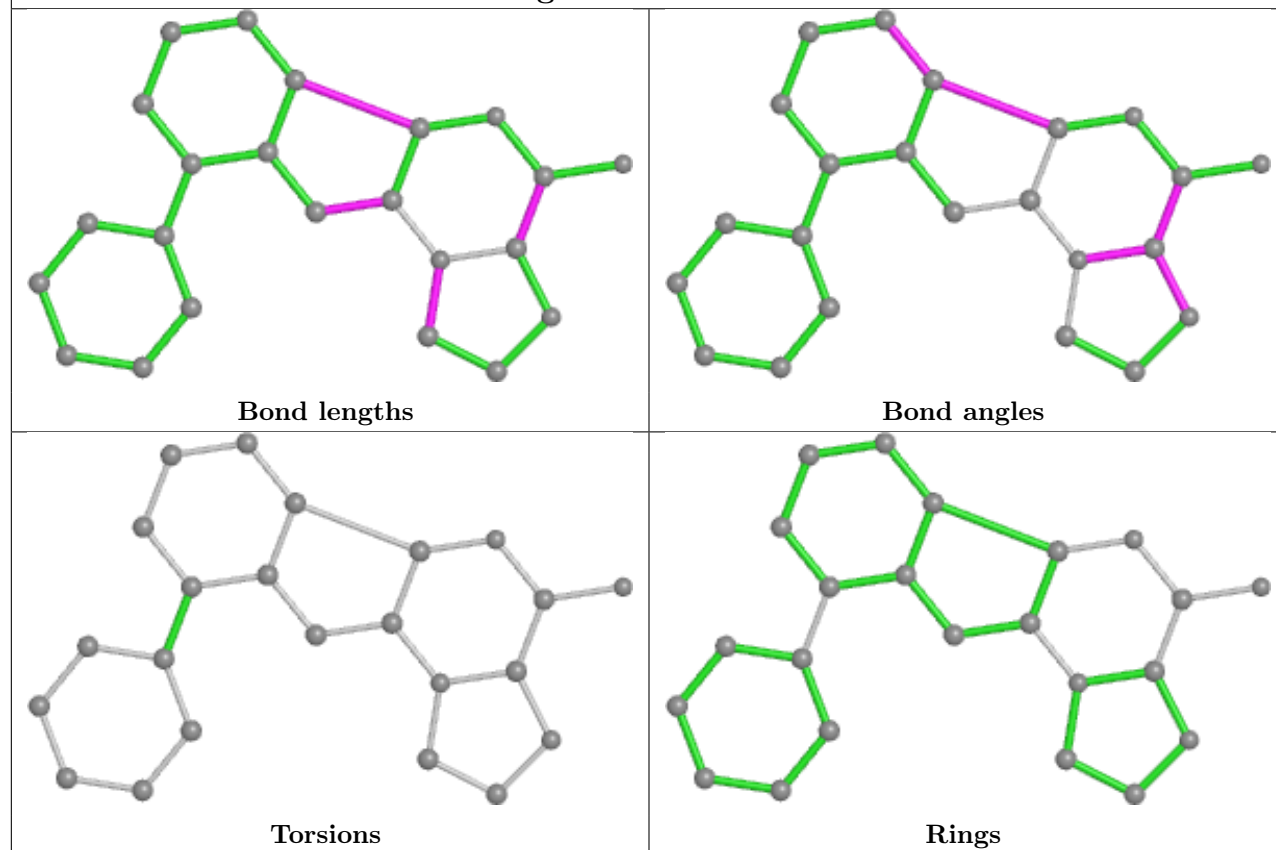
Ligand 2K9 S 900



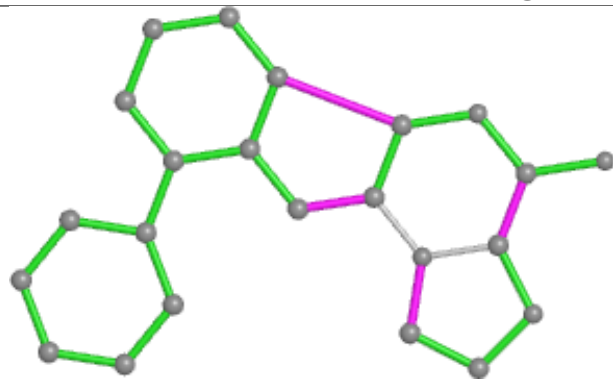
Ligand 2K9 P 900



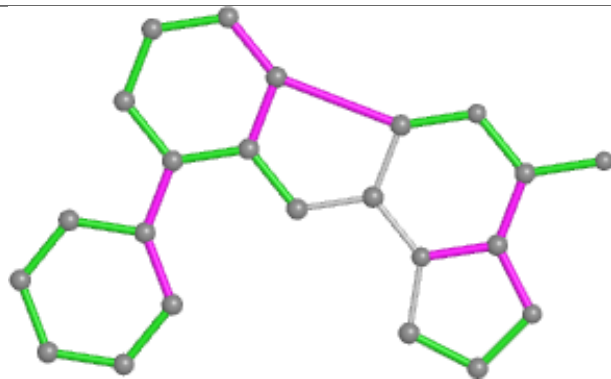
Ligand 2K9 R 900



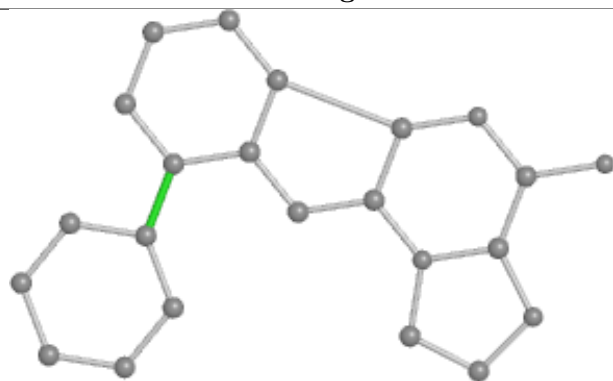
Ligand 2K9 U 900



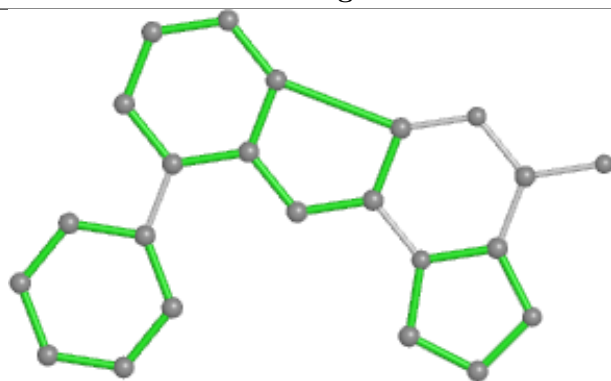
Bond lengths



Bond angles

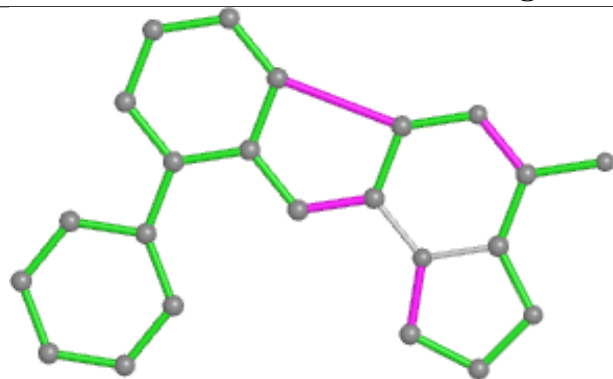


Torsions

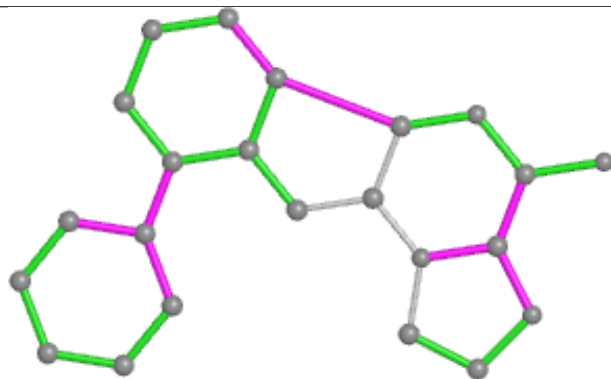


Rings

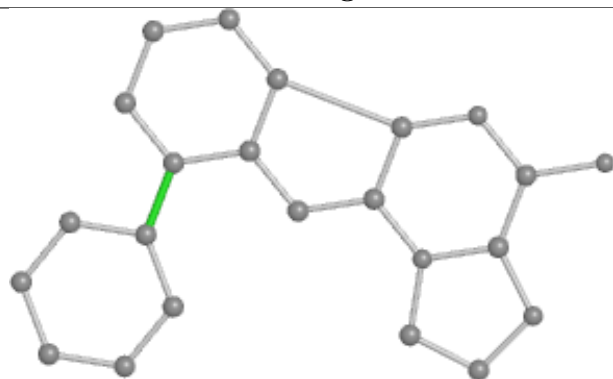
Ligand 2K9 D 900



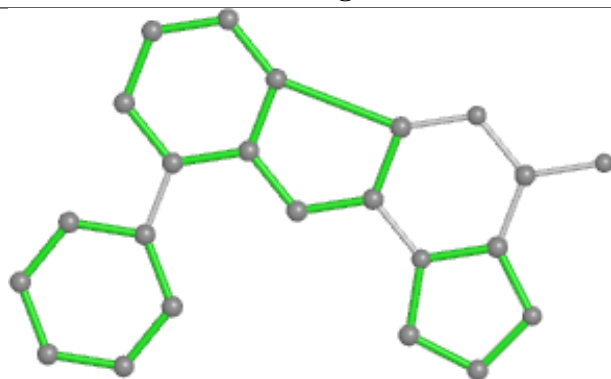
Bond lengths



Bond angles

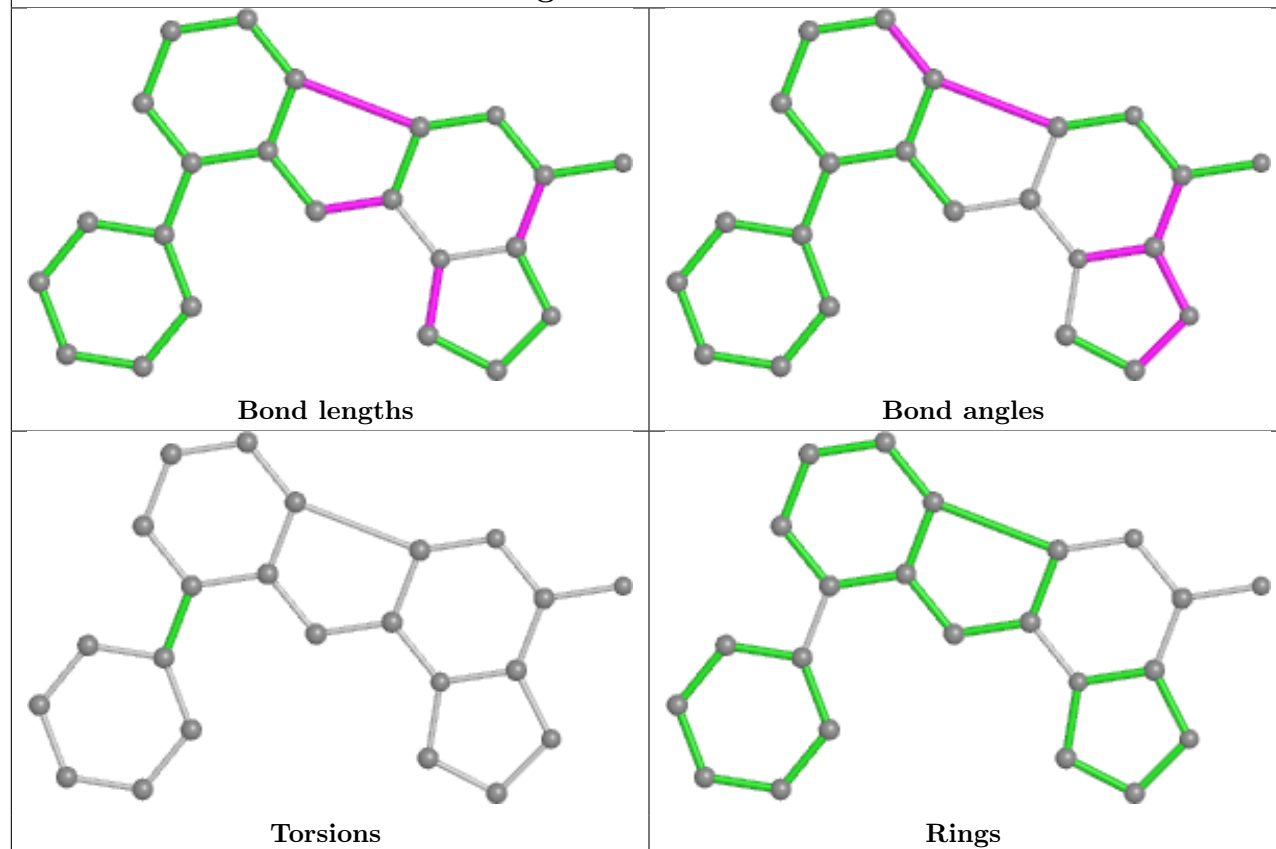


Torsions

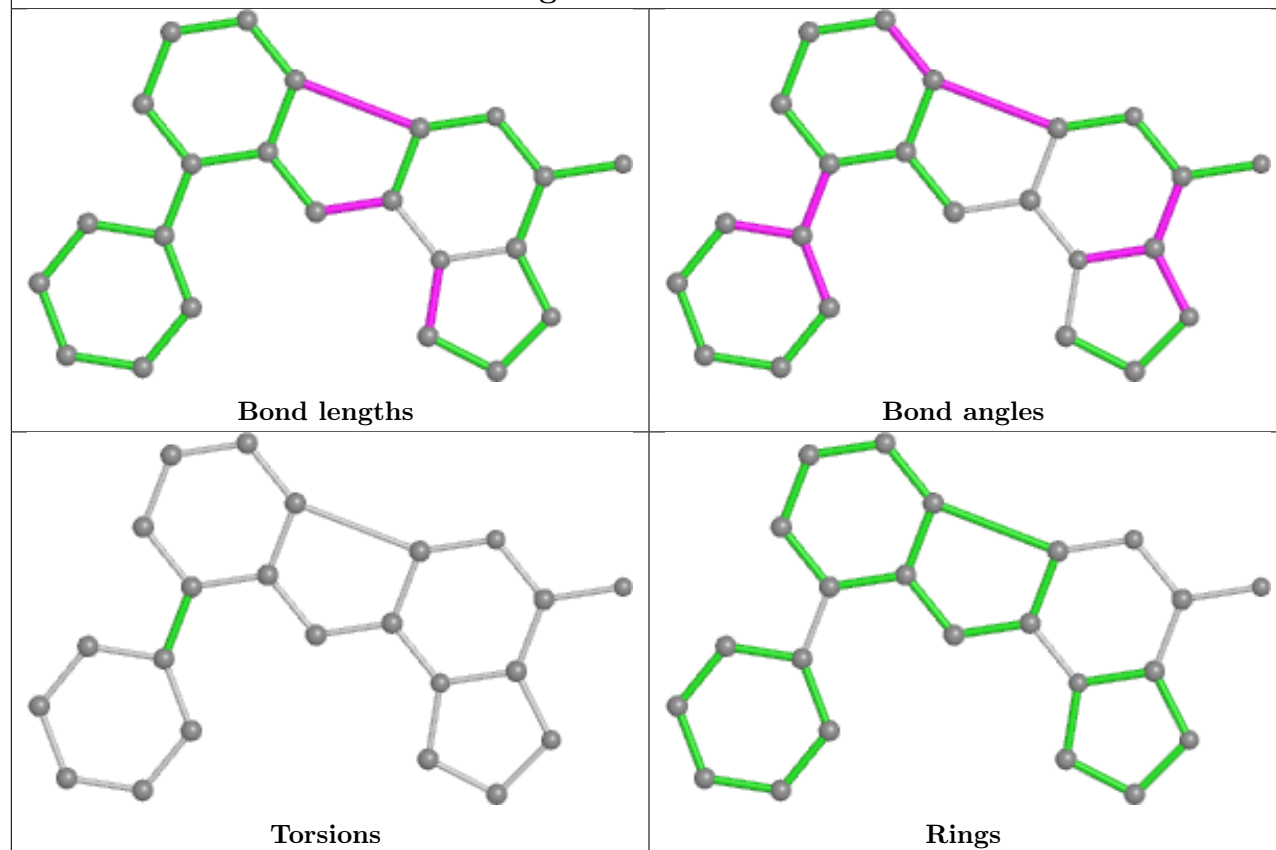


Rings

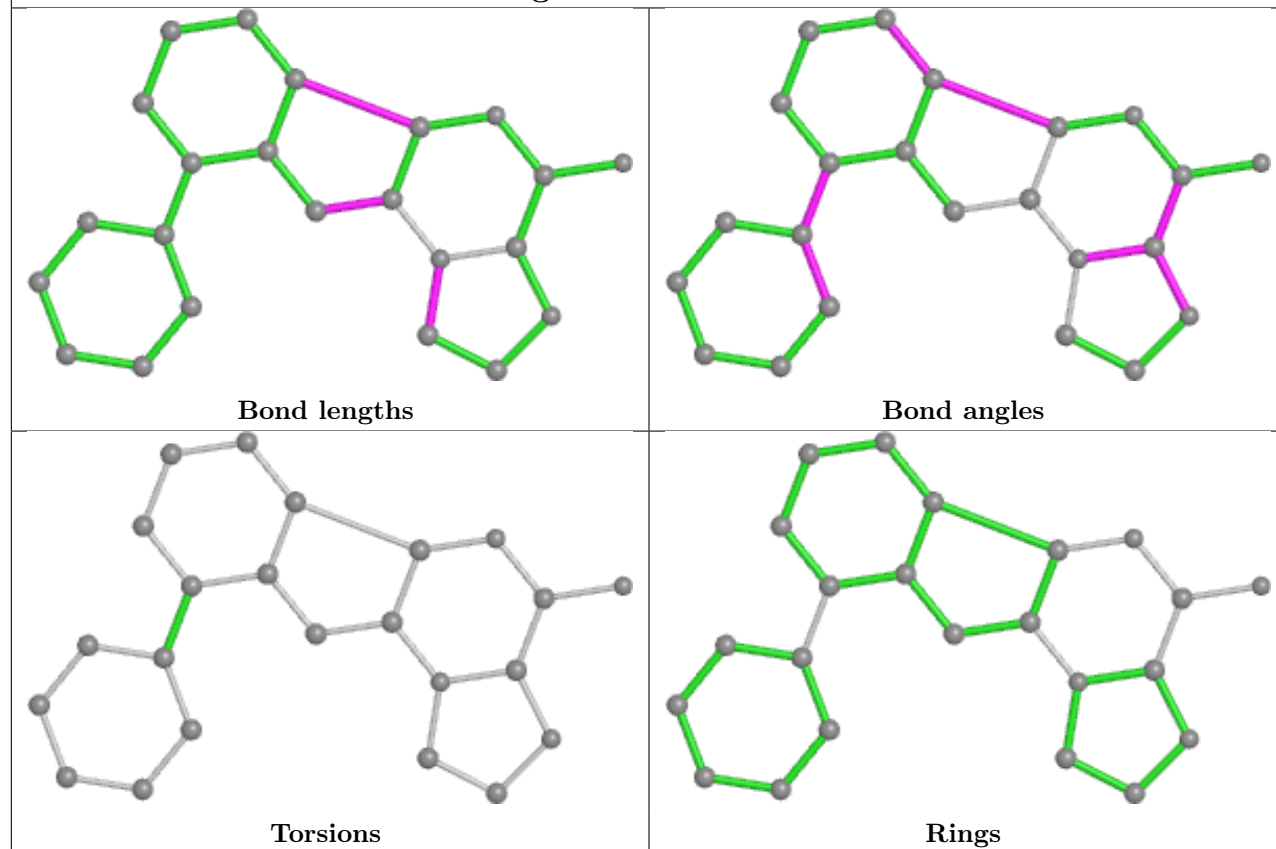
Ligand 2K9 X 900



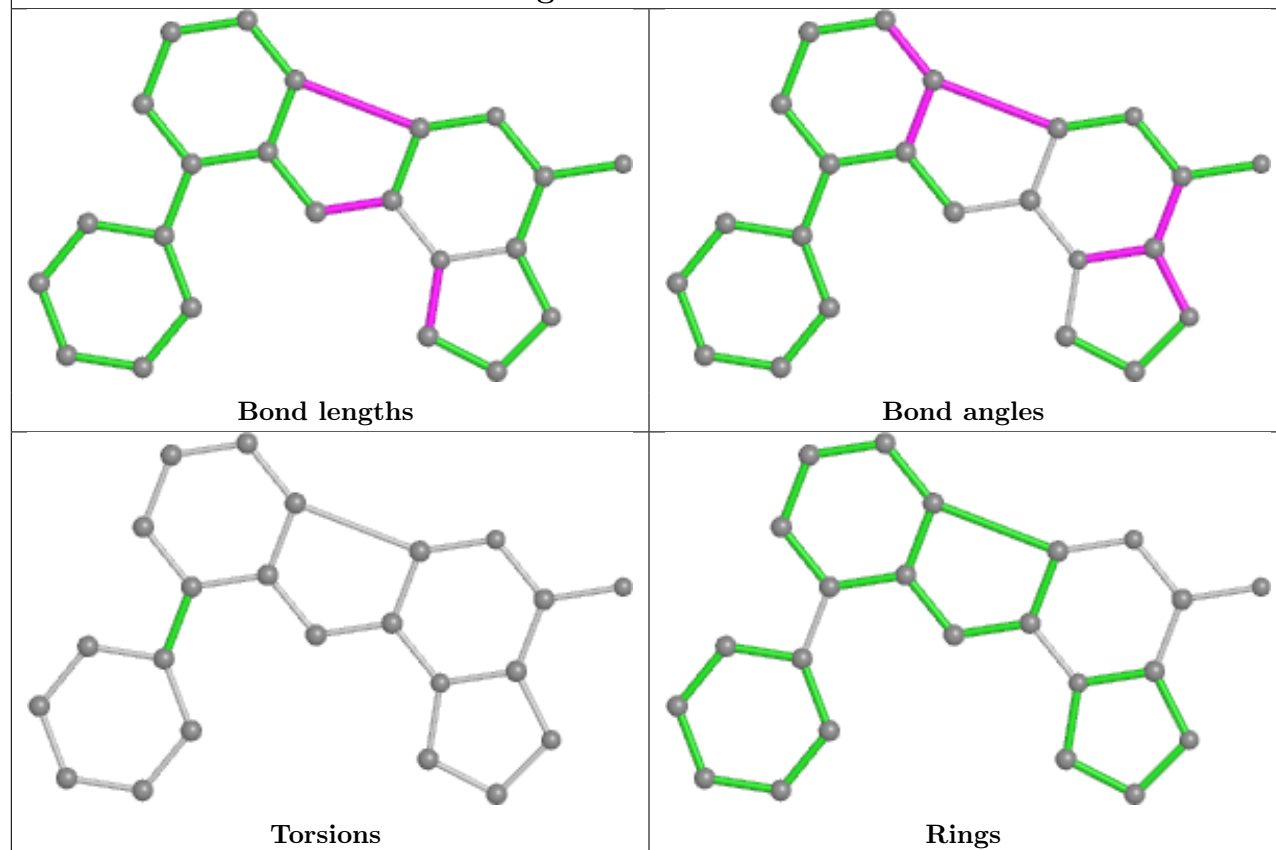
Ligand 2K9 F 900



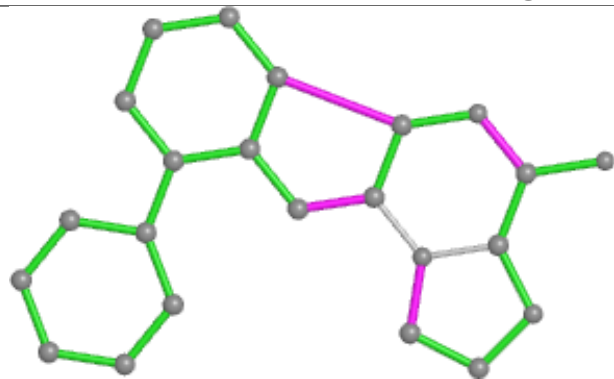
Ligand 2K9 W 900



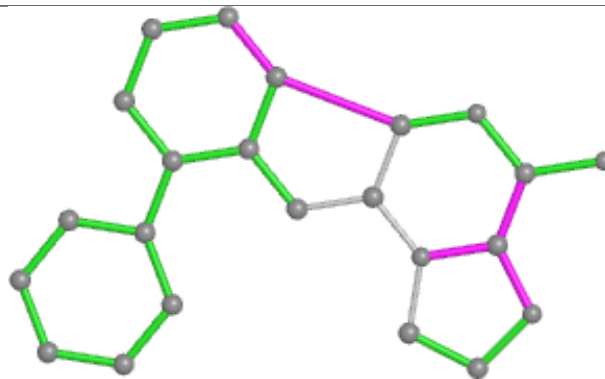
Ligand 2K9 O 900



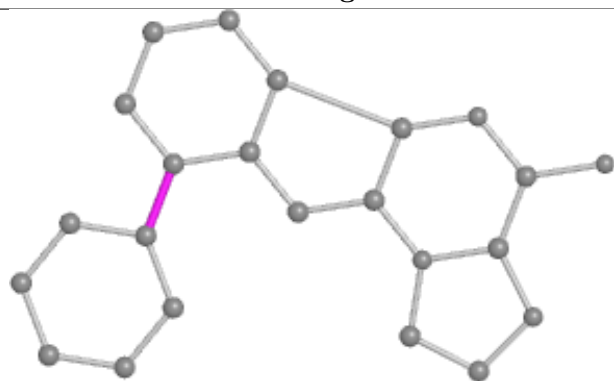
Ligand 2K9 B 900



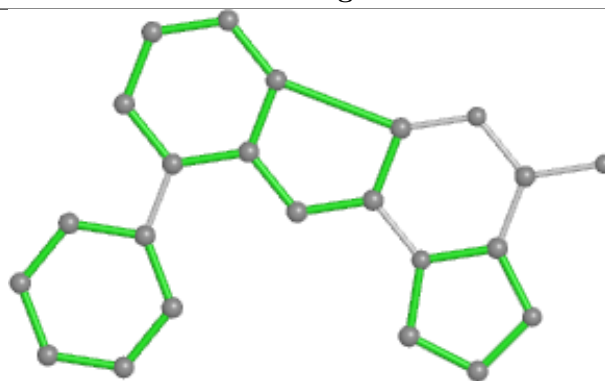
Bond lengths



Bond angles

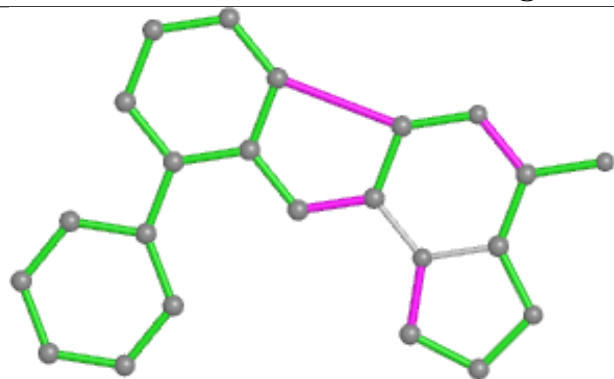


Torsions

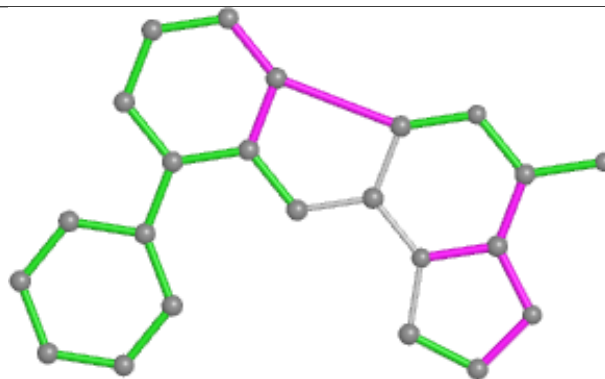


Rings

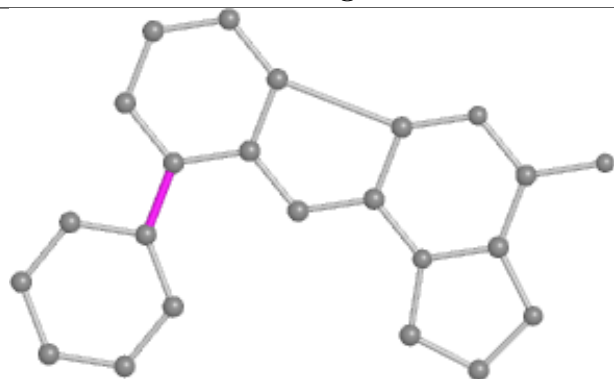
Ligand 2K9 H 900



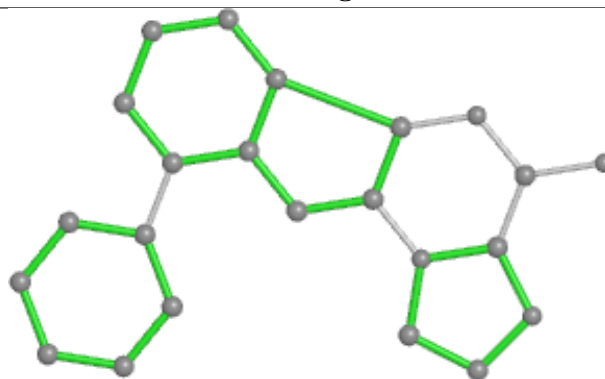
Bond lengths



Bond angles

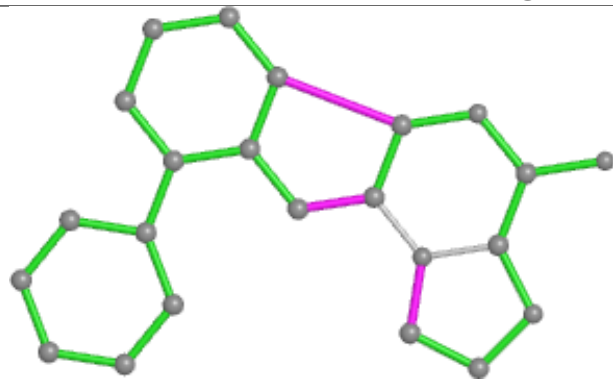


Torsions

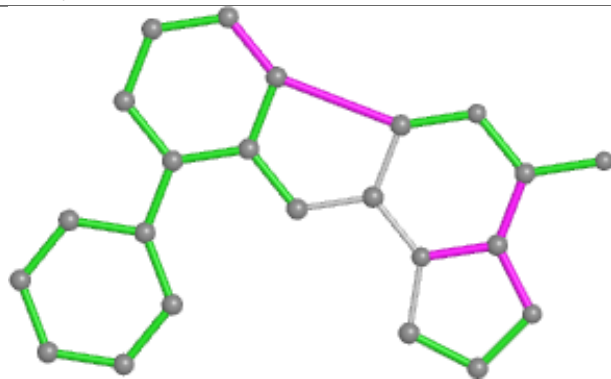


Rings

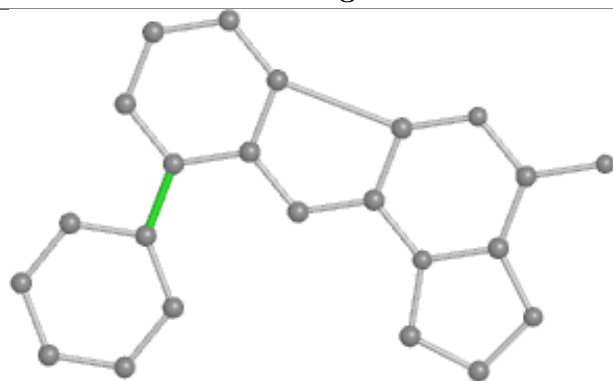
Ligand 2K9 Q 900



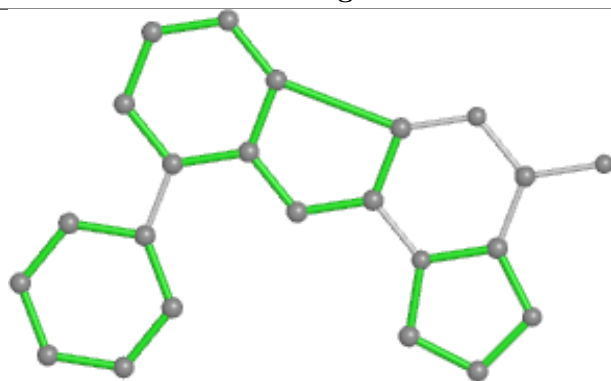
Bond lengths



Bond angles

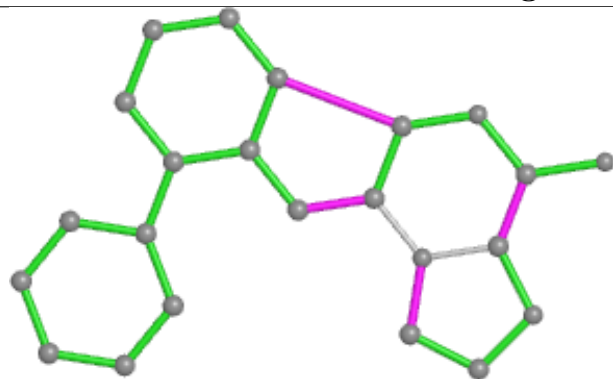


Torsions

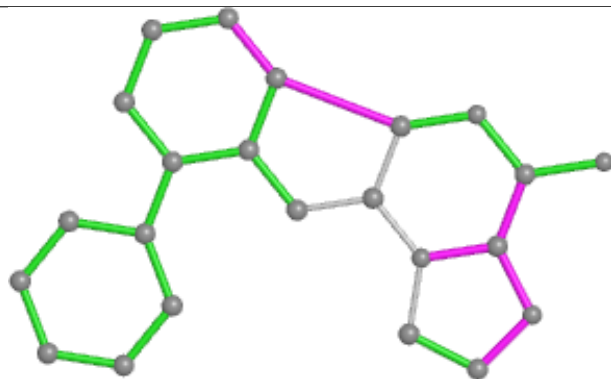


Rings

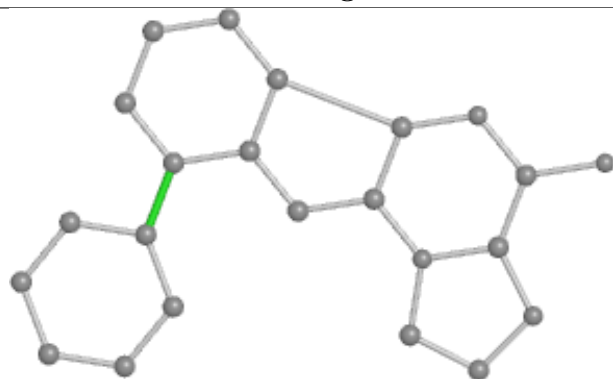
Ligand 2K9 T 900



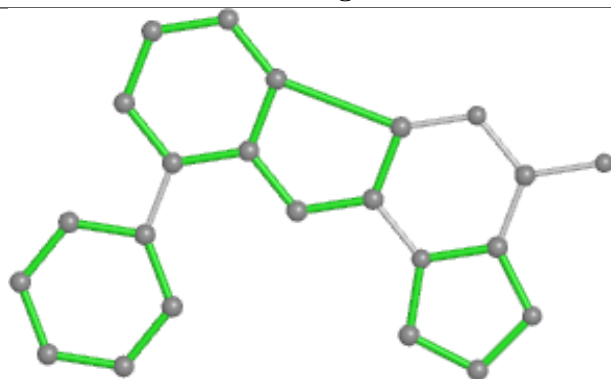
Bond lengths



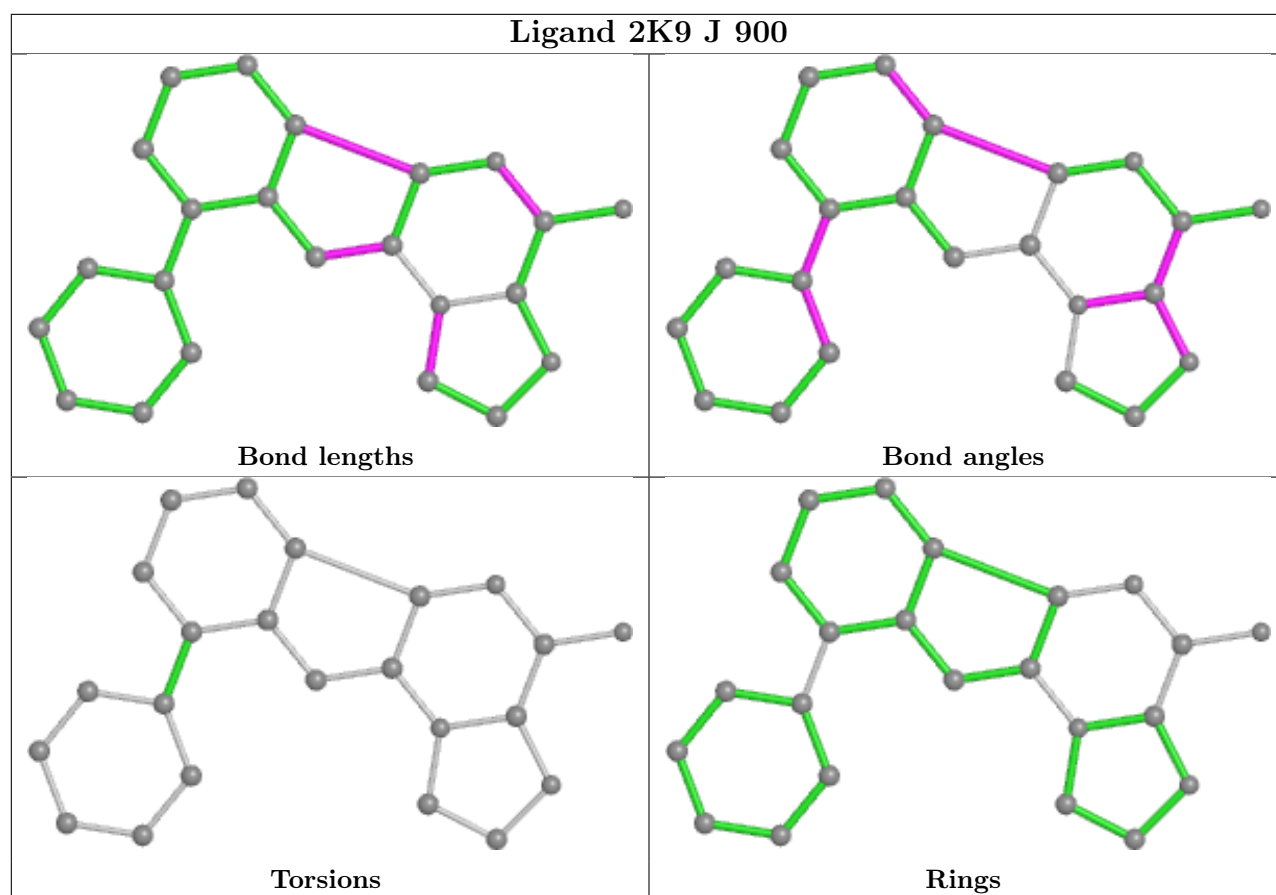
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	466/478 (97%)	-0.18	17 (3%) 42 40	31, 54, 85, 128	0
1	B	464/478 (97%)	-0.11	15 (3%) 47 46	33, 55, 85, 125	0
1	C	460/478 (96%)	-0.20	5 (1%) 80 81	32, 53, 83, 124	0
1	D	466/478 (97%)	-0.17	8 (1%) 70 68	31, 52, 82, 124	0
1	E	463/478 (96%)	-0.21	5 (1%) 80 81	31, 52, 82, 124	0
1	F	467/478 (97%)	-0.19	5 (1%) 80 81	31, 54, 85, 124	0
1	G	466/478 (97%)	-0.18	11 (2%) 59 56	31, 54, 84, 124	0
1	H	464/478 (97%)	-0.20	12 (2%) 56 53	32, 54, 84, 124	0
1	I	460/478 (96%)	-0.26	7 (1%) 73 72	32, 53, 82, 124	0
1	J	466/478 (97%)	-0.25	8 (1%) 70 68	31, 52, 82, 124	0
1	K	463/478 (96%)	-0.16	8 (1%) 70 68	31, 53, 82, 124	0
1	L	467/478 (97%)	-0.25	5 (1%) 80 81	32, 53, 84, 124	0
1	M	466/478 (97%)	-0.10	13 (2%) 53 51	33, 54, 85, 124	0
1	N	464/478 (97%)	-0.23	6 (1%) 77 77	32, 53, 83, 124	0
1	O	460/478 (96%)	-0.20	9 (1%) 65 64	32, 54, 83, 124	0
1	P	466/478 (97%)	-0.23	10 (2%) 63 62	32, 54, 83, 124	0
1	Q	463/478 (96%)	-0.17	9 (1%) 66 65	34, 55, 83, 125	0
1	R	467/478 (97%)	-0.20	11 (2%) 59 56	32, 53, 84, 124	0
1	S	466/478 (97%)	-0.17	11 (2%) 59 56	33, 54, 84, 124	0
1	T	464/478 (97%)	-0.22	7 (1%) 73 72	32, 54, 83, 124	0
1	U	460/478 (96%)	-0.22	8 (1%) 70 68	32, 53, 83, 124	0
1	V	466/478 (97%)	-0.28	9 (1%) 66 65	31, 53, 82, 124	0
1	W	463/478 (96%)	-0.25	6 (1%) 77 77	33, 54, 82, 124	0
1	X	467/478 (97%)	-0.22	9 (1%) 66 65	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%)	-0.20	214 (1%) 66 65	31, 54, 84, 128	0

All (214) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	402	TYR	6.6
1	O	406	PRO	5.6
1	M	405	PRO	4.7
1	M	406	PRO	4.6
1	A	61	HIS	4.6
1	R	406	PRO	4.5
1	L	51	GLY	4.4
1	D	406	PRO	4.3
1	M	402	TYR	4.3
1	D	402	TYR	4.3
1	B	406	PRO	4.3
1	M	403	GLU	4.2
1	P	406	PRO	4.2
1	O	405	PRO	4.1
1	U	406	PRO	4.1
1	G	407	GLU	4.1
1	H	407	GLU	4.1
1	D	51	GLY	4.0
1	A	402	TYR	4.0
1	Q	406	PRO	4.0
1	S	406	PRO	3.9
1	I	406	PRO	3.9
1	O	51	GLY	3.9
1	X	51	GLY	3.8
1	C	403	GLU	3.8
1	V	406	PRO	3.8
1	R	51	GLY	3.8
1	G	405	PRO	3.8
1	S	400	ASP	3.7
1	U	402	TYR	3.7
1	D	407	GLU	3.7
1	B	329	GLY	3.7
1	G	406	PRO	3.7
1	G	51	GLY	3.6
1	T	406	PRO	3.6
1	T	403	GLU	3.5
1	H	406	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	Q	405	PRO	3.5
1	N	402	TYR	3.5
1	L	407	GLU	3.4
1	U	51	GLY	3.4
1	E	406	PRO	3.4
1	K	402	TYR	3.4
1	R	401	LEU	3.4
1	V	407	GLU	3.4
1	M	401	LEU	3.3
1	S	401	LEU	3.3
1	K	403	GLU	3.3
1	X	407	GLU	3.3
1	P	405	PRO	3.3
1	B	407	GLU	3.3
1	Q	402	TYR	3.3
1	N	406	PRO	3.2
1	A	400	ASP	3.2
1	C	406	PRO	3.2
1	P	-2	THR	3.2
1	N	403	GLU	3.2
1	R	407	GLU	3.2
1	G	401	LEU	3.2
1	N	51	GLY	3.1
1	W	63	SER	3.1
1	A	405	PRO	3.1
1	P	407	GLU	3.1
1	X	330	TYR	3.1
1	B	51	GLY	3.1
1	M	61	HIS	3.1
1	L	406	PRO	3.1
1	J	406	PRO	3.1
1	W	402	TYR	3.1
1	E	405	PRO	3.1
1	M	400	ASP	3.0
1	I	407	GLU	3.0
1	S	405	PRO	3.0
1	A	403	GLU	3.0
1	S	403	GLU	3.0
1	T	402	TYR	3.0
1	K	401	LEU	3.0
1	F	402	TYR	2.9
1	S	61	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	T	407	GLU	2.9
1	R	405	PRO	2.9
1	O	407	GLU	2.9
1	E	63	SER	2.9
1	Q	63	SER	2.9
1	F	407	GLU	2.9
1	W	403	GLU	2.9
1	J	407	GLU	2.8
1	A	413	PRO	2.8
1	A	407	GLU	2.8
1	S	402	TYR	2.8
1	G	408	GLU	2.8
1	D	400	ASP	2.8
1	X	406	PRO	2.8
1	T	405	PRO	2.8
1	A	406	PRO	2.8
1	Q	403	GLU	2.8
1	H	330	TYR	2.8
1	I	403	GLU	2.7
1	P	402	TYR	2.7
1	N	405	PRO	2.7
1	C	402	TYR	2.7
1	R	354	SER	2.7
1	L	402	TYR	2.7
1	A	401	LEU	2.7
1	V	405	PRO	2.7
1	H	402	TYR	2.7
1	Q	407	GLU	2.7
1	H	331	GLU	2.7
1	G	402	TYR	2.7
1	R	330	TYR	2.7
1	G	404	LEU	2.7
1	P	404	LEU	2.7
1	D	403	GLU	2.7
1	G	400	ASP	2.6
1	V	408	GLU	2.6
1	S	354	SER	2.6
1	O	402	TYR	2.6
1	A	408	GLU	2.5
1	R	403	GLU	2.5
1	D	-1	GLU	2.5
1	P	399	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	409	ALA	2.5
1	A	404	LEU	2.5
1	P	411	SER	2.5
1	E	402	TYR	2.5
1	I	402	TYR	2.5
1	B	330	TYR	2.5
1	Q	409	ALA	2.5
1	F	403	GLU	2.5
1	B	403	GLU	2.5
1	H	403	GLU	2.5
1	U	180	GLY	2.4
1	B	399	LYS	2.4
1	M	407	GLU	2.4
1	H	405	PRO	2.4
1	K	400	ASP	2.4
1	M	289	THR	2.4
1	G	180	GLY	2.4
1	A	410	ALA	2.4
1	A	62	GLU	2.4
1	S	404	LEU	2.4
1	J	403	GLU	2.4
1	B	331	GLU	2.4
1	B	45	ASP	2.4
1	C	410	ALA	2.4
1	F	406	PRO	2.4
1	K	406	PRO	2.4
1	V	400	ASP	2.3
1	X	400	ASP	2.3
1	S	399	LYS	2.3
1	B	402	TYR	2.3
1	X	61	HIS	2.3
1	B	409	ALA	2.3
1	M	63	SER	2.3
1	U	403	GLU	2.3
1	U	407	GLU	2.3
1	A	354	SER	2.3
1	O	354	SER	2.3
1	E	407	GLU	2.3
1	X	401	LEU	2.3
1	B	353	GLY	2.3
1	R	331	GLU	2.3
1	B	11	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	405	PRO	2.3
1	N	407	GLU	2.2
1	V	402	TYR	2.2
1	P	354	SER	2.2
1	M	296	ASP	2.2
1	U	399	LYS	2.2
1	X	402	TYR	2.2
1	B	44	ASP	2.2
1	C	409	ALA	2.2
1	V	404	LEU	2.2
1	H	45	ASP	2.2
1	A	356	PRO	2.2
1	H	413	PRO	2.2
1	J	63	SER	2.2
1	X	354	SER	2.2
1	K	405	PRO	2.2
1	W	406	PRO	2.2
1	A	412	ILE	2.2
1	V	180	GLY	2.2
1	W	407	GLU	2.2
1	H	412	ILE	2.1
1	L	405	PRO	2.1
1	F	400	ASP	2.1
1	M	404	LEU	2.1
1	J	330	TYR	2.1
1	K	413	PRO	2.1
1	Q	336	LEU	2.1
1	K	164	THR	2.1
1	O	180	GLY	2.1
1	H	411	SER	2.1
1	I	7	LYS	2.1
1	G	409	ALA	2.1
1	H	400	ASP	2.1
1	U	280	ASP	2.1
1	J	410	ALA	2.1
1	A	51	GLY	2.1
1	O	7	LYS	2.1
1	S	407	GLU	2.1
1	V	51	GLY	2.1
1	O	280	ASP	2.1
1	R	289	THR	2.0
1	T	399	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	M	354	SER	2.0
1	W	405	PRO	2.0
1	T	62	GLU	2.0
1	B	404	LEU	2.0
1	J	51	GLY	2.0
1	P	63	SER	2.0
1	Q	411	SER	2.0
1	D	405	PRO	2.0
1	J	402	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	F	900	23/23	0.90	0.27	64,67,67,68	0
2	2K9	O	900	23/23	0.90	0.44	82,85,88,88	0
2	2K9	M	900	23/23	0.91	0.27	85,86,87,88	0
2	2K9	Q	900	23/23	0.92	0.24	113,114,114,114	0
2	2K9	W	900	23/23	0.92	0.22	76,77,77,78	0
2	2K9	B	900	23/23	0.93	0.26	100,102,103,104	0
2	2K9	S	900	23/23	0.93	0.22	67,69,71,72	0
2	2K9	U	900	23/23	0.93	0.32	69,73,75,77	0
2	2K9	P	900	23/23	0.93	0.27	64,65,66,67	0
2	2K9	H	900	23/23	0.94	0.27	90,90,91,92	0
2	2K9	G	900	23/23	0.94	0.26	54,54,56,57	0
2	2K9	N	900	23/23	0.94	0.24	58,60,61,62	0
2	2K9	R	900	23/23	0.95	0.31	57,58,59,59	0
2	2K9	K	900	23/23	0.95	0.20	46,48,49,50	0

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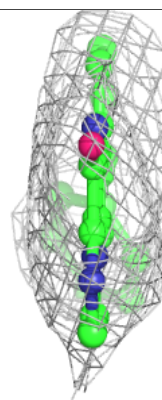
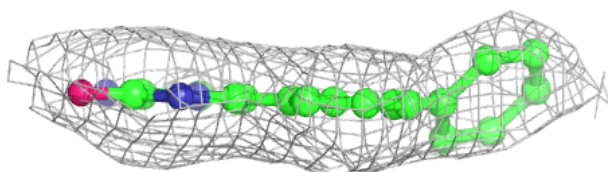
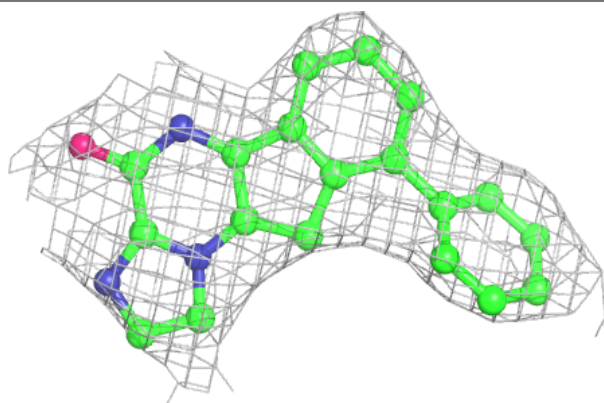
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	2K9	D	900	23/23	0.95	0.22	47,51,53,54	0
2	2K9	V	900	23/23	0.95	0.23	39,43,45,47	0
2	2K9	I	900	23/23	0.95	0.19	54,55,57,57	0
2	2K9	X	900	23/23	0.95	0.28	60,61,61,62	0
2	2K9	A	900	23/23	0.96	0.27	58,60,62,62	0
2	2K9	L	900	23/23	0.96	0.24	50,51,52,53	0
2	2K9	J	900	23/23	0.96	0.24	56,58,60,60	0
2	2K9	T	900	23/23	0.96	0.24	75,75,76,76	0
2	2K9	E	900	23/23	0.97	0.25	43,44,46,46	0
2	2K9	C	900	23/23	0.97	0.20	47,48,49,50	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.

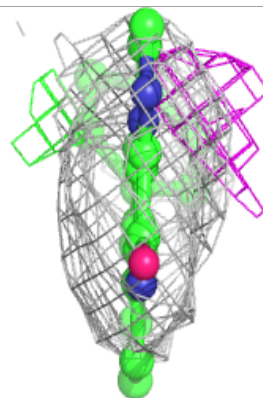
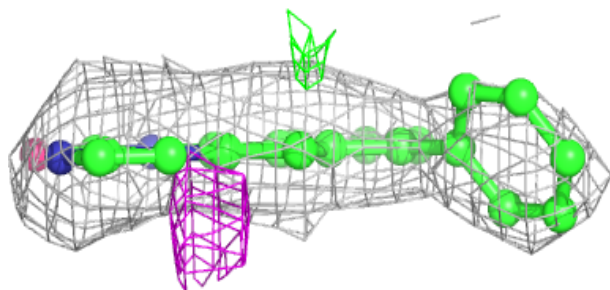
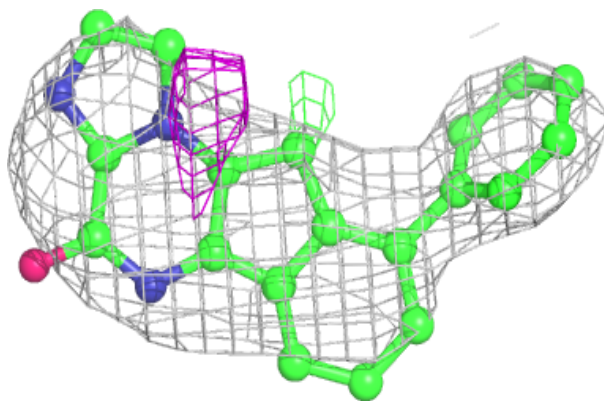
Electron density around 2K9 F 900:

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

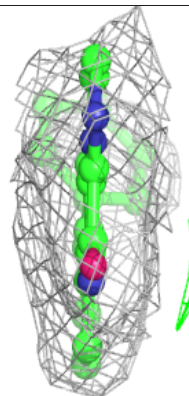
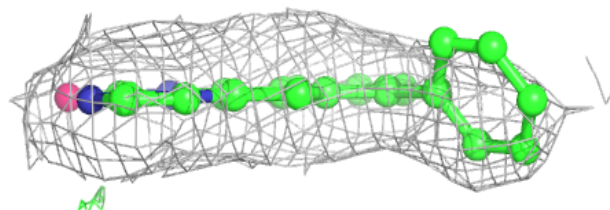
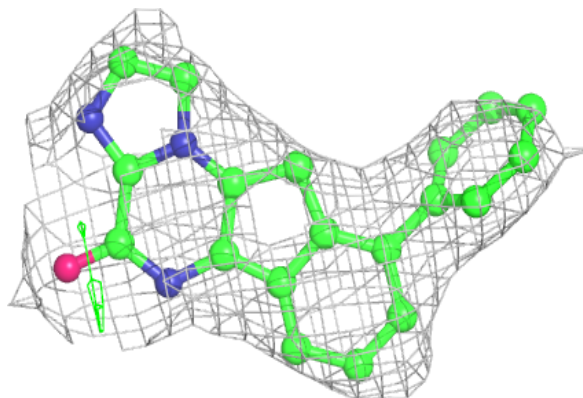


Electron density around 2K9 O 900:

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

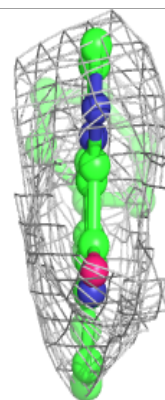
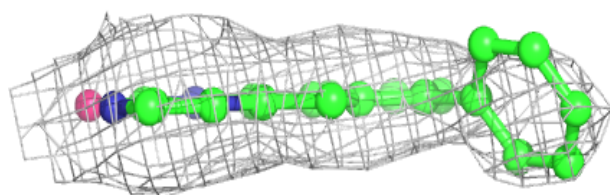
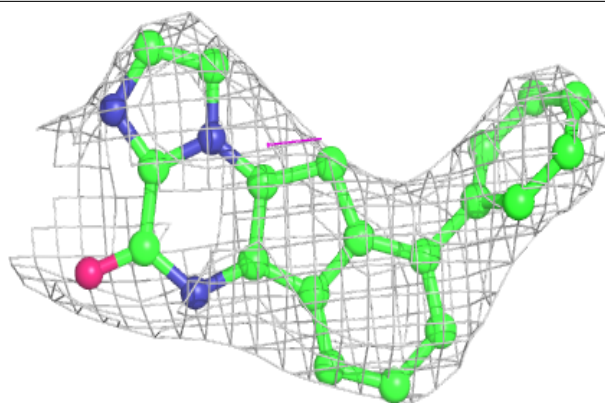
**Electron density around 2K9 M 900:**

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

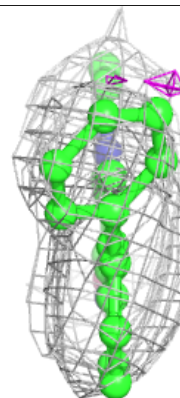
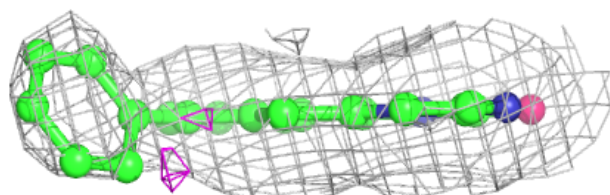
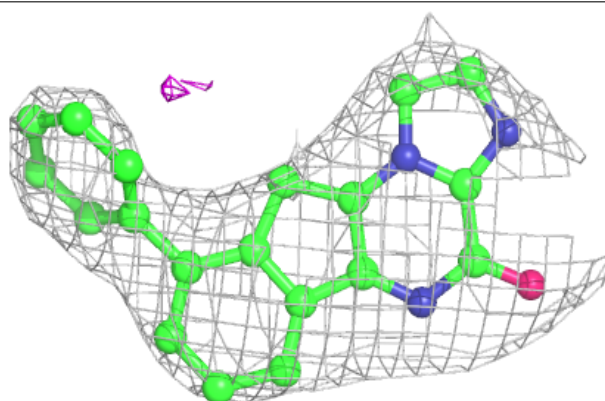


Electron density around 2K9 Q 900:

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

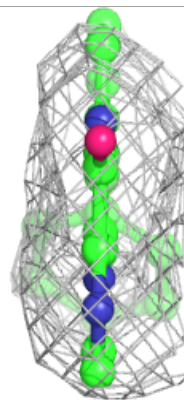
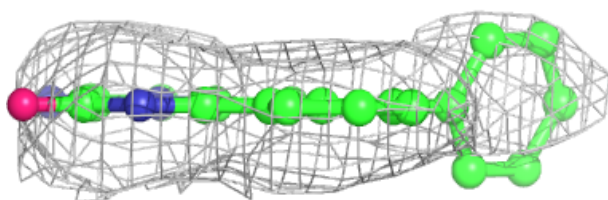
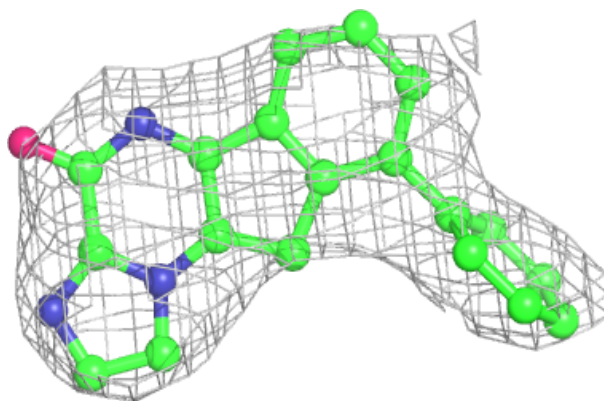
**Electron density around 2K9 W 900:**

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

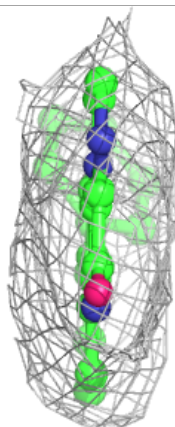
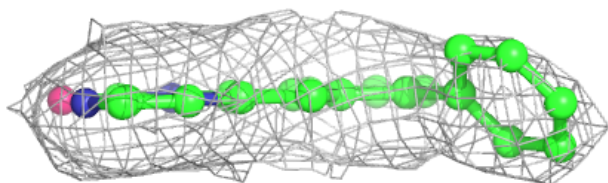
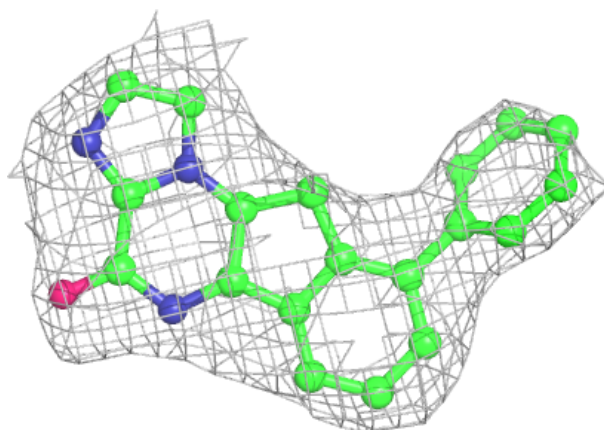


Electron density around 2K9 B 900:

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

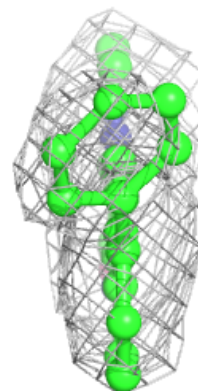
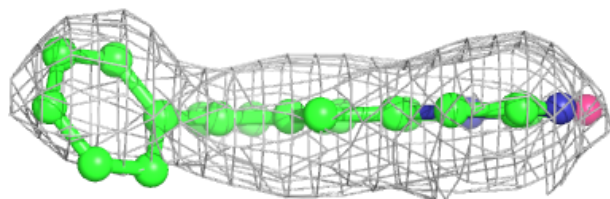
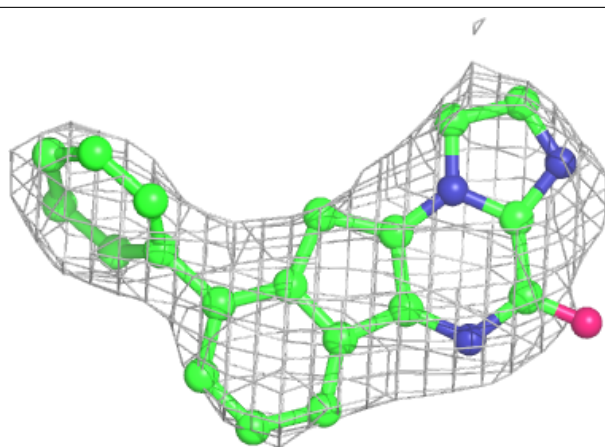
**Electron density around 2K9 S 900:**

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

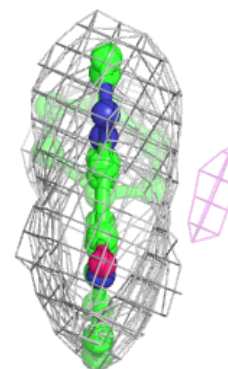
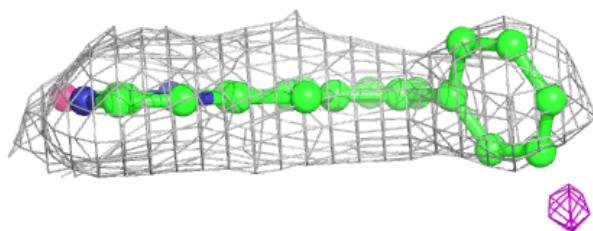
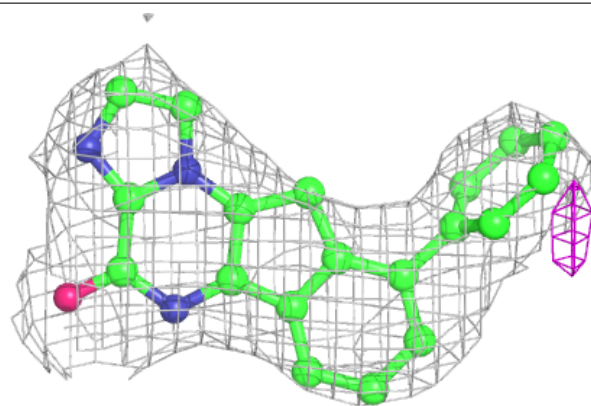


Electron density around 2K9 U 900:

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and green (positive)

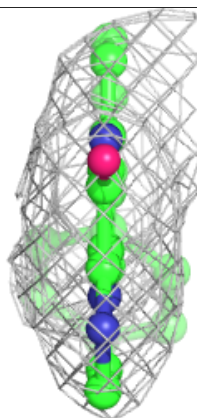
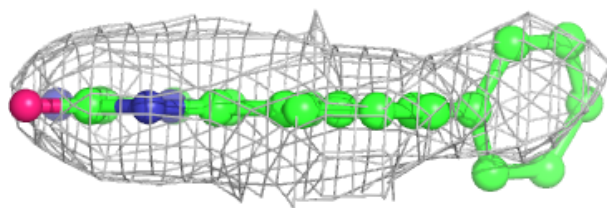
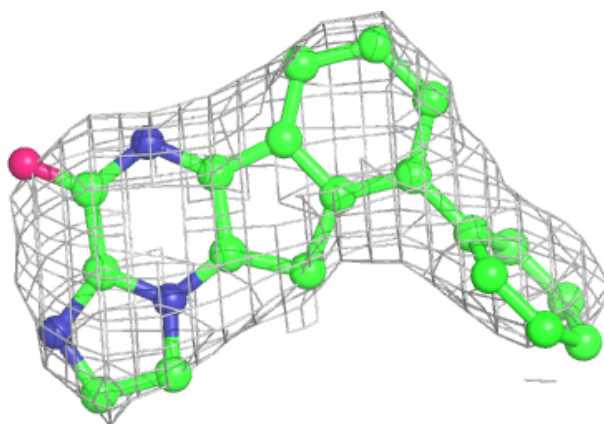
**Electron density around 2K9 P 900:**

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



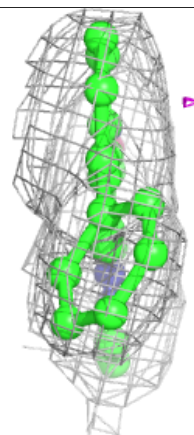
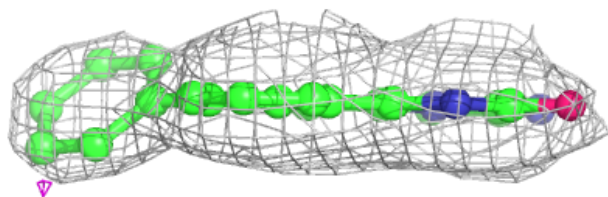
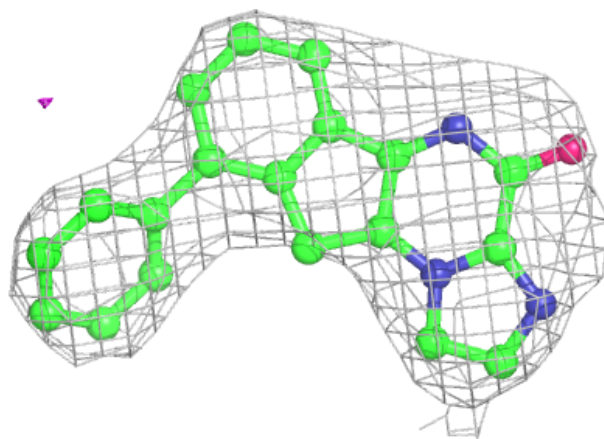
Electron density around 2K9 H 900:

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and green (positive)

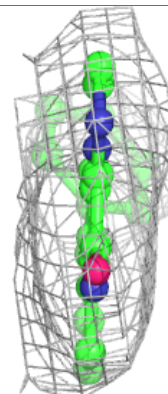
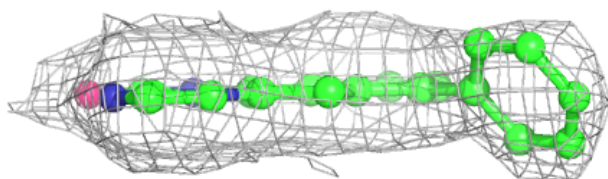
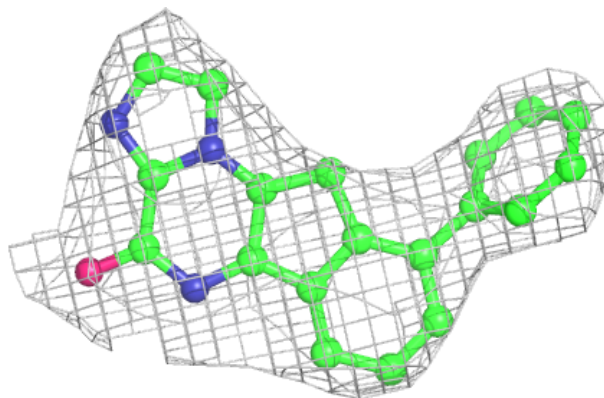


Electron density around 2K9 G 900:

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

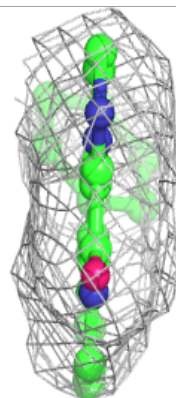
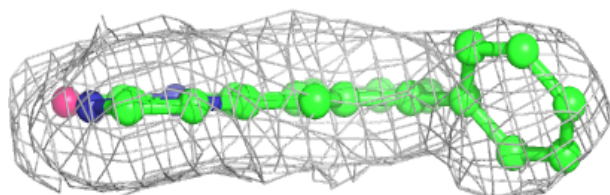
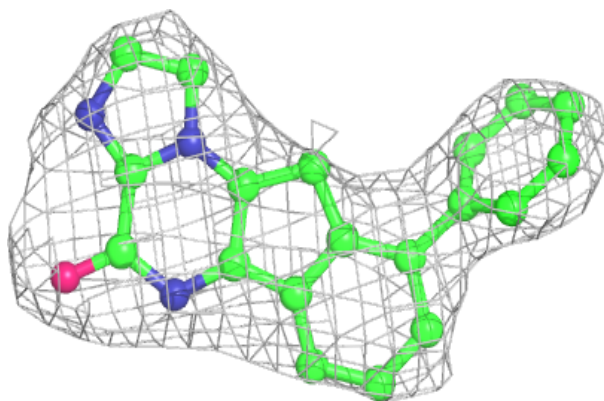
**Electron density around 2K9 N 900:**

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and green (positive)

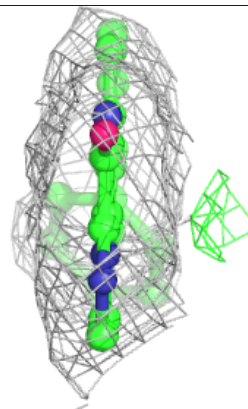
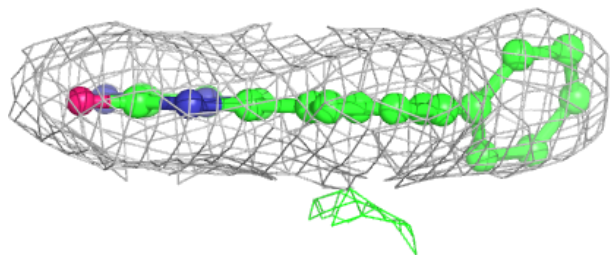
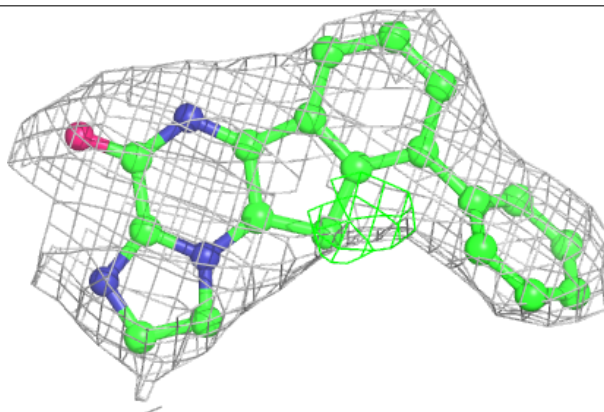


Electron density around 2K9 R 900:

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and green (positive)

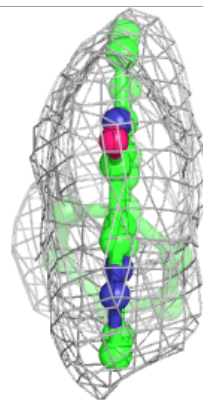
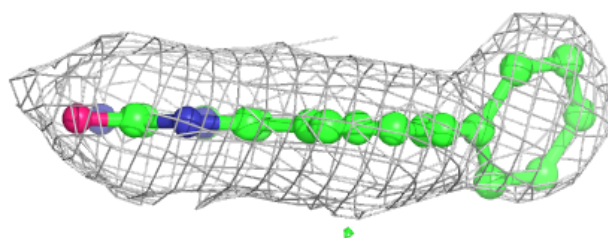
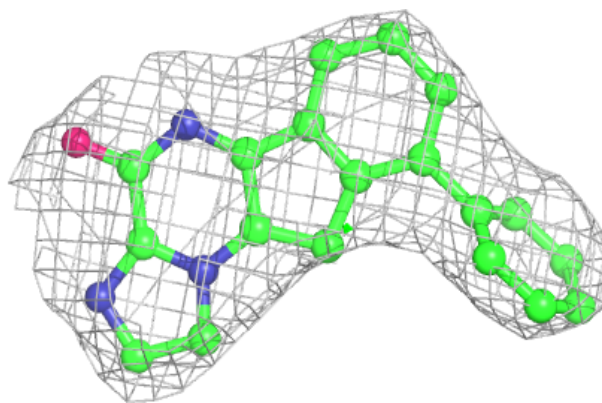
**Electron density around 2K9 K 900:**

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and green (positive)

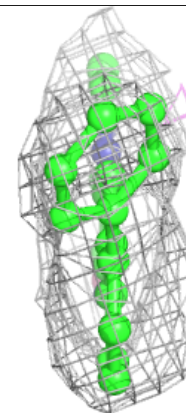
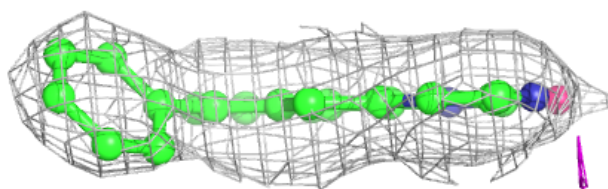
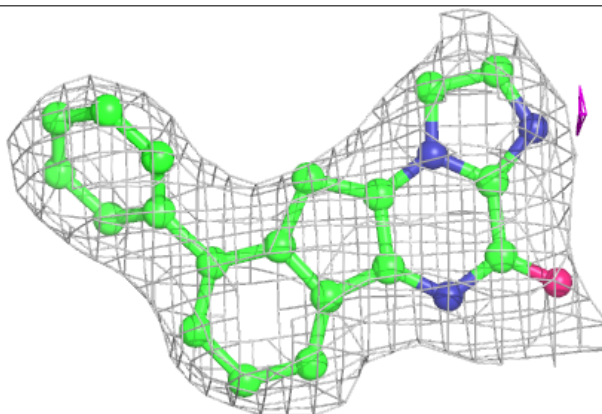


Electron density around 2K9 D 900:

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and green (positive)

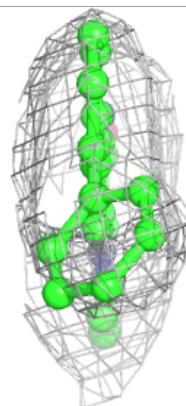
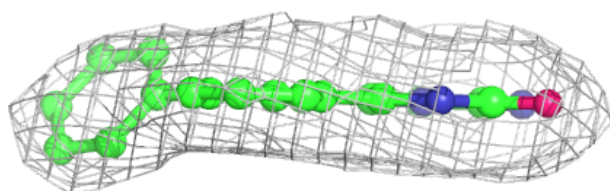
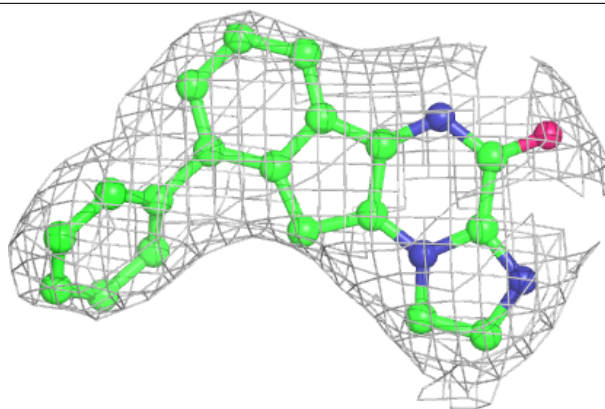
**Electron density around 2K9 V 900:**

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and green (positive)

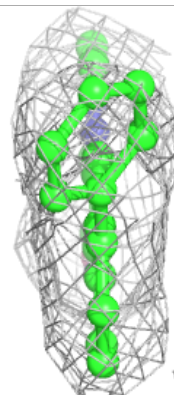
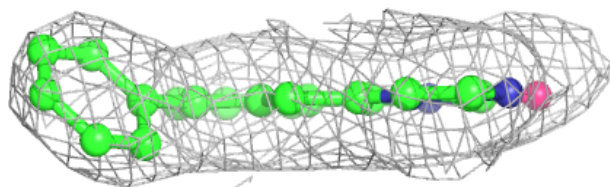
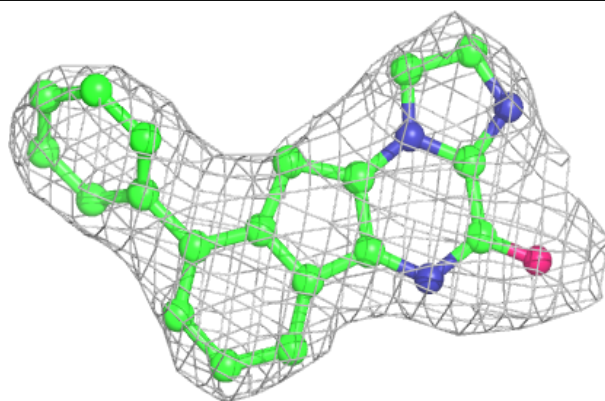


Electron density around 2K9 I 900:

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

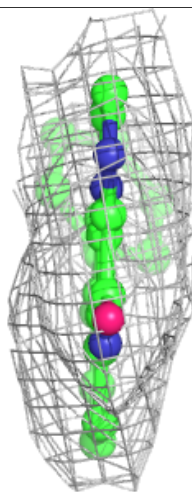
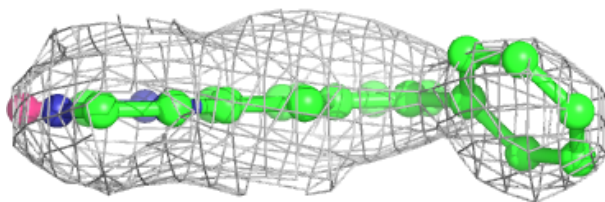
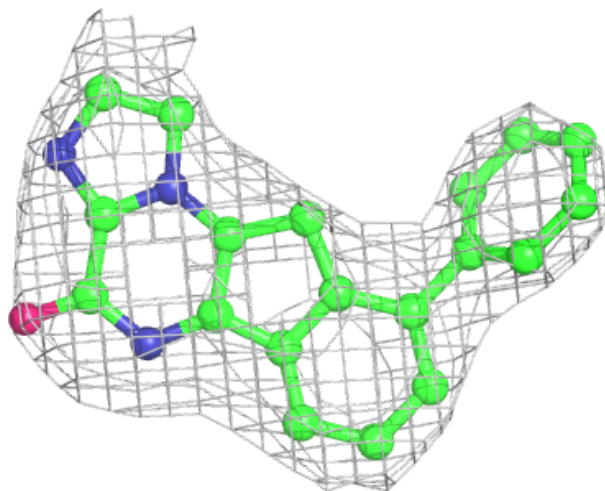
**Electron density around 2K9 X 900:**

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



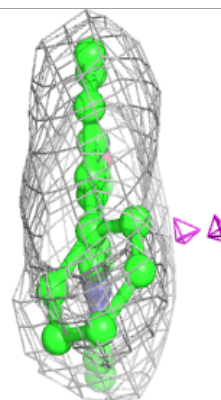
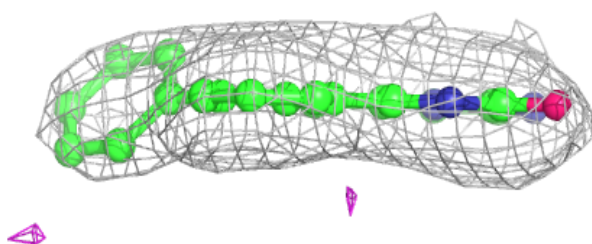
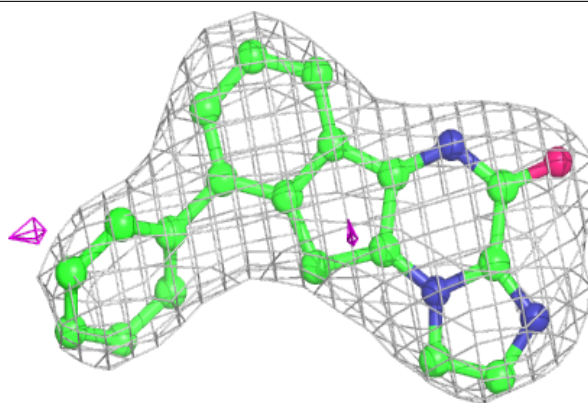
Electron density around 2K9 A 900:

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

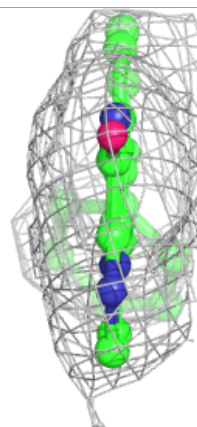
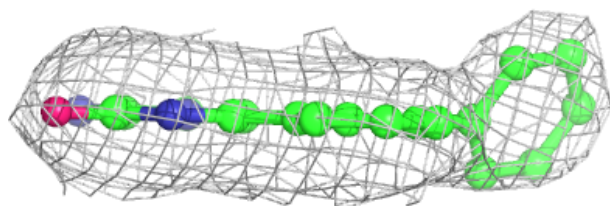
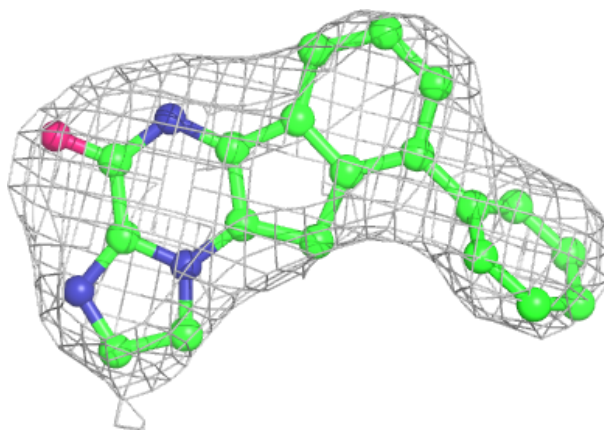


Electron density around 2K9 L 900:

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

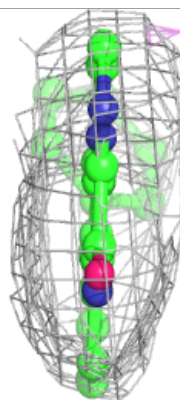
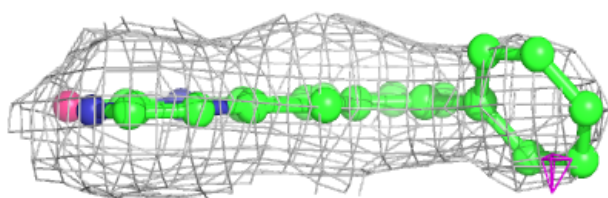
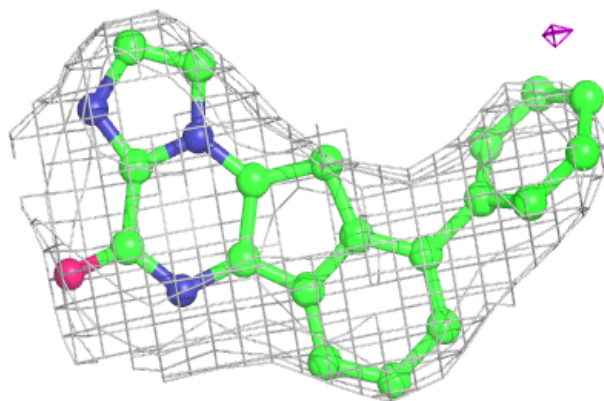
**Electron density around 2K9 J 900:**

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

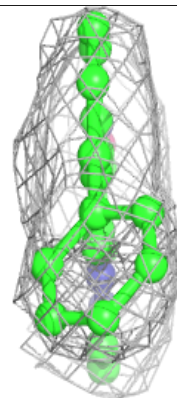
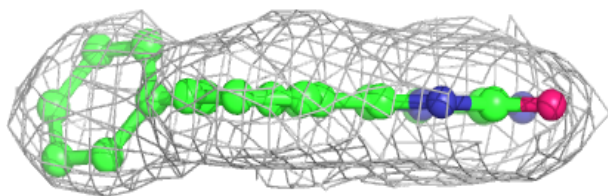
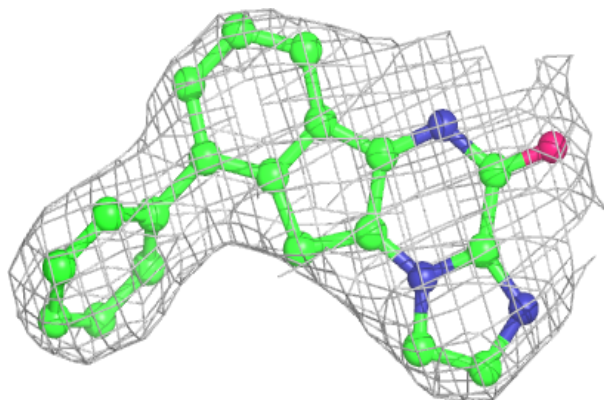


Electron density around 2K9 T 900:

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

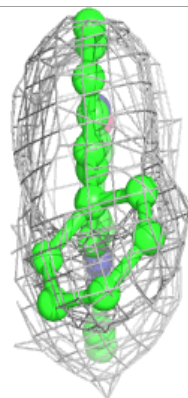
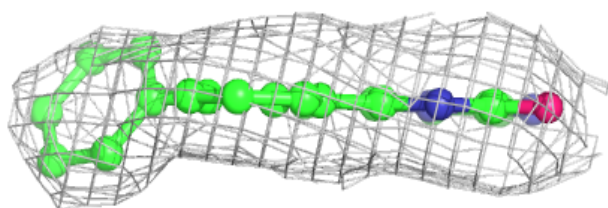
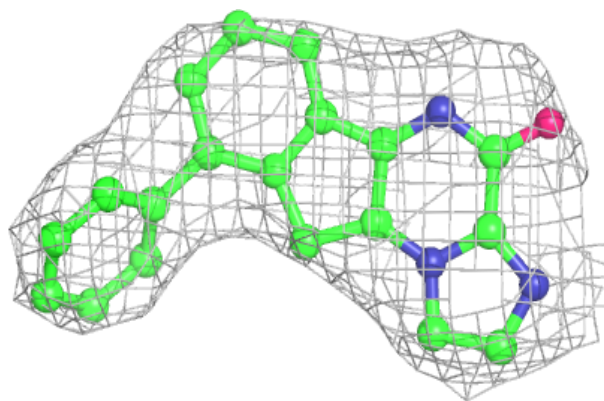
**Electron density around 2K9 E 900:**

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.