



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:06 PM UTC

PDB ID : 5C1A / pdb_00005c1a
Title : p97-N750D/R753D/M757D/Q760D in complex with ATP-gamma-S
Authors : Haenzelmann, P.; Schindelin, H.
Deposited on : 2015-06-13
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

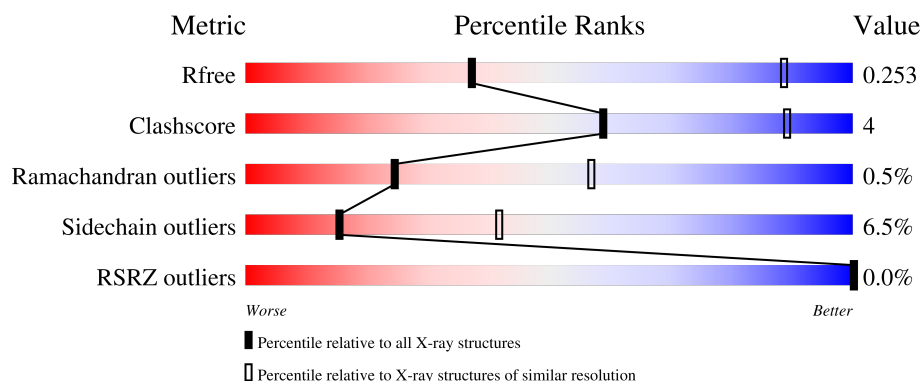
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	805	 78% 12% • 9%
1	B	805	 75% 15% • 9%
1	C	805	 78% 12% • 9%
1	D	805	 79% 12% • 9%
1	E	805	 77% 13% • 9%

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Mol	Chain	Length	Quality of chain
1	F	805	 78%12% • 9%
1	G	805	 77%14% • 9%
1	H	805	 77%13% • 9%
1	I	805	 76%13% • 9%
1	J	805	 78%12% • 9%
1	K	805	 74%16% • 8%
1	L	805	 77%13% • 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 140261 atoms, of which 70187 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 Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	735	Total	C	H	N	O	S	0	0	0
			11578	3616	5814	1019	1100	29			
1	B	735	Total	C	H	N	O	S	0	0	0
			11590	3623	5819	1019	1100	29			
1	C	735	Total	C	H	N	O	S	0	0	0
			11589	3623	5818	1019	1100	29			
1	D	735	Total	C	H	N	O	S	0	0	0
			11591	3623	5820	1019	1100	29			
1	E	735	Total	C	H	N	O	S	0	0	0
			11589	3623	5818	1019	1100	29			
1	F	735	Total	C	H	N	O	S	0	0	0
			11589	3623	5818	1019	1100	29			
1	G	735	Total	C	H	N	O	S	0	0	0
			11576	3616	5812	1019	1100	29			
1	H	735	Total	C	H	N	O	S	0	0	0
			11590	3623	5819	1019	1100	29			
1	I	735	Total	C	H	N	O	S	0	0	0
			11589	3623	5818	1019	1100	29			
1	J	735	Total	C	H	N	O	S	0	0	0
			11590	3623	5819	1019	1100	29			
1	K	744	Total	C	H	N	O	S	0	0	0
			11719	3663	5880	1029	1117	30			
1	L	735	Total	C	H	N	O	S	0	0	0
			11591	3623	5820	1019	1100	29			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	750	ASP	ASN	engineered mutation	UNP P55072
A	753	ASP	ARG	engineered mutation	UNP P55072
A	757	ASP	MET	engineered mutation	UNP P55072
A	760	ASP	GLN	engineered mutation	UNP P55072
B	750	ASP	ASN	engineered mutation	UNP P55072

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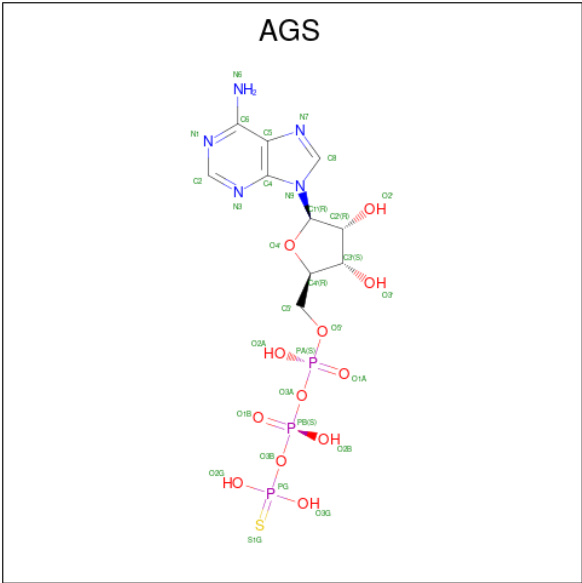
Chain	Residue	Modelled	Actual	Comment	Reference
B	753	ASP	ARG	engineered mutation	UNP P55072
B	757	ASP	MET	engineered mutation	UNP P55072
B	760	ASP	GLN	engineered mutation	UNP P55072
C	750	ASP	ASN	engineered mutation	UNP P55072
C	753	ASP	ARG	engineered mutation	UNP P55072
C	757	ASP	MET	engineered mutation	UNP P55072
C	760	ASP	GLN	engineered mutation	UNP P55072
D	750	ASP	ASN	engineered mutation	UNP P55072
D	753	ASP	ARG	engineered mutation	UNP P55072
D	757	ASP	MET	engineered mutation	UNP P55072
D	760	ASP	GLN	engineered mutation	UNP P55072
E	750	ASP	ASN	engineered mutation	UNP P55072
E	753	ASP	ARG	engineered mutation	UNP P55072
E	757	ASP	MET	engineered mutation	UNP P55072
E	760	ASP	GLN	engineered mutation	UNP P55072
F	750	ASP	ASN	engineered mutation	UNP P55072
F	753	ASP	ARG	engineered mutation	UNP P55072
F	757	ASP	MET	engineered mutation	UNP P55072
F	760	ASP	GLN	engineered mutation	UNP P55072
G	750	ASP	ASN	engineered mutation	UNP P55072
G	753	ASP	ARG	engineered mutation	UNP P55072
G	757	ASP	MET	engineered mutation	UNP P55072
G	760	ASP	GLN	engineered mutation	UNP P55072
H	750	ASP	ASN	engineered mutation	UNP P55072
H	753	ASP	ARG	engineered mutation	UNP P55072
H	757	ASP	MET	engineered mutation	UNP P55072
H	760	ASP	GLN	engineered mutation	UNP P55072
I	750	ASP	ASN	engineered mutation	UNP P55072
I	753	ASP	ARG	engineered mutation	UNP P55072
I	757	ASP	MET	engineered mutation	UNP P55072
I	760	ASP	GLN	engineered mutation	UNP P55072
J	750	ASP	ASN	engineered mutation	UNP P55072
J	753	ASP	ARG	engineered mutation	UNP P55072
J	757	ASP	MET	engineered mutation	UNP P55072
J	760	ASP	GLN	engineered mutation	UNP P55072
K	750	ASP	ASN	engineered mutation	UNP P55072
K	753	ASP	ARG	engineered mutation	UNP P55072
K	757	ASP	MET	engineered mutation	UNP P55072
K	760	ASP	GLN	engineered mutation	UNP P55072
L	750	ASP	ASN	engineered mutation	UNP P55072
L	753	ASP	ARG	engineered mutation	UNP P55072
L	757	ASP	MET	engineered mutation	UNP P55072

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Chain	Residue	Modelled	Actual	Comment	Reference
L	760	ASP	GLN	engineered mutation	UNP P55072

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



Mol	Chain	Residues	Atoms								ZeroOcc	AltConf
			Total	C	H	N	O	P	S			
2	A	1	Total	C	H	N	O	P	S		0	0
			44	10	13	5	12	3	1			
2	A	1	Total	C	H	N	O	P	S		0	0
			44	10	13	5	12	3	1			
2	B	1	Total	C	H	N	O	P	S		0	0
			44	10	13	5	12	3	1			
2	B	1	Total	C	H	N	O	P	S		0	0
			44	10	13	5	12	3	1			
2	C	1	Total	C	H	N	O	P	S		0	0
			44	10	13	5	12	3	1			
2	C	1	Total	C	H	N	O	P	S		0	0
			44	10	13	5	12	3	1			
2	D	1	Total	C	H	N	O	P	S		0	0
			44	10	13	5	12	3	1			
2	D	1	Total	C	H	N	O	P	S		0	0
			44	10	13	5	12	3	1			
2	E	1	Total	C	H	N	O	P	S		0	0
			44	10	13	5	12	3	1			
2	E	1	Total	C	H	N	O	P	S		0	0
			44	10	13	5	12	3	1			

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Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	F	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	F	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	G	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	G	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	H	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	H	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	I	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	I	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	J	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	J	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	K	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	K	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	L	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	L	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		
3	B	2	Total	Mg	0	0
			2	2		
3	C	2	Total	Mg	0	0
			2	2		
3	D	2	Total	Mg	0	0
			2	2		
3	E	2	Total	Mg	0	0
			2	2		

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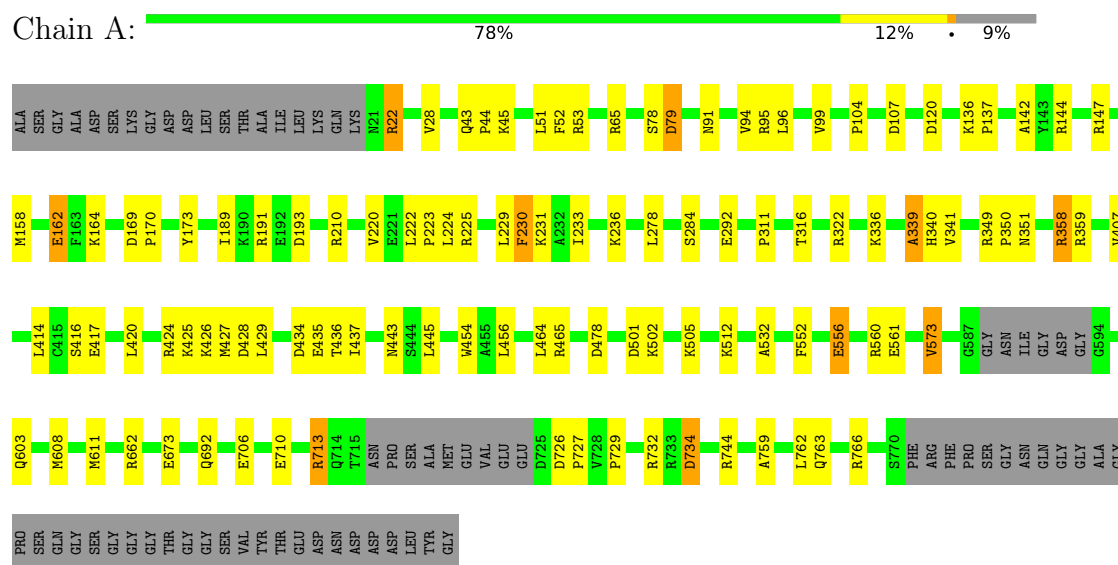
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	2	Total 2	Mg 2	0	0
3	G	2	Total 2	Mg 2	0	0
3	H	2	Total 2	Mg 2	0	0
3	I	2	Total 2	Mg 2	0	0
3	J	2	Total 2	Mg 2	0	0
3	K	2	Total 2	Mg 2	0	0
3	L	2	Total 2	Mg 2	0	0

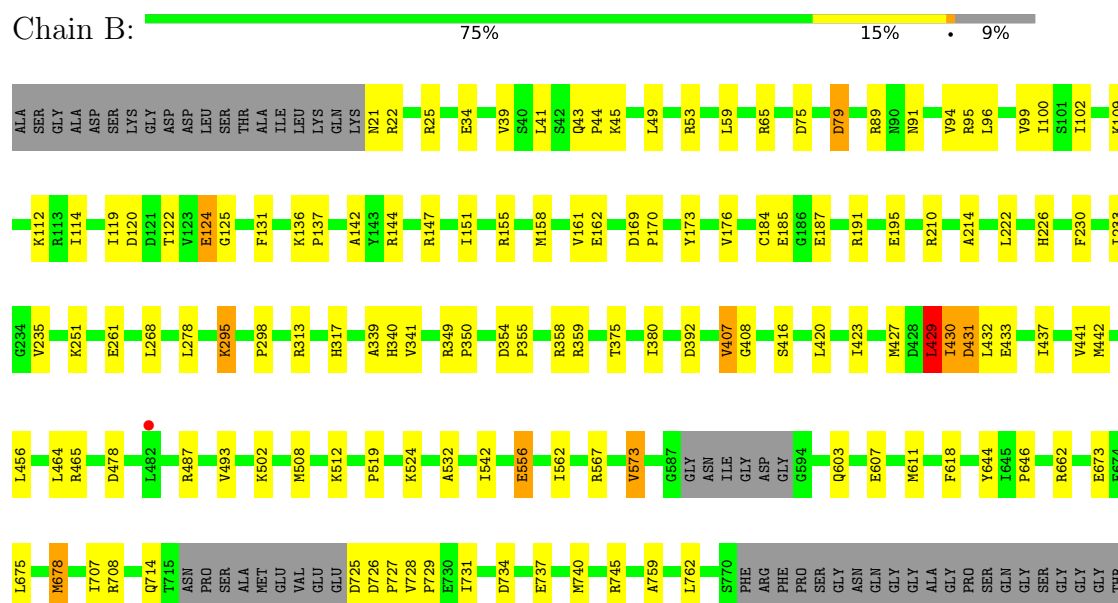
3 Residue-property plots

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

- Molecule 1: Transitional endoplasmic reticulum ATPase



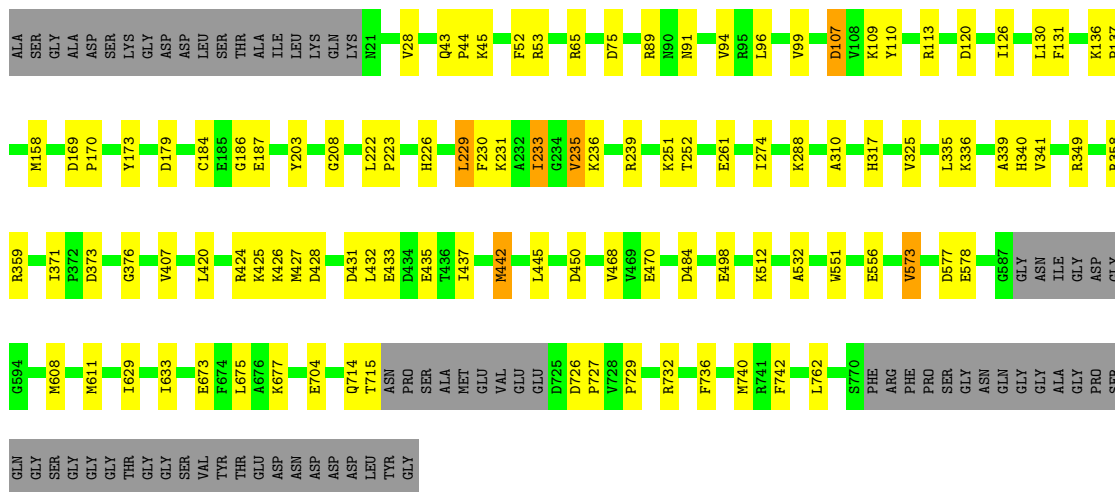
- Molecule 1: Transitional endoplasmic reticulum ATPase



GLY
GLY
SER
VAL
THR
GLU
ASP
ASN
ASP
ASP
LEU
TYR
GLY

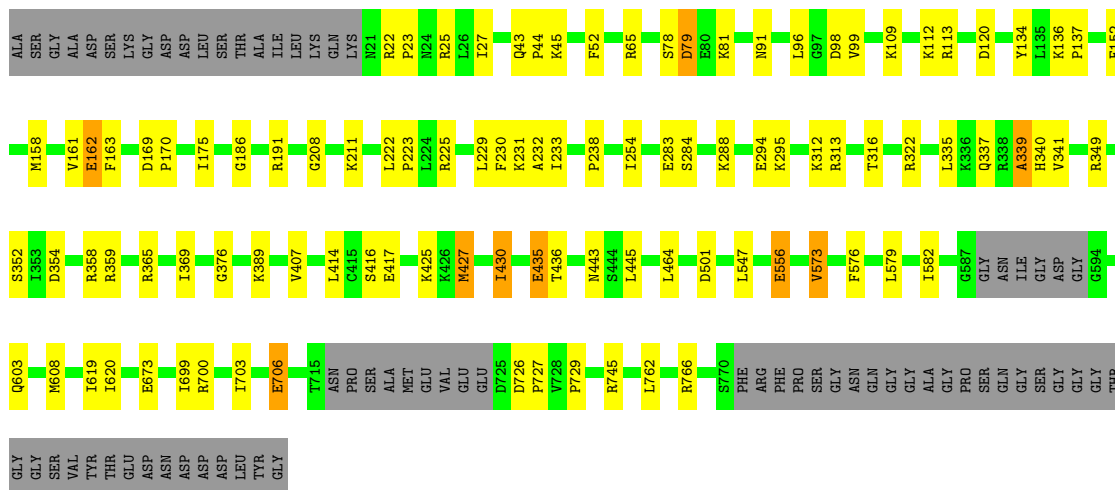
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain C: 78% 12% 9%



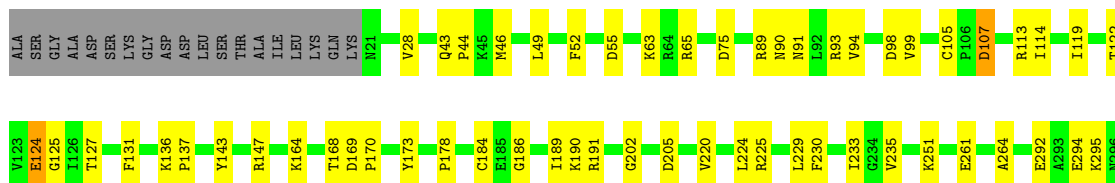
• Molecule 1: Transitional endoplasmic reticulum ATPase

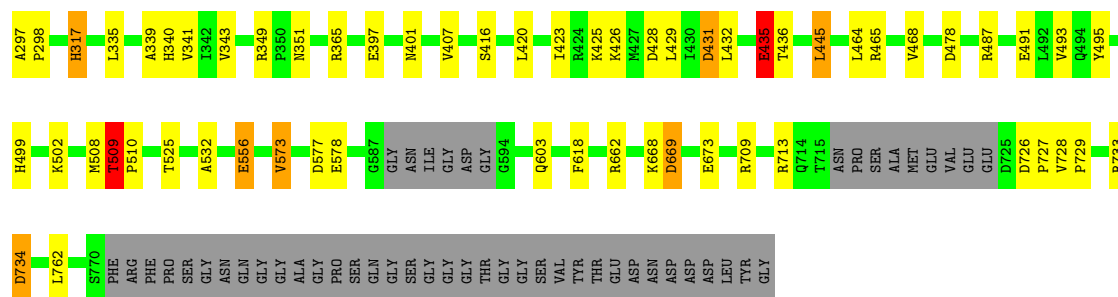
Chain D: 79% 12% 9%



• Molecule 1: Transitional endoplasmic reticulum ATPase

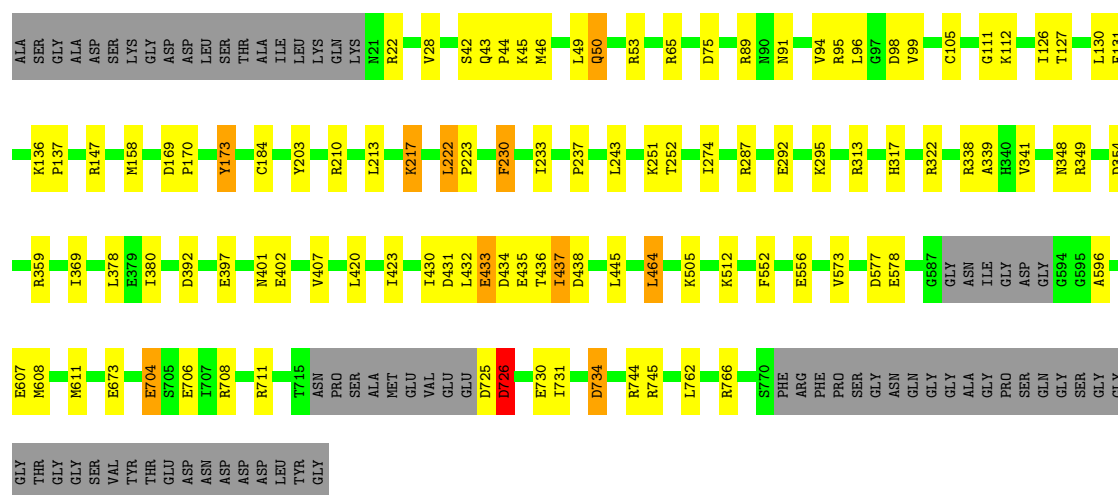
Chain E: 77% 13% 9%





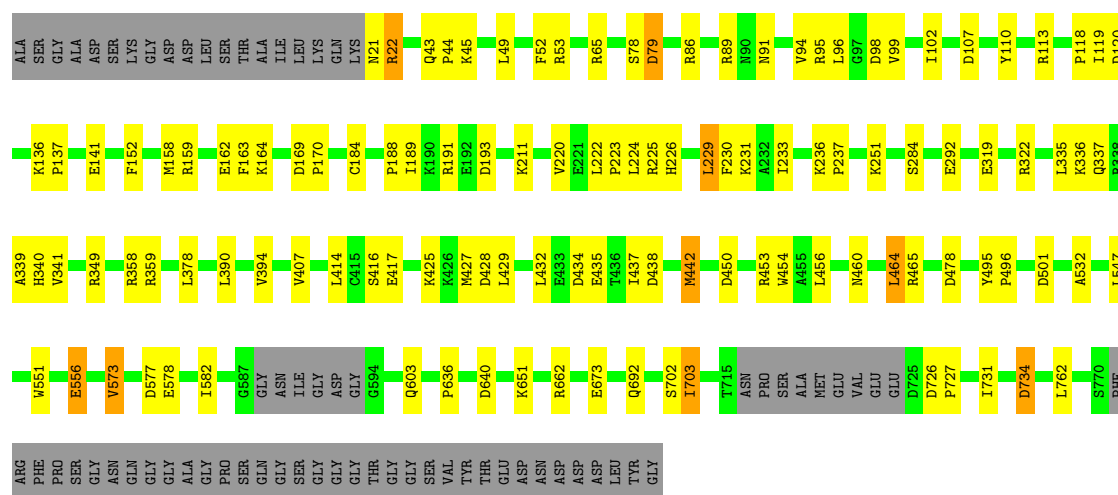
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain F: 78% 12% 9%



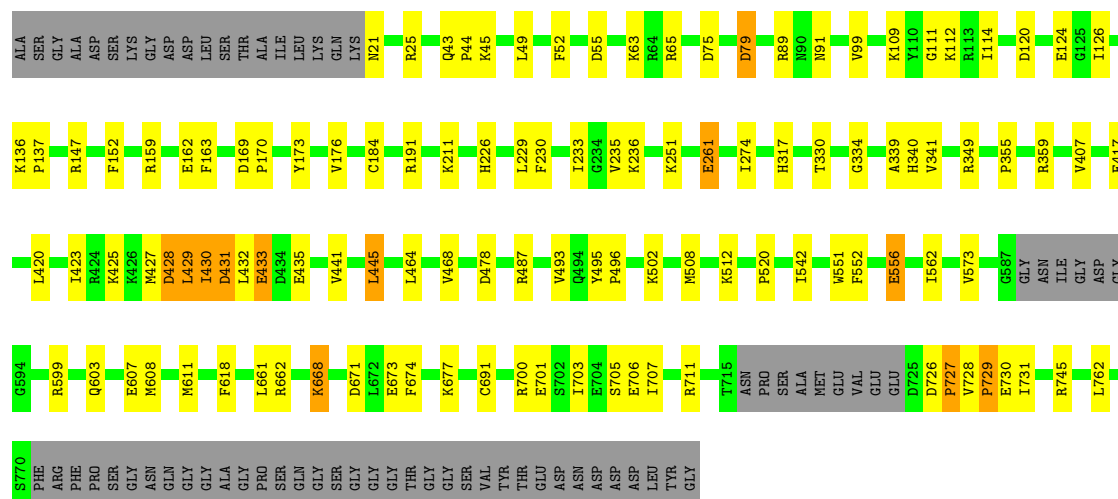
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain G: 77% 14% 9%



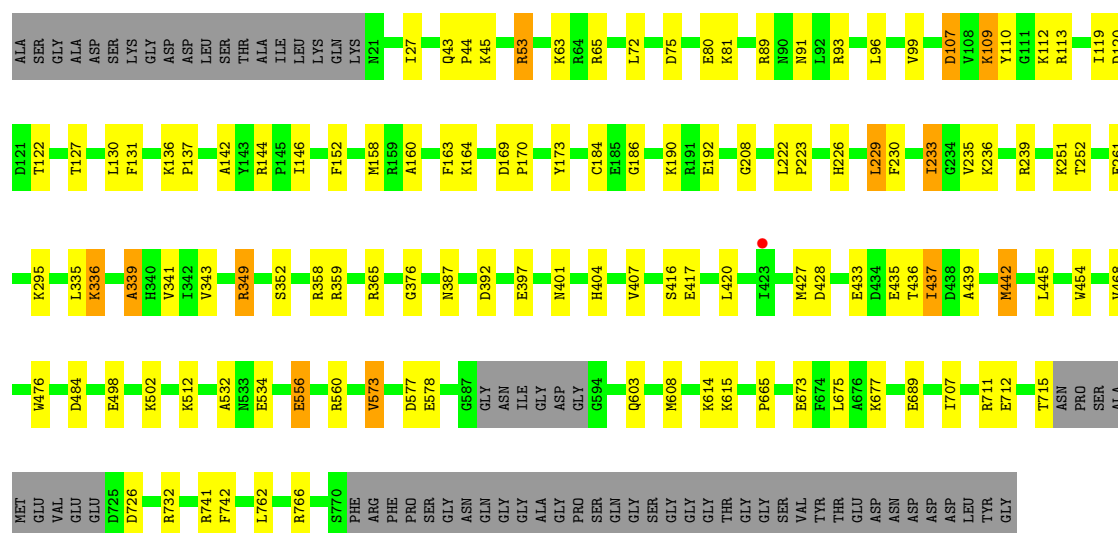
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain H: 77% 13% 9%



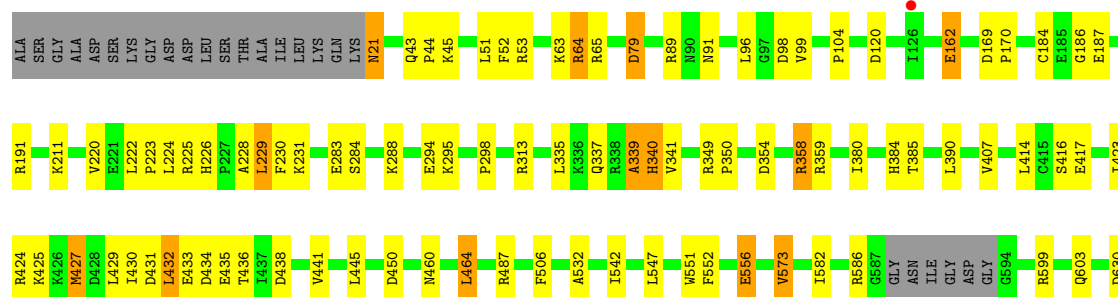
- Molecule 1: Transitional endoplasmic reticulum ATPase

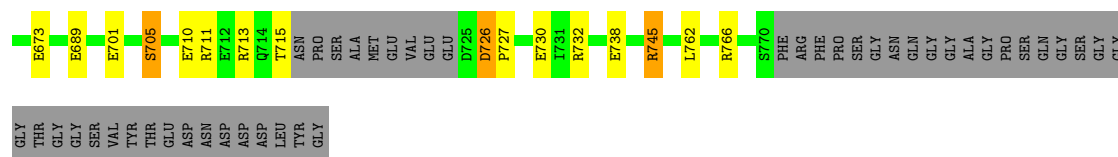
Chain I: 76% 13% 9%



- Molecule 1: Transitional endoplasmic reticulum ATPase

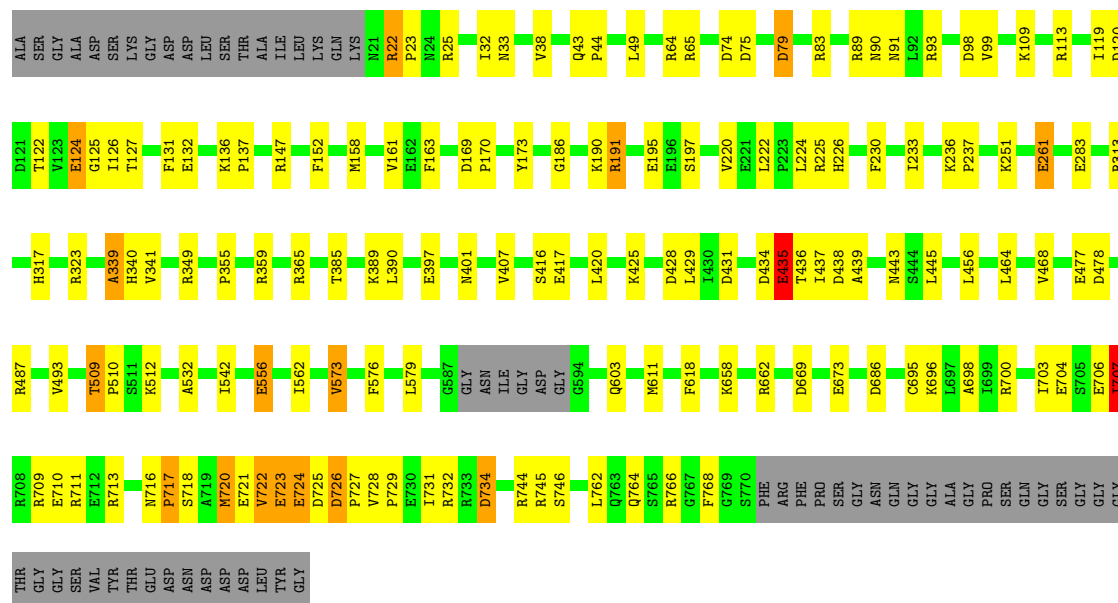
Chain J: 78% 12% 9%





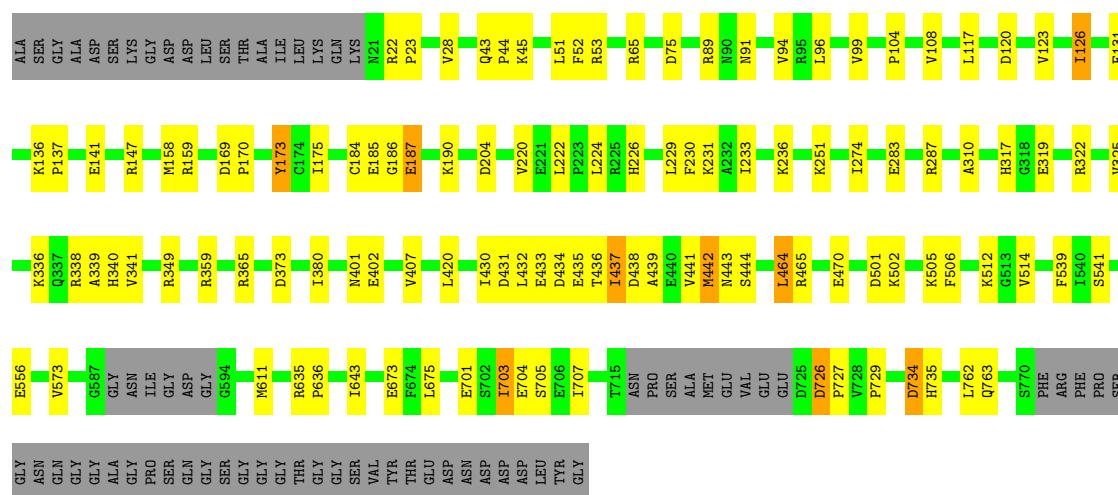
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain K: 74% 16% 8%



• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain L: 77% 13% 9%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	182.67Å 145.47Å 251.40Å 90.00° 109.77° 90.00°	Depositor
Resolution (Å)	49.05 – 3.80 49.05 – 3.80	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.05-3.80) 98.7 (49.05-3.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 3.77Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.190 , 0.254 0.196 , 0.253	Depositor DCC
R_{free} test set	6037 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	148.8	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 140.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.059 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	140261	wwPDB-VP
Average B, all atoms (Å ²)	199.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.88% of the height of the origin peak. No significant pseudotranslation is detected.*

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: AGS, MG

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	0.39	0/5856	0.78	5/7906 (0.1%)
1	B	0.40	0/5864	0.79	4/7917 (0.1%)
1	C	0.38	0/5864	0.81	2/7917 (0.0%)
1	D	0.37	0/5864	0.78	2/7917 (0.0%)
1	E	0.39	0/5864	0.80	6/7917 (0.1%)
1	F	0.41	0/5864	0.82	5/7917 (0.1%)
1	G	0.39	0/5856	0.82	5/7906 (0.1%)
1	H	0.39	0/5864	0.78	2/7917 (0.0%)
1	I	0.38	0/5863	0.79	4/7913 (0.1%)
1	J	0.39	0/5864	0.80	6/7917 (0.1%)
1	K	0.41	0/5934	0.80	4/8014 (0.0%)
1	L	0.39	0/5864	0.79	4/7917 (0.1%)
All	All	0.39	0/70421	0.80	49/95075 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	F	0	1
All	All	0	2

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	435	GLU	N-CA-C	-7.52	103.02	111.07
1	D	339	ALA	N-CA-C	-7.50	99.21	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	728	VAL	N-CA-C	7.29	115.40	107.60
1	F	726	ASP	CA-C-N	-7.03	113.46	120.21
1	F	726	ASP	C-N-CA	-7.03	113.46	120.21
1	J	187	GLU	CA-C-N	6.60	126.55	120.21
1	J	187	GLU	C-N-CA	6.60	126.55	120.21
1	I	339	ALA	N-CA-C	-6.44	100.50	110.10
1	G	22	ARG	CA-C-N	6.33	125.95	119.56
1	G	22	ARG	C-N-CA	6.33	125.95	119.56
1	L	464	LEU	N-CA-C	-6.18	105.00	112.54
1	I	726	ASP	CA-C-N	-6.14	114.31	120.21
1	I	726	ASP	C-N-CA	-6.14	114.31	120.21
1	A	436	THR	N-CA-C	6.04	118.67	109.62
1	L	726	ASP	CA-C-N	-6.01	114.08	120.03
1	L	726	ASP	C-N-CA	-6.01	114.08	120.03
1	A	22	ARG	CA-C-N	5.99	125.61	119.56
1	A	22	ARG	C-N-CA	5.99	125.61	119.56
1	C	53	ARG	N-CA-C	5.96	118.55	111.33
1	K	32	ILE	N-CA-C	-5.91	107.15	112.12
1	F	22	ARG	CA-C-N	-5.89	113.61	119.56
1	F	22	ARG	C-N-CA	-5.89	113.61	119.56
1	I	428	ASP	N-CA-C	-5.88	104.95	111.36
1	J	339	ALA	N-CA-C	-5.85	101.64	110.24
1	B	726	ASP	CA-C-N	-5.80	114.77	120.52
1	B	726	ASP	C-N-CA	-5.80	114.77	120.52
1	J	726	ASP	CA-C-N	-5.79	114.65	120.21
1	J	726	ASP	C-N-CA	-5.79	114.65	120.21
1	A	339	ALA	N-CA-C	-5.58	102.37	110.24
1	E	726	ASP	CA-C-N	-5.57	114.51	120.03
1	E	726	ASP	C-N-CA	-5.57	114.51	120.03
1	K	339	ALA	N-CA-C	-5.45	102.23	110.24
1	F	22	ARG	N-CA-C	-5.42	102.31	109.84
1	E	105	CYS	CA-C-N	5.41	125.10	119.64
1	E	105	CYS	C-N-CA	5.41	125.10	119.64
1	L	705	SER	N-CA-C	-5.38	105.85	112.90
1	E	509	THR	CA-C-N	-5.37	115.04	120.31
1	E	509	THR	C-N-CA	-5.37	115.04	120.31
1	H	435	GLU	N-CA-C	-5.32	105.38	111.07
1	H	55	ASP	N-CA-C	5.24	117.05	110.24
1	J	53	ARG	N-CA-C	5.22	116.97	111.28
1	A	53	ARG	N-CA-C	5.21	116.95	111.28
1	G	53	ARG	N-CA-C	5.20	116.94	111.28
1	G	702	SER	N-CA-C	5.12	116.86	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	336	LYS	N-CA-C	-5.10	106.16	112.38
1	C	428	ASP	N-CA-C	-5.10	105.80	111.36
1	B	22	ARG	CA-C-N	5.06	124.67	119.56
1	B	22	ARG	C-N-CA	5.06	124.67	119.56
1	K	120	ASP	N-CA-C	5.03	117.15	111.11

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	429	LEU	Peptide
1	F	49	LEU	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	5764	5814	5812	52	0
1	B	5771	5819	5819	66	0
1	C	5771	5818	5818	44	0
1	D	5771	5820	5820	48	0
1	E	5771	5818	5818	55	0
1	F	5771	5818	5819	57	0
1	G	5764	5812	5811	54	0
1	H	5771	5819	5819	64	0
1	I	5771	5818	5818	51	0
1	J	5771	5819	5819	49	0
1	K	5839	5880	5879	73	0
1	L	5771	5820	5819	56	0
2	A	62	26	24	0	0
2	B	62	26	24	4	0
2	C	62	26	24	3	0
2	D	62	26	24	0	0
2	E	62	26	24	3	0
2	F	62	26	24	6	0
2	G	62	26	24	2	0
2	H	62	26	24	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	62	26	24	4	0
2	J	62	26	23	4	0
2	K	62	26	24	2	0
2	L	62	26	24	4	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
All	All	70074	70187	70158	622	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 4.

All (622) 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:429:LEU:O	1:H:431:ASP:N	2.15	0.79
1:B:89:ARG:NH1	1:B:261:GLU:OE2	2.17	0.78
1:J:313:ARG:NE	1:J:354:ASP:OD2	2.19	0.75
1:B:429:LEU:O	1:B:431:ASP:N	2.21	0.74
1:H:65:ARG:NH1	1:H:91:ASN:O	2.20	0.73
1:B:124:GLU:OE2	1:C:231:LYS:NZ	2.21	0.73
1:G:434:ASP:OD2	1:H:226:HIS:ND1	2.21	0.73
1:J:745:ARG:O	1:K:764:GLN:NE2	2.21	0.73
1:K:709:ARG:NH1	1:K:720:MET:SD	2.62	0.73
1:L:65:ARG:NH1	1:L:91:ASN:O	2.22	0.73
1:A:502:LYS:NZ	1:F:706:GLU:OE2	2.22	0.73
2:E:902:AGS:O3G	1:F:766:ARG:NH1	2.21	0.73
1:K:355:PRO:O	1:K:359:ARG:NH1	2.22	0.72
1:G:692:GLN:NE2	1:H:508:MET:SD	2.64	0.71
1:K:417:GLU:OE1	1:L:365:ARG:NH2	2.24	0.70
1:D:162:GLU:OE1	1:D:191:ARG:NH2	2.25	0.70
1:G:339:ALA:O	1:G:341:VAL:N	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:339:ALA:O	1:K:341:VAL:N	2.25	0.70
1:J:417:GLU:OE1	1:K:365:ARG:NH2	2.25	0.70
1:A:339:ALA:O	1:A:341:VAL:N	2.25	0.69
1:A:744:ARG:NH2	1:B:759:ALA:O	2.25	0.69
1:B:65:ARG:NH1	1:B:91:ASN:O	2.25	0.68
1:D:706:GLU:OE2	1:E:502:LYS:NZ	2.26	0.68
1:E:65:ARG:NH1	1:E:91:ASN:O	2.26	0.68
1:G:65:ARG:NH1	1:G:91:ASN:O	2.26	0.68
1:F:65:ARG:NH1	1:F:91:ASN:O	2.27	0.68
1:E:89:ARG:NH1	1:E:261:GLU:OE2	2.27	0.67
1:D:313:ARG:NE	1:D:354:ASP:OD2	2.27	0.67
1:J:162:GLU:OE1	1:J:191:ARG:NH2	2.27	0.66
1:E:673:GLU:N	1:E:673:GLU:OE1	2.27	0.66
1:C:107:ASP:N	1:C:107:ASP:OD1	2.25	0.66
1:G:465:ARG:NH2	1:H:607:GLU:OE1	2.29	0.66
1:H:417:GLU:OE1	1:I:365:ARG:NH2	2.29	0.66
1:L:734:ASP:OD1	1:L:734:ASP:N	2.29	0.65
1:E:317:HIS:O	1:F:322:ARG:NH2	2.29	0.64
1:B:230:PHE:HA	1:B:233:ILE:HG22	1.80	0.64
1:H:339:ALA:O	1:H:341:VAL:N	2.31	0.64
1:C:673:GLU:N	1:C:673:GLU:OE1	2.31	0.64
1:J:339:ALA:O	1:J:341:VAL:N	2.31	0.64
1:F:339:ALA:O	1:F:341:VAL:N	2.32	0.63
1:K:79:ASP:OD1	1:K:79:ASP:N	2.29	0.63
1:F:46:MET:O	1:F:50:GLN:HA	1.99	0.63
1:A:79:ASP:OD1	1:A:79:ASP:N	2.29	0.62
1:C:339:ALA:O	1:C:341:VAL:N	2.32	0.62
1:H:552:PHE:O	1:H:599:ARG:NH2	2.32	0.62
1:K:478:ASP:OD1	1:K:662:ARG:NH2	2.32	0.62
1:J:294:GLU:OE2	1:J:337:GLN:NE2	2.32	0.62
1:G:49:LEU:HD21	1:G:102:ILE:HG23	1.81	0.62
1:K:65:ARG:NH1	1:K:91:ASN:O	2.32	0.62
1:G:673:GLU:N	1:G:673:GLU:OE1	2.33	0.62
1:J:79:ASP:OD1	1:J:79:ASP:N	2.29	0.62
1:F:512:LYS:NZ	1:F:608:MET:O	2.31	0.61
1:D:700:ARG:NE	1:E:491:GLU:OE2	2.34	0.61
1:L:673:GLU:N	1:L:673:GLU:OE1	2.33	0.61
1:B:350:PRO:O	1:B:358:ARG:NH2	2.34	0.61
1:L:432:LEU:O	1:L:434:ASP:N	2.34	0.61
2:G:902:AGS:O2G	2:G:902:AGS:O2B	2.18	0.60
1:J:701:GLU:O	1:J:705:SER:OG	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:673:GLU:OE1	1:F:673:GLU:N	2.35	0.60
1:I:65:ARG:NH1	1:I:91:ASN:O	2.35	0.60
1:A:759:ALA:O	1:F:744:ARG:NH1	2.34	0.60
1:F:251:LYS:NZ	2:F:901:AGS:O2B	2.34	0.60
1:H:162:GLU:OE1	1:H:191:ARG:NH2	2.34	0.60
1:J:98:ASP:OD1	1:J:225:ARG:NH1	2.33	0.60
1:E:339:ALA:O	1:E:341:VAL:N	2.34	0.60
1:K:512:LYS:NZ	1:K:611:MET:O	2.23	0.60
1:C:65:ARG:NH1	1:C:91:ASN:O	2.35	0.60
1:J:556:GLU:O	1:J:603:GLN:NE2	2.35	0.59
1:D:316:THR:O	1:D:322:ARG:NH2	2.35	0.59
1:I:251:LYS:NZ	2:I:901:AGS:O1B	2.36	0.59
1:A:673:GLU:OE1	1:A:673:GLU:N	2.35	0.59
1:H:478:ASP:OD1	1:H:662:ARG:NH2	2.35	0.59
1:D:79:ASP:N	1:D:79:ASP:OD1	2.32	0.59
1:L:339:ALA:O	1:L:341:VAL:N	2.36	0.59
1:C:251:LYS:NZ	2:C:901:AGS:O2B	2.36	0.59
1:L:251:LYS:NZ	2:L:901:AGS:O1B	2.36	0.59
1:K:98:ASP:OD1	1:K:225:ARG:NH2	2.35	0.58
1:D:339:ALA:O	1:D:341:VAL:N	2.36	0.58
1:F:313:ARG:NE	1:F:354:ASP:OD2	2.36	0.58
1:B:355:PRO:O	1:B:359:ARG:NH1	2.36	0.58
1:C:512:LYS:NZ	1:C:611:MET:O	2.35	0.58
1:L:432:LEU:C	1:L:434:ASP:H	2.11	0.58
2:J:902:AGS:O3G	1:K:766:ARG:NH1	2.36	0.57
1:A:434:ASP:OD2	1:B:226:HIS:ND1	2.37	0.57
1:A:222:LEU:HB2	1:A:223:PRO:HD3	1.87	0.57
1:B:673:GLU:N	1:B:673:GLU:OE1	2.35	0.57
1:H:701:GLU:O	1:H:705:SER:N	2.36	0.57
1:H:673:GLU:N	1:H:673:GLU:OE1	2.38	0.57
1:K:704:GLU:HA	1:K:707:ILE:HD11	1.87	0.57
1:B:124:GLU:OE1	1:B:125:GLY:N	2.38	0.56
1:K:119:ILE:O	1:K:122:THR:OG1	2.20	0.56
1:K:724:GLU:O	1:K:726:ASP:N	2.39	0.56
1:C:431:ASP:OD2	1:D:25:ARG:NH2	2.39	0.56
1:E:202:GLY:N	1:E:205:ASP:OD2	2.37	0.56
1:H:251:LYS:NZ	2:H:901:AGS:O1B	2.39	0.56
1:J:65:ARG:NH1	1:J:91:ASN:O	2.39	0.56
1:L:512:LYS:NZ	1:L:611:MET:O	2.31	0.56
1:J:701:GLU:OE1	1:J:732:ARG:NH2	2.38	0.56
1:E:556:GLU:O	1:E:603:GLN:NE2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:124:GLU:OE1	1:E:125:GLY:N	2.40	0.55
1:B:512:LYS:NZ	1:B:611:MET:O	2.37	0.55
1:D:294:GLU:OE2	1:D:337:GLN:NE2	2.39	0.55
1:K:673:GLU:OE1	1:K:673:GLU:N	2.39	0.55
1:B:79:ASP:N	1:B:79:ASP:OD1	2.40	0.55
1:H:706:GLU:OE1	1:I:502:LYS:NZ	2.39	0.55
1:L:434:ASP:C	1:L:436:THR:H	2.14	0.55
1:B:313:ARG:NE	1:B:354:ASP:OD2	2.40	0.55
1:B:556:GLU:O	1:B:603:GLN:NE2	2.40	0.55
1:G:556:GLU:O	1:G:603:GLN:NE2	2.38	0.55
1:B:119:ILE:O	1:B:122:THR:OG1	2.24	0.55
1:I:673:GLU:OE1	1:I:673:GLU:N	2.39	0.55
1:F:423:ILE:HG12	1:F:445:LEU:HD21	1.89	0.55
1:I:512:LYS:NZ	1:I:608:MET:O	2.39	0.55
2:I:902:AGS:S1G	1:J:766:ARG:NH1	2.81	0.54
1:A:556:GLU:O	1:A:603:GLN:NE2	2.41	0.54
1:F:734:ASP:OD1	1:F:734:ASP:N	2.32	0.54
1:F:112:LYS:HB2	1:F:169:ASP:HB3	1.90	0.54
1:G:96:LEU:O	1:G:225:ARG:NH2	2.40	0.54
1:E:169:ASP:HB3	1:E:170:PRO:HD3	1.90	0.54
1:J:284:SER:OG	1:J:288:LYS:NZ	2.41	0.54
1:K:556:GLU:O	1:K:603:GLN:NE2	2.40	0.54
1:K:720:MET:SD	1:K:721:GLU:N	2.74	0.54
1:F:432:LEU:C	1:F:434:ASP:H	2.16	0.53
1:I:252:THR:OG1	2:I:901:AGS:O2B	2.25	0.53
1:A:734:ASP:OD1	1:A:734:ASP:N	2.30	0.53
1:H:726:ASP:N	1:H:727:PRO:HD3	2.23	0.53
1:J:464:LEU:HD12	1:J:464:LEU:H	1.72	0.53
1:C:169:ASP:HB3	1:C:170:PRO:HD3	1.91	0.53
1:C:736:PHE:O	1:C:740:MET:N	2.41	0.53
1:H:512:LYS:NZ	1:H:611:MET:O	2.40	0.53
1:A:478:ASP:OD1	1:A:662:ARG:NH2	2.40	0.53
1:B:162:GLU:OE1	1:B:191:ARG:NH2	2.41	0.53
1:H:79:ASP:OD1	1:H:79:ASP:N	2.39	0.53
1:I:339:ALA:O	1:I:341:VAL:N	2.42	0.53
1:D:389:LYS:HD3	1:D:443:ASN:O	2.08	0.52
1:K:191:ARG:NH1	1:K:195:GLU:O	2.41	0.52
1:D:673:GLU:OE1	1:D:673:GLU:N	2.42	0.52
1:C:252:THR:OG1	2:C:901:AGS:O1B	2.27	0.52
1:F:136:LYS:HB3	1:F:137:PRO:HD3	1.92	0.52
1:G:547:LEU:HD12	1:G:582:ILE:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:717:PRO:N	1:K:718:SER:HA	2.24	0.52
1:F:430:ILE:O	1:F:433:GLU:N	2.32	0.52
1:H:89:ARG:NH1	1:H:261:GLU:OE2	2.41	0.52
1:K:169:ASP:HB3	1:K:170:PRO:HD3	1.90	0.52
1:E:525:THR:OG1	1:E:577:ASP:OD2	2.28	0.52
1:F:512:LYS:NZ	1:F:611:MET:O	2.39	0.52
1:G:169:ASP:HB3	1:G:170:PRO:HD3	1.92	0.52
1:G:442:MET:HA	1:G:442:MET:CE	2.40	0.52
1:B:142:ALA:HB1	1:B:144:ARG:HG3	1.91	0.52
1:L:43:GLN:N	1:L:44:PRO:HD2	2.25	0.51
1:H:230:PHE:HA	1:H:233:ILE:HG22	1.92	0.51
1:F:434:ASP:C	1:F:436:THR:H	2.17	0.51
1:K:509:THR:HG22	1:K:510:PRO:HD2	1.92	0.51
2:L:902:AGS:O1A	2:L:902:AGS:O2G	2.28	0.51
1:B:727:PRO:O	1:B:729:PRO:HD3	2.11	0.51
1:H:427:MET:HG2	1:H:427:MET:O	2.09	0.51
1:K:716:ASN:C	1:K:718:SER:HA	2.35	0.51
1:A:692:GLN:NE2	1:B:508:MET:SD	2.83	0.51
1:G:43:GLN:N	1:G:44:PRO:HD2	2.26	0.51
1:C:424:ARG:HG3	1:D:222:LEU:HD11	1.92	0.51
1:E:107:ASP:N	1:E:107:ASP:OD1	2.43	0.51
1:H:114:ILE:CD1	1:H:176:VAL:HG22	2.41	0.51
1:D:230:PHE:HA	1:D:233:ILE:HG22	1.92	0.51
1:B:478:ASP:OD1	1:B:662:ARG:NH2	2.44	0.51
1:B:432:LEU:HD22	1:C:226:HIS:CE1	2.46	0.50
2:B:902:AGS:O2G	2:B:902:AGS:O2A	2.28	0.50
1:C:96:LEU:HD23	1:C:261:GLU:HG3	1.93	0.50
1:D:65:ARG:NH1	1:D:91:ASN:O	2.44	0.50
1:G:432:LEU:O	1:H:25:ARG:NH1	2.44	0.50
1:L:169:ASP:HB3	1:L:170:PRO:HD3	1.93	0.50
1:F:147:ARG:HG2	1:F:173:TYR:HB3	1.94	0.50
1:K:722:VAL:O	1:K:724:GLU:N	2.44	0.50
1:A:169:ASP:HB3	1:A:170:PRO:HD3	1.94	0.50
1:C:442:MET:HA	1:C:442:MET:CE	2.41	0.50
1:D:284:SER:OG	1:D:288:LYS:NZ	2.44	0.50
1:I:397:GLU:O	1:I:401:ASN:ND2	2.44	0.50
1:J:96:LEU:O	1:J:225:ARG:NH2	2.44	0.50
1:C:726:ASP:N	1:C:727:PRO:HD3	2.24	0.50
1:J:552:PHE:O	1:J:599:ARG:NH2	2.45	0.50
1:E:532:ALA:HB2	1:E:573:VAL:HG11	1.93	0.50
1:F:173:TYR:CD1	1:F:173:TYR:N	2.80	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:728:VAL:N	1:H:729:PRO:CD	2.75	0.50
1:L:441:VAL:O	1:L:444:SER:OG	2.26	0.50
1:A:136:LYS:HB3	1:A:137:PRO:HD3	1.94	0.50
1:E:43:GLN:N	1:E:44:PRO:HD2	2.27	0.50
1:H:169:ASP:HB3	1:H:170:PRO:HD3	1.92	0.50
1:H:728:VAL:O	1:H:730:GLU:N	2.45	0.49
1:J:551:TRP:CZ2	1:K:556:GLU:HG2	2.47	0.49
1:K:576:PHE:HB3	1:K:579:LEU:HD21	1.95	0.49
1:L:727:PRO:HB2	1:L:729:PRO:HD3	1.94	0.49
1:D:208:GLY:HA2	1:D:376:GLY:HA2	1.95	0.49
1:D:556:GLU:O	1:D:603:GLN:NE2	2.45	0.49
1:E:734:ASP:OD1	1:E:734:ASP:N	2.44	0.49
1:G:734:ASP:OD1	1:G:734:ASP:N	2.31	0.49
1:I:43:GLN:N	1:I:44:PRO:HD2	2.27	0.49
1:I:169:ASP:HB3	1:I:170:PRO:HD3	1.93	0.49
1:I:239:ARG:NH1	1:I:336:LYS:HD2	2.27	0.49
1:J:673:GLU:OE1	1:J:673:GLU:N	2.43	0.49
1:B:339:ALA:O	1:B:341:VAL:N	2.45	0.49
1:E:119:ILE:O	1:E:122:THR:OG1	2.30	0.49
1:B:169:ASP:HB3	1:B:170:PRO:HD3	1.93	0.49
1:B:734:ASP:N	1:B:734:ASP:OD1	2.42	0.49
1:L:147:ARG:HG2	1:L:173:TYR:HB3	1.95	0.49
1:B:158:MET:HE1	1:B:423:ILE:HD11	1.95	0.49
1:I:89:ARG:NH1	1:I:261:GLU:OE1	2.45	0.49
1:K:230:PHE:HA	1:K:233:ILE:HG22	1.94	0.49
1:B:493:VAL:HG13	1:B:618:PHE:CD2	2.48	0.48
1:B:43:GLN:N	1:B:44:PRO:HD2	2.28	0.48
1:F:252:THR:OG1	2:F:901:AGS:O1B	2.31	0.48
1:G:222:LEU:HB2	1:G:223:PRO:HD3	1.94	0.48
1:K:493:VAL:HG13	1:K:618:PHE:CD2	2.48	0.48
1:L:439:ALA:O	1:L:443:ASN:N	2.41	0.48
1:C:233:ILE:HG22	1:C:235:VAL:H	1.77	0.48
1:E:431:ASP:OD1	1:E:432:LEU:N	2.46	0.48
1:I:107:ASP:OD1	1:I:107:ASP:N	2.46	0.48
1:J:120:ASP:OD1	1:J:120:ASP:N	2.46	0.48
1:E:499:HIS:HB3	1:E:502:LYS:HG3	1.96	0.48
1:J:222:LEU:HB2	1:J:223:PRO:HD3	1.95	0.48
1:K:43:GLN:N	1:K:44:PRO:HD2	2.28	0.48
1:K:75:ASP:N	1:K:75:ASP:OD1	2.47	0.48
1:E:233:ILE:HG23	1:E:235:VAL:H	1.78	0.48
1:G:478:ASP:OD1	1:G:662:ARG:NH2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:51:LEU:HD21	1:L:104:PRO:HB3	1.95	0.48
1:C:442:MET:HA	1:C:442:MET:HE2	1.95	0.48
1:G:464:LEU:HD12	1:G:464:LEU:H	1.79	0.48
1:A:142:ALA:HB1	1:A:144:ARG:HG3	1.95	0.48
1:C:75:ASP:OD1	1:C:75:ASP:N	2.46	0.48
1:F:437:ILE:N	1:F:437:ILE:HD13	2.29	0.48
1:E:230:PHE:HA	1:E:233:ILE:HG22	1.96	0.48
1:H:43:GLN:N	1:H:44:PRO:HD2	2.28	0.48
1:K:136:LYS:HB3	1:K:137:PRO:HD3	1.96	0.48
1:I:136:LYS:HB3	1:I:137:PRO:HD3	1.96	0.48
1:E:147:ARG:HG2	1:E:173:TYR:HB3	1.96	0.47
1:J:169:ASP:HB3	1:J:170:PRO:HD3	1.95	0.47
1:B:112:LYS:HB2	1:B:169:ASP:HB3	1.96	0.47
1:F:169:ASP:HB3	1:F:170:PRO:HD3	1.95	0.47
1:A:43:GLN:N	1:A:44:PRO:HD2	2.30	0.47
1:D:27:ILE:HB	1:D:81:LYS:HG2	1.97	0.47
1:E:397:GLU:O	1:E:401:ASN:ND2	2.47	0.47
1:F:230:PHE:HA	1:F:233:ILE:HG22	1.96	0.47
1:G:136:LYS:HB3	1:G:137:PRO:HD3	1.96	0.47
2:L:902:AGS:O2G	2:L:902:AGS:O2B	2.33	0.47
1:B:120:ASP:N	1:B:120:ASP:OD1	2.47	0.47
1:D:96:LEU:O	1:D:225:ARG:NH2	2.47	0.47
1:D:152:PHE:CZ	1:D:163:PHE:HB2	2.49	0.47
1:G:726:ASP:N	1:G:727:PRO:HD3	2.29	0.47
1:E:75:ASP:OD1	1:E:75:ASP:N	2.45	0.47
1:F:432:LEU:O	1:F:434:ASP:N	2.48	0.47
1:A:512:LYS:NZ	1:A:611:MET:O	2.38	0.47
1:D:547:LEU:HD12	1:D:582:ILE:HD11	1.97	0.47
1:E:220:VAL:CG1	1:E:224:LEU:HD22	2.43	0.47
1:F:725:ASP:O	1:F:726:ASP:HB2	2.15	0.47
1:H:430:ILE:HG23	1:H:431:ASP:N	2.30	0.47
1:K:435:GLU:HG3	1:K:436:THR:H	1.79	0.47
1:A:311:PRO:HD2	1:A:316:THR:HG22	1.97	0.47
2:C:902:AGS:S1G	1:D:766:ARG:NH1	2.88	0.47
1:E:709:ARG:HH22	1:E:727:PRO:HB3	1.80	0.47
1:H:493:VAL:HG13	1:H:618:PHE:CD2	2.50	0.47
1:K:698:ALA:HB1	1:K:731:ILE:HG22	1.95	0.47
1:C:310:ALA:HA	1:C:325:VAL:HG22	1.97	0.47
1:G:577:ASP:OD1	1:G:578:GLU:N	2.48	0.47
1:G:703:ILE:HG22	1:H:502:LYS:HD2	1.97	0.47
1:G:94:VAL:HG13	1:G:98:ASP:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:119:ILE:O	1:I:122:THR:OG1	2.32	0.47
1:J:21:ASN:OD1	1:J:21:ASN:N	2.48	0.47
1:F:75:ASP:N	1:F:75:ASP:OD1	2.47	0.46
1:H:427:MET:O	1:H:428:ASP:C	2.57	0.46
1:E:224:LEU:HD23	1:E:264:ALA:HB2	1.97	0.46
1:F:43:GLN:N	1:F:44:PRO:HD2	2.31	0.46
1:G:79:ASP:N	1:G:79:ASP:OD1	2.48	0.46
1:H:556:GLU:O	1:H:603:GLN:NE2	2.48	0.46
1:H:668:LYS:HA	1:H:668:LYS:HE3	1.98	0.46
1:K:435:GLU:CG	1:K:436:THR:H	2.28	0.46
1:D:312:LYS:N	1:D:352:SER:O	2.49	0.46
1:D:417:GLU:OE1	1:E:365:ARG:NH2	2.49	0.46
1:G:233:ILE:HD13	1:L:442:MET:SD	2.55	0.46
1:L:437:ILE:HD13	1:L:437:ILE:N	2.30	0.46
1:B:158:MET:HE2	1:B:442:MET:HE1	1.97	0.46
1:C:425:LYS:HE2	1:C:426:LYS:HE2	1.98	0.46
1:E:465:ARG:NH2	1:F:607:GLU:OE2	2.49	0.46
1:G:442:MET:HA	1:G:442:MET:HE2	1.97	0.46
1:I:142:ALA:HB1	1:I:144:ARG:HG3	1.97	0.46
1:D:576:PHE:HB3	1:D:579:LEU:HD21	1.98	0.46
1:F:89:ARG:NH1	1:F:96:LEU:HD21	2.31	0.46
1:F:111:GLY:HA2	1:F:170:PRO:HG2	1.97	0.46
1:F:378:LEU:HD13	1:F:397:GLU:HA	1.97	0.46
1:H:728:VAL:O	1:H:729:PRO:C	2.59	0.46
1:A:158:MET:SD	1:B:233:ILE:HD11	2.56	0.46
1:H:112:LYS:HB2	1:H:169:ASP:HB3	1.98	0.46
1:F:348:ASN:ND2	2:F:901:AGS:S1G	2.89	0.46
1:G:95:ARG:HB2	1:G:225:ARG:NH2	2.30	0.46
1:I:96:LEU:HD23	1:I:261:GLU:HG3	1.98	0.46
1:H:703:ILE:HG22	1:H:707:ILE:HD12	1.98	0.46
1:J:43:GLN:N	1:J:44:PRO:HD2	2.31	0.46
1:A:28:VAL:HG21	1:A:94:VAL:HG11	1.96	0.46
1:D:231:LYS:HG2	1:D:232:ALA:N	2.30	0.46
1:J:350:PRO:O	1:J:358:ARG:NH2	2.49	0.46
1:K:686:ASP:OD1	1:K:746:SER:OG	2.25	0.46
2:K:902:AGS:O2G	2:K:902:AGS:O2B	2.33	0.46
1:F:577:ASP:OD1	1:F:578:GLU:N	2.48	0.46
1:K:152:PHE:CZ	1:K:163:PHE:HB2	2.51	0.46
1:A:136:LYS:HB3	1:A:137:PRO:CD	2.46	0.45
1:B:725:ASP:C	1:B:727:PRO:HD3	2.41	0.45
1:D:136:LYS:HB3	1:D:137:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:136:LYS:HB3	1:L:137:PRO:HD3	1.98	0.45
1:A:164:LYS:HE2	1:A:189:ILE:CD1	2.46	0.45
1:B:532:ALA:HB2	1:B:573:VAL:HG11	1.98	0.45
1:H:147:ARG:HG2	1:H:173:TYR:HB3	1.98	0.45
1:D:43:GLN:N	1:D:44:PRO:HD2	2.31	0.45
1:E:28:VAL:HG21	1:E:94:VAL:HG11	1.98	0.45
1:G:251:LYS:N	2:G:901:AGS:O1B	2.46	0.45
1:I:63:LYS:HD3	1:I:93:ARG:HG3	1.97	0.45
1:E:423:ILE:HG12	1:E:445:LEU:HD11	1.98	0.45
1:F:251:LYS:NZ	2:F:901:AGS:S1G	2.89	0.45
1:L:373:ASP:HB3	1:L:470:GLU:HB3	1.99	0.45
1:B:437:ILE:HG12	1:C:229:LEU:CD1	2.47	0.45
1:C:727:PRO:C	1:C:729:PRO:HD3	2.41	0.45
1:D:134:TYR:CD2	1:D:161:VAL:HG11	2.51	0.45
1:G:152:PHE:CZ	1:G:163:PHE:HB2	2.51	0.45
1:H:551:TRP:CZ2	1:I:556:GLU:HG2	2.52	0.45
1:L:703:ILE:O	1:L:707:ILE:HG13	2.17	0.45
1:B:41:LEU:HD11	1:B:102:ILE:HD13	1.98	0.45
1:B:75:ASP:OD1	1:B:75:ASP:N	2.49	0.45
1:C:43:GLN:N	1:C:44:PRO:HD2	2.31	0.45
1:C:203:TYR:CE2	1:C:261:GLU:HG2	2.52	0.45
1:E:136:LYS:HB3	1:E:137:PRO:HD3	1.98	0.45
1:G:164:LYS:HE2	1:G:189:ILE:CD1	2.47	0.45
1:G:442:MET:SD	1:H:233:ILE:HD13	2.56	0.45
1:K:707:ILE:O	1:K:711:ARG:HG3	2.16	0.45
1:L:231:LYS:HD2	1:L:231:LYS:O	2.17	0.45
1:B:114:ILE:CD1	1:B:176:VAL:HG22	2.46	0.45
1:D:169:ASP:HB3	1:D:170:PRO:HD3	1.98	0.45
1:E:98:ASP:OD1	1:E:225:ARG:NH2	2.49	0.45
1:H:423:ILE:O	1:H:427:MET:N	2.49	0.45
1:A:532:ALA:HB2	1:A:573:VAL:HG11	1.99	0.45
1:C:136:LYS:HB3	1:C:137:PRO:HD3	1.98	0.45
1:E:509:THR:HG22	1:E:510:PRO:HD2	1.99	0.45
1:F:222:LEU:HB3	1:F:223:PRO:HD3	1.98	0.45
1:H:728:VAL:N	1:H:729:PRO:HD2	2.32	0.45
1:J:89:ARG:NH1	1:J:96:LEU:HD21	2.31	0.45
1:A:230:PHE:HA	1:A:233:ILE:HG22	1.98	0.45
1:H:430:ILE:HG23	1:H:431:ASP:H	1.82	0.45
1:J:532:ALA:HB2	1:J:573:VAL:HG11	1.99	0.45
1:L:310:ALA:HA	1:L:325:VAL:HG22	1.97	0.45
1:E:143:TYR:CE1	1:E:178:PRO:HD3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:294:GLU:HG3	1:E:339:ALA:HB3	1.99	0.45
1:K:230:PHE:CZ	1:K:237:PRO:HB3	2.52	0.45
1:C:512:LYS:NZ	1:C:608:MET:O	2.46	0.44
1:H:551:TRP:CE2	1:I:556:GLU:HG2	2.51	0.44
1:L:75:ASP:OD1	1:L:75:ASP:N	2.49	0.44
1:L:120:ASP:N	1:L:120:ASP:OD1	2.50	0.44
1:A:220:VAL:CG1	1:A:224:LEU:HD12	2.47	0.44
1:E:669:ASP:OD1	1:E:733:ARG:NH1	2.50	0.44
1:F:42:SER:O	1:F:46:MET:N	2.44	0.44
1:G:390:LEU:HD23	1:G:394:VAL:HG11	1.99	0.44
1:L:126:ILE:CD1	1:L:159:ARG:HD3	2.48	0.44
1:L:438:ASP:OD1	1:L:438:ASP:N	2.51	0.44
1:L:439:ALA:HA	1:L:442:MET:HB3	1.99	0.44
1:B:430:ILE:HD11	1:B:441:VAL:HG11	1.99	0.44
1:H:542:ILE:HD13	1:H:562:ILE:HD13	1.98	0.44
1:A:424:ARG:HG3	1:B:222:LEU:HD22	1.99	0.44
1:B:298:PRO:HA	1:B:340:HIS:O	2.17	0.44
1:I:484:ASP:OD1	1:I:484:ASP:N	2.51	0.44
1:G:120:ASP:N	1:G:120:ASP:OD1	2.51	0.44
1:G:532:ALA:HB2	1:G:573:VAL:HG11	1.98	0.44
1:J:51:LEU:CD2	1:J:104:PRO:HB3	2.47	0.44
1:I:404:HIS:NE2	1:I:468:VAL:HG21	2.32	0.44
1:J:431:ASP:HA	1:J:434:ASP:HB2	1.98	0.44
1:B:89:ARG:CZ	1:B:96:LEU:HD21	2.48	0.44
1:H:75:ASP:OD1	1:H:75:ASP:N	2.49	0.44
1:I:160:ALA:HB2	1:I:387:ASN:HD21	1.82	0.44
1:J:427:MET:HE1	1:K:226:HIS:NE2	2.32	0.44
1:A:120:ASP:OD1	1:A:120:ASP:N	2.51	0.44
1:B:644:TYR:CE2	1:B:646:PRO:HB3	2.52	0.44
1:D:112:LYS:HB2	1:D:169:ASP:HB3	1.99	0.44
1:G:89:ARG:NH1	1:G:96:LEU:HD21	2.32	0.44
1:H:431:ASP:C	1:H:433:GLU:H	2.26	0.44
1:H:727:PRO:HB2	1:H:729:PRO:CD	2.48	0.44
1:K:713:ARG:HB2	1:K:720:MET:HE2	2.00	0.44
1:K:734:ASP:OD1	1:K:734:ASP:N	2.50	0.44
1:C:89:ARG:NH1	1:C:96:LEU:HD21	2.32	0.44
1:D:222:LEU:HB2	1:D:223:PRO:HD3	1.99	0.44
1:D:699:ILE:O	1:D:703:ILE:HD12	2.18	0.44
1:F:173:TYR:N	1:F:173:TYR:HD1	2.15	0.44
1:C:484:ASP:OD1	1:C:484:ASP:N	2.51	0.43
1:E:425:LYS:HE3	1:E:426:LYS:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:105:CYS:SG	1:F:173:TYR:HE2	2.41	0.43
1:L:185:GLU:O	1:L:187:GLU:N	2.51	0.43
1:L:501:ASP:OD1	1:L:502:LYS:N	2.51	0.43
1:A:465:ARG:NH2	1:B:607:GLU:OE1	2.51	0.43
1:B:122:THR:HB	1:B:161:VAL:HA	2.00	0.43
1:F:552:PHE:CE1	1:F:596:ALA:HB2	2.53	0.43
1:G:450:ASP:OD1	1:G:453:ARG:NH1	2.51	0.43
1:I:222:LEU:HB3	1:I:223:PRO:HD3	2.00	0.43
1:K:532:ALA:HB2	1:K:573:VAL:HG11	2.00	0.43
1:K:744:ARG:NH2	1:L:763:GLN:OE1	2.51	0.43
1:A:65:ARG:NH1	1:A:91:ASN:O	2.44	0.43
1:D:703:ILE:HD13	1:E:495:TYR:CE2	2.54	0.43
1:G:233:ILE:HD11	1:L:158:MET:HE3	1.99	0.43
1:H:512:LYS:NZ	1:H:608:MET:O	2.43	0.43
1:I:75:ASP:OD1	1:I:75:ASP:N	2.49	0.43
1:J:726:ASP:N	1:J:727:PRO:HD3	2.33	0.43
1:K:124:GLU:OE1	1:K:125:GLY:N	2.51	0.43
1:K:158:MET:HB2	1:L:233:ILE:HD11	2.01	0.43
1:L:539:PHE:CE2	1:L:541:SER:HB2	2.53	0.43
1:B:542:ILE:HD13	1:B:562:ILE:HD13	2.01	0.43
1:D:22:ARG:HB3	1:D:23:PRO:HD2	1.99	0.43
1:E:478:ASP:OD2	1:E:662:ARG:NH2	2.51	0.43
1:I:233:ILE:HG22	1:I:235:VAL:H	1.83	0.43
2:J:902:AGS:O2B	2:J:902:AGS:O2G	2.35	0.43
1:E:493:VAL:HG13	1:E:618:PHE:CD2	2.53	0.43
1:I:208:GLY:HA2	1:I:376:GLY:HA2	2.00	0.43
1:K:126:ILE:HG21	1:K:439:ALA:HB2	1.99	0.43
1:K:385:THR:HB	1:K:390:LEU:HD11	2.01	0.43
1:L:28:VAL:HG21	1:L:94:VAL:HG11	2.00	0.43
1:C:136:LYS:HB3	1:C:137:PRO:CD	2.48	0.43
1:F:94:VAL:HG13	1:F:98:ASP:HB2	2.01	0.43
1:I:707:ILE:O	1:I:711:ARG:HG3	2.18	0.43
1:K:707:ILE:HD12	1:K:707:ILE:N	2.34	0.43
1:B:427:MET:CG	1:B:432:LEU:HD21	2.48	0.43
1:J:586:ARG:NH1	1:J:630:ASP:OD2	2.46	0.43
1:K:220:VAL:CG1	1:K:224:LEU:HD22	2.48	0.43
1:L:117:LEU:HD21	1:L:185:GLU:H	1.84	0.43
1:A:426:LYS:HG3	1:A:445:LEU:CD1	2.49	0.43
1:F:230:PHE:CZ	1:F:237:PRO:HB3	2.54	0.43
1:I:349:ARG:HG3	1:I:352:SER:CB	2.49	0.43
1:I:532:ALA:HB2	1:I:573:VAL:HG11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:519:PRO:O	1:B:524:LYS:NZ	2.51	0.43
1:B:675:LEU:CD2	1:B:740:MET:HE3	2.49	0.43
1:C:120:ASP:OD1	1:C:120:ASP:N	2.52	0.43
1:D:427:MET:HG2	1:D:430:ILE:HG22	2.00	0.43
1:F:28:VAL:HG21	1:F:94:VAL:HG11	2.01	0.43
1:F:136:LYS:HB3	1:F:137:PRO:CD	2.49	0.43
1:H:423:ILE:HG12	1:H:445:LEU:HD21	2.01	0.43
1:A:233:ILE:HD11	1:F:158:MET:HB2	2.00	0.42
1:E:114:ILE:HG12	1:E:168:THR:HG22	2.01	0.42
1:F:704:GLU:O	1:F:708:ARG:HG3	2.19	0.42
1:J:226:HIS:HB3	1:J:229:LEU:HG	2.00	0.42
1:K:90:ASN:O	1:K:93:ARG:NH1	2.50	0.42
1:L:380:ILE:HD12	2:L:901:AGS:N1	2.34	0.42
1:A:233:ILE:HD11	1:F:158:MET:HE3	2.01	0.42
1:A:766:ARG:NH1	2:F:902:AGS:O3G	2.50	0.42
1:B:295:LYS:HE3	1:B:295:LYS:HA	2.00	0.42
1:C:373:ASP:HB3	1:C:470:GLU:HB3	2.00	0.42
1:I:560:ARG:HG3	1:I:603:GLN:HE21	1.84	0.42
1:L:703:ILE:HD12	1:L:704:GLU:N	2.33	0.42
1:A:51:LEU:HD21	1:A:104:PRO:HG3	2.01	0.42
1:A:556:GLU:OE1	1:A:560:ARG:NH1	2.51	0.42
1:C:371:ILE:HD11	1:C:468:VAL:HG22	2.01	0.42
1:G:49:LEU:HG	1:G:49:LEU:O	2.19	0.42
1:H:520:PRO:HB3	1:I:766:ARG:NH1	2.35	0.42
1:H:542:ILE:HD12	1:H:562:ILE:HG21	2.01	0.42
1:I:226:HIS:HB3	1:I:229:LEU:HG	2.02	0.42
1:I:442:MET:HE2	1:I:442:MET:HA	2.01	0.42
1:I:577:ASP:OD1	1:I:578:GLU:N	2.49	0.42
1:J:424:ARG:HG3	1:K:222:LEU:HD11	2.02	0.42
1:K:703:ILE:HA	1:L:502:LYS:HZ2	1.84	0.42
1:L:123:VAL:HA	1:L:126:ILE:HG13	2.01	0.42
1:D:608:MET:HG2	1:D:619:ILE:HD13	2.01	0.42
1:E:251:LYS:NZ	2:E:901:AGS:S1G	2.93	0.42
1:H:126:ILE:HG13	1:H:159:ARG:HD2	2.01	0.42
1:I:164:LYS:NZ	1:I:192:GLU:OE1	2.50	0.42
1:J:423:ILE:HD11	1:K:233:ILE:CD1	2.49	0.42
1:K:317:HIS:O	1:L:322:ARG:NH2	2.50	0.42
1:L:514:VAL:HG11	1:L:643:ILE:HD12	2.00	0.42
1:B:185:GLU:C	1:B:187:GLU:H	2.26	0.42
1:B:210:ARG:O	1:B:214:ALA:N	2.49	0.42
1:C:96:LEU:N	1:C:96:LEU:HD22	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:438:ASP:OD1	1:F:438:ASP:N	2.51	0.42
1:I:53:ARG:HB2	1:I:72:LEU:HD23	2.01	0.42
1:A:96:LEU:O	1:A:225:ARG:NH2	2.53	0.42
1:C:222:LEU:HB3	1:C:223:PRO:HD3	2.02	0.42
1:E:727:PRO:O	1:E:729:PRO:HD3	2.18	0.42
1:G:119:ILE:HG21	1:G:191:ARG:HG2	2.01	0.42
1:G:158:MET:SD	1:H:233:ILE:HD11	2.59	0.42
1:J:433:GLU:O	1:J:433:GLU:HG3	2.19	0.42
1:K:397:GLU:O	1:K:401:ASN:ND2	2.52	0.42
1:A:727:PRO:C	1:A:729:PRO:HD3	2.44	0.42
1:B:151:ILE:HD11	1:B:195:GLU:CD	2.45	0.42
1:E:90:ASN:O	1:E:93:ARG:NH1	2.52	0.42
1:G:136:LYS:HB3	1:G:137:PRO:CD	2.49	0.42
1:H:52:PHE:CD1	1:H:52:PHE:N	2.87	0.42
1:H:671:ASP:HB3	1:H:674:PHE:HB3	2.02	0.42
1:K:89:ARG:NH1	1:K:261:GLU:OE2	2.51	0.42
1:K:434:ASP:O	1:K:435:GLU:CG	2.68	0.42
1:L:108:VAL:HG11	1:L:175:ILE:HG13	2.02	0.42
1:L:635:ARG:NH1	1:L:636:PRO:O	2.53	0.42
1:E:63:LYS:O	1:E:63:LYS:HG2	2.20	0.42
1:F:127:THR:HG22	1:F:437:ILE:HB	2.02	0.42
1:G:110:TYR:N	1:G:110:TYR:CD1	2.88	0.42
1:J:710:GLU:OE2	1:J:713:ARG:NH2	2.52	0.42
1:B:407:VAL:CG1	1:B:408:GLY:N	2.83	0.42
1:D:109:LYS:O	1:D:175:ILE:N	2.43	0.42
1:F:203:TYR:CE2	1:F:217:LYS:HD3	2.54	0.42
1:G:429:LEU:HD12	1:G:429:LEU:H	1.84	0.42
1:I:335:LEU:HD11	1:I:343:VAL:CG2	2.49	0.42
1:I:437:ILE:N	1:I:437:ILE:CD1	2.82	0.42
1:J:427:MET:HE1	1:K:226:HIS:CD2	2.54	0.42
1:L:434:ASP:C	1:L:436:THR:N	2.78	0.42
1:A:726:ASP:N	1:A:727:PRO:HD3	2.35	0.42
1:D:98:ASP:OD1	1:D:225:ARG:NH1	2.37	0.42
1:E:164:LYS:HD3	1:E:189:ILE:HD11	2.02	0.42
1:J:298:PRO:HA	1:J:340:HIS:O	2.20	0.42
1:E:251:LYS:NZ	2:E:901:AGS:O2B	2.52	0.41
1:F:464:LEU:H	1:F:464:LEU:HD12	1.85	0.41
1:A:28:VAL:HG21	1:A:94:VAL:CG1	2.50	0.41
1:D:501:ASP:OD1	1:D:501:ASP:N	2.53	0.41
1:E:335:LEU:HD11	1:E:343:VAL:CG2	2.49	0.41
1:H:330:THR:O	1:H:334:GLY:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:542:ILE:CD1	1:K:562:ILE:HG21	2.50	0.41
1:K:695:CYS:SG	1:L:506:PHE:HB3	2.60	0.41
1:A:706:GLU:OE1	1:B:502:LYS:NZ	2.50	0.41
1:B:136:LYS:HB3	1:B:137:PRO:HD3	2.02	0.41
1:C:28:VAL:HG21	1:C:94:VAL:HG11	2.02	0.41
1:D:120:ASP:N	1:D:120:ASP:OD1	2.53	0.41
1:G:335:LEU:C	1:G:337:GLN:N	2.74	0.41
1:J:380:ILE:HG23	2:J:901:AGS:C2	2.50	0.41
1:K:438:ASP:OD1	1:K:438:ASP:N	2.53	0.41
1:A:95:ARG:HB2	1:A:225:ARG:NH2	2.35	0.41
1:A:501:ASP:OD1	1:A:501:ASP:N	2.53	0.41
1:B:567:ARG:CG	1:B:611:MET:HE1	2.50	0.41
1:C:208:GLY:HA2	1:C:376:GLY:HA2	2.02	0.41
1:D:726:ASP:N	1:D:727:PRO:HD3	2.34	0.41
1:G:501:ASP:N	1:G:501:ASP:OD1	2.52	0.41
1:H:495:TYR:N	1:H:496:PRO:HD2	2.35	0.41
1:L:226:HIS:HB3	1:L:229:LEU:HG	2.03	0.41
1:A:94:VAL:HG12	1:A:95:ARG:N	2.35	0.41
1:A:512:LYS:NZ	1:A:608:MET:O	2.44	0.41
1:C:532:ALA:HB2	1:C:573:VAL:HG11	2.03	0.41
1:C:577:ASP:OD1	1:C:578:GLU:N	2.52	0.41
1:F:434:ASP:C	1:F:436:THR:N	2.78	0.41
1:G:220:VAL:CG1	1:G:224:LEU:HD12	2.51	0.41
1:H:63:LYS:HG2	1:H:63:LYS:O	2.20	0.41
1:I:27:ILE:HB	1:I:81:LYS:HG2	2.02	0.41
1:D:158:MET:HE2	1:E:235:VAL:HG21	2.03	0.41
1:E:577:ASP:OD1	1:E:578:GLU:N	2.52	0.41
1:G:118:PRO:HG2	1:G:188:PRO:HB3	2.03	0.41
1:G:226:HIS:HB3	1:G:229:LEU:HG	2.00	0.41
1:G:417:GLU:HG3	1:G:454:TRP:HZ3	1.85	0.41
1:H:152:PHE:CZ	1:H:163:PHE:HB2	2.56	0.41
1:J:385:THR:HB	1:J:390:LEU:HD11	2.02	0.41
1:L:204:ASP:OD1	1:L:204:ASP:N	2.54	0.41
1:D:254:ILE:HD12	1:D:369:ILE:HD13	2.03	0.41
1:F:94:VAL:HG12	1:F:95:ARG:N	2.35	0.41
1:I:136:LYS:HB3	1:I:137:PRO:CD	2.51	0.41
1:J:220:VAL:CG1	1:J:224:LEU:HD12	2.50	0.41
1:K:122:THR:HB	1:K:161:VAL:HA	2.01	0.41
1:K:706:GLU:O	1:K:707:ILE:C	2.64	0.41
1:L:123:VAL:O	1:L:126:ILE:N	2.50	0.41
1:L:726:ASP:N	1:L:727:PRO:HD3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:GLU:HG3	1:A:454:TRP:HZ3	1.86	0.41
1:A:710:GLU:HA	1:A:713:ARG:HD3	2.02	0.41
1:C:110:TYR:N	1:C:110:TYR:CD1	2.89	0.41
1:H:120:ASP:OD1	1:H:120:ASP:N	2.53	0.41
1:I:127:THR:O	1:I:439:ALA:N	2.46	0.41
1:I:417:GLU:HG3	1:I:454:TRP:HZ3	1.85	0.41
1:K:389:LYS:HD3	1:K:443:ASN:O	2.21	0.41
1:L:136:LYS:HB3	1:L:137:PRO:CD	2.51	0.41
1:A:162:GLU:OE1	1:A:191:ARG:NH2	2.54	0.41
1:A:350:PRO:O	1:A:358:ARG:NH2	2.53	0.41
1:B:59:LEU:HD22	1:B:100:ILE:HD13	2.02	0.41
1:B:147:ARG:HG2	1:B:173:TYR:HB3	2.01	0.41
1:C:158:MET:HE3	1:D:233:ILE:HD11	2.03	0.41
1:C:629:ILE:HG12	1:C:633:ILE:HD12	2.02	0.41
1:D:573:VAL:HG23	1:D:620:ILE:HD13	2.03	0.41
1:F:243:LEU:HD22	1:F:369:ILE:HD11	2.03	0.41
1:F:380:ILE:HD12	2:F:901:AGS:N1	2.36	0.41
1:G:495:TYR:N	1:G:496:PRO:HD2	2.36	0.41
1:J:438:ASP:HB3	1:J:441:VAL:HB	2.03	0.41
1:J:547:LEU:HD12	1:J:582:ILE:HD11	2.03	0.41
1:K:283:GLU:OE1	1:K:323:ARG:NH1	2.53	0.41
1:A:147:ARG:HG2	1:A:173:TYR:HB3	2.03	0.41
1:B:251:LYS:NZ	2:B:901:AGS:O2B	2.51	0.41
1:D:727:PRO:C	1:D:729:PRO:HD3	2.46	0.41
1:E:43:GLN:HG3	1:E:46:MET:HE2	2.03	0.41
1:F:432:LEU:C	1:F:434:ASP:N	2.79	0.41
1:G:86:ARG:HG3	1:G:89:ARG:NH1	2.36	0.41
1:G:390:LEU:HD12	1:G:390:LEU:N	2.36	0.41
1:I:158:MET:N	1:I:387:ASN:O	2.53	0.41
1:K:251:LYS:NZ	2:K:901:AGS:O1B	2.53	0.41
1:A:429:LEU:H	1:A:429:LEU:HD12	1.85	0.40
1:B:94:VAL:HG12	1:B:95:ARG:N	2.36	0.40
1:D:238:PRO:HB3	1:D:365:ARG:HE	1.86	0.40
1:E:435:GLU:CG	1:E:436:THR:H	2.35	0.40
1:G:636:PRO:HA	1:G:640:ASP:HB3	2.03	0.40
1:I:476:TRP:NE1	1:I:534:GLU:HB2	2.36	0.40
1:I:665:PRO:HD2	1:J:506:PHE:HA	2.04	0.40
1:J:432:LEU:HG	1:K:25:ARG:NH1	2.35	0.40
1:L:701:GLU:OE2	1:L:735:HIS:NE2	2.43	0.40
1:C:432:LEU:HG	1:C:433:GLU:N	2.36	0.40
1:H:661:LEU:HD21	1:H:691:CYS:SG	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:228:ALA:HA	1:J:231:LYS:HD3	2.04	0.40
1:J:384:HIS:HE1	2:J:901:AGS:N3	2.20	0.40
1:K:147:ARG:HG2	1:K:173:TYR:HB3	2.03	0.40
1:K:191:ARG:NH2	1:K:197:SER:HA	2.36	0.40
1:L:89:ARG:NH1	1:L:96:LEU:HD21	2.35	0.40
1:A:420:LEU:HD22	1:B:222:LEU:HD23	2.02	0.40
1:B:678:MET:HE2	1:B:678:MET:HA	2.04	0.40
1:G:230:PHE:CE1	1:G:237:PRO:HB3	2.57	0.40
1:H:111:GLY:HA2	1:H:170:PRO:HG2	2.03	0.40
1:H:355:PRO:O	1:H:359:ARG:NH1	2.55	0.40
1:H:430:ILE:HD11	1:H:441:VAL:HG11	2.04	0.40
1:I:152:PHE:CZ	1:I:163:PHE:HB2	2.56	0.40
1:I:335:LEU:HD11	1:I:343:VAL:HG23	2.03	0.40
1:K:22:ARG:CG	1:K:23:PRO:HD2	2.52	0.40
1:K:136:LYS:HB3	1:K:137:PRO:CD	2.52	0.40
1:B:39:VAL:HG11	1:B:59:LEU:HD11	2.03	0.40
1:B:408:GLY:HA3	2:B:901:AGS:N7	2.37	0.40
1:E:297:ALA:HA	1:E:298:PRO:C	2.47	0.40
1:H:136:LYS:HB3	1:H:137:PRO:HD3	2.03	0.40
1:I:120:ASP:OD1	1:I:120:ASP:N	2.54	0.40
1:L:220:VAL:CG1	1:L:224:LEU:HD12	2.52	0.40
1:L:430:ILE:N	1:L:430:ILE:HD12	2.37	0.40
1:A:763:GLN:H	1:A:763:GLN:CD	2.29	0.40
1:B:380:ILE:HD12	2:B:901:AGS:C6	2.52	0.40
1:C:239:ARG:NH1	1:C:335:LEU:O	2.55	0.40
1:E:52:PHE:HD1	1:E:55:ASP:OD1	2.05	0.40
1:I:109:LYS:HD2	1:I:110:TYR:N	2.36	0.40
2:I:902:AGS:O2G	2:I:902:AGS:O2A	2.40	0.40
1:J:63:LYS:C	1:J:64:ARG:HG2	2.47	0.40
1:K:33:ASN:ND2	1:K:38:VAL:HG11	2.36	0.40
1:K:74:ASP:OD2	1:K:83:ARG:NE	2.48	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	729/805 (91%)	705 (97%)	23 (3%)	1 (0%)	48	79
1	B	729/805 (91%)	703 (96%)	23 (3%)	3 (0%)	30	62
1	C	729/805 (91%)	704 (97%)	23 (3%)	2 (0%)	36	67
1	D	729/805 (91%)	707 (97%)	20 (3%)	2 (0%)	36	67
1	E	729/805 (91%)	704 (97%)	20 (3%)	5 (1%)	18	51
1	F	729/805 (91%)	703 (96%)	22 (3%)	4 (0%)	24	57
1	G	729/805 (91%)	706 (97%)	22 (3%)	1 (0%)	48	79
1	H	729/805 (91%)	702 (96%)	21 (3%)	6 (1%)	16	48
1	I	727/805 (90%)	705 (97%)	21 (3%)	1 (0%)	48	79
1	J	729/805 (91%)	707 (97%)	20 (3%)	2 (0%)	36	67
1	K	740/805 (92%)	700 (95%)	27 (4%)	13 (2%)	6	33
1	L	729/805 (91%)	706 (97%)	18 (2%)	5 (1%)	18	51
All	All	8757/9660 (91%)	8452 (96%)	260 (3%)	45 (0%)	24	57

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	430	ILE
1	B	431	ASP
1	B	728	VAL
1	D	186	GLY
1	E	435	GLU
1	F	433	GLU
1	F	726	ASP
1	H	428	ASP
1	H	430	ILE
1	H	431	ASP
1	H	729	PRO
1	K	435	GLU
1	K	723	GLU
1	K	724	GLU
1	K	725	ASP
1	L	433	GLU
1	A	340	HIS
1	E	728	VAL
1	F	50	GLN

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Mol	Chain	Res	Type
1	F	435	GLU
1	J	186	GLY
1	K	707	ILE
1	K	729	PRO
1	L	435	GLU
1	D	340	HIS
1	E	431	ASP
1	H	727	PRO
1	J	340	HIS
1	K	340	HIS
1	K	717	PRO
1	G	340	HIS
1	K	431	ASP
1	L	340	HIS
1	C	340	HIS
1	E	340	HIS
1	H	340	HIS
1	K	186	GLY
1	K	720	MET
1	K	727	PRO
1	L	186	GLY
1	L	23	PRO
1	E	186	GLY
1	I	186	GLY
1	C	186	GLY
1	K	726	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	627/677 (93%)	584 (93%)	43 (7%)	14	40
1	B	628/677 (93%)	588 (94%)	40 (6%)	16	42
1	C	628/677 (93%)	583 (93%)	45 (7%)	13	39
1	D	628/677 (93%)	598 (95%)	30 (5%)	23	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	628/677 (93%)	593 (94%)	35 (6%)	19	45
1	F	628/677 (93%)	589 (94%)	39 (6%)	16	42
1	G	627/677 (93%)	580 (92%)	47 (8%)	12	38
1	H	628/677 (93%)	593 (94%)	35 (6%)	19	45
1	I	628/677 (93%)	580 (92%)	48 (8%)	12	37
1	J	628/677 (93%)	585 (93%)	43 (7%)	14	40
1	K	636/677 (94%)	589 (93%)	47 (7%)	13	38
1	L	628/677 (93%)	588 (94%)	40 (6%)	16	42
All	All	7542/8124 (93%)	7050 (94%)	492 (6%)	15	42

All (492) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ARG
1	A	45	LYS
1	A	52	PHE
1	A	78	SER
1	A	79	ASP
1	A	99	VAL
1	A	107	ASP
1	A	162	GLU
1	A	193	ASP
1	A	210	ARG
1	A	229	LEU
1	A	230	PHE
1	A	231	LYS
1	A	236	LYS
1	A	278	LEU
1	A	284	SER
1	A	292	GLU
1	A	322	ARG
1	A	336	LYS
1	A	349	ARG
1	A	351	ASN
1	A	358	ARG
1	A	359	ARG
1	A	407	VAL
1	A	414	LEU
1	A	416	SER

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Mol	Chain	Res	Type
1	A	425	LYS
1	A	427	MET
1	A	428	ASP
1	A	435	GLU
1	A	437	ILE
1	A	443	ASN
1	A	456	LEU
1	A	464	LEU
1	A	505	LYS
1	A	552	PHE
1	A	556	GLU
1	A	561	GLU
1	A	573	VAL
1	A	713	ARG
1	A	732	ARG
1	A	734	ASP
1	A	762	LEU
1	B	21	ASN
1	B	25	ARG
1	B	34	GLU
1	B	45	LYS
1	B	49	LEU
1	B	53	ARG
1	B	79	ASP
1	B	99	VAL
1	B	109	LYS
1	B	124	GLU
1	B	131	PHE
1	B	155	ARG
1	B	184	CYS
1	B	235	VAL
1	B	268	LEU
1	B	278	LEU
1	B	295	LYS
1	B	317	HIS
1	B	349	ARG
1	B	375	THR
1	B	392	ASP
1	B	407	VAL
1	B	416	SER
1	B	420	LEU
1	B	429	LEU

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Mol	Chain	Res	Type
1	B	433	GLU
1	B	456	LEU
1	B	464	LEU
1	B	465	ARG
1	B	487	ARG
1	B	556	GLU
1	B	573	VAL
1	B	678	MET
1	B	707	ILE
1	B	708	ARG
1	B	714	GLN
1	B	731	ILE
1	B	737	GLU
1	B	745	ARG
1	B	762	LEU
1	C	45	LYS
1	C	52	PHE
1	C	99	VAL
1	C	107	ASP
1	C	109	LYS
1	C	113	ARG
1	C	126	ILE
1	C	130	LEU
1	C	131	PHE
1	C	173	TYR
1	C	179	ASP
1	C	184	CYS
1	C	187	GLU
1	C	229	LEU
1	C	230	PHE
1	C	233	ILE
1	C	235	VAL
1	C	236	LYS
1	C	274	ILE
1	C	288	LYS
1	C	317	HIS
1	C	336	LYS
1	C	349	ARG
1	C	358	ARG
1	C	359	ARG
1	C	407	VAL
1	C	420	LEU

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Mol	Chain	Res	Type
1	C	427	MET
1	C	435	GLU
1	C	437	ILE
1	C	442	MET
1	C	445	LEU
1	C	450	ASP
1	C	498	GLU
1	C	551	TRP
1	C	556	GLU
1	C	573	VAL
1	C	675	LEU
1	C	677	LYS
1	C	704	GLU
1	C	714	GLN
1	C	715	THR
1	C	732	ARG
1	C	742	PHE
1	C	762	LEU
1	D	45	LYS
1	D	52	PHE
1	D	78	SER
1	D	79	ASP
1	D	99	VAL
1	D	113	ARG
1	D	162	GLU
1	D	211	LYS
1	D	229	LEU
1	D	283	GLU
1	D	295	LYS
1	D	335	LEU
1	D	349	ARG
1	D	358	ARG
1	D	359	ARG
1	D	407	VAL
1	D	414	LEU
1	D	416	SER
1	D	425	LYS
1	D	427	MET
1	D	430	ILE
1	D	435	GLU
1	D	436	THR
1	D	445	LEU

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Mol	Chain	Res	Type
1	D	464	LEU
1	D	556	GLU
1	D	573	VAL
1	D	706	GLU
1	D	745	ARG
1	D	762	LEU
1	E	49	LEU
1	E	99	VAL
1	E	107	ASP
1	E	113	ARG
1	E	124	GLU
1	E	127	THR
1	E	131	PHE
1	E	184	CYS
1	E	190	LYS
1	E	191	ARG
1	E	229	LEU
1	E	292	GLU
1	E	295	LYS
1	E	317	HIS
1	E	349	ARG
1	E	351	ASN
1	E	407	VAL
1	E	416	SER
1	E	420	LEU
1	E	428	ASP
1	E	429	LEU
1	E	435	GLU
1	E	445	LEU
1	E	464	LEU
1	E	468	VAL
1	E	487	ARG
1	E	508	MET
1	E	509	THR
1	E	556	GLU
1	E	573	VAL
1	E	668	LYS
1	E	669	ASP
1	E	713	ARG
1	E	734	ASP
1	E	762	LEU
1	F	45	LYS

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Mol	Chain	Res	Type
1	F	53	ARG
1	F	99	VAL
1	F	126	ILE
1	F	130	LEU
1	F	131	PHE
1	F	173	TYR
1	F	184	CYS
1	F	210	ARG
1	F	213	LEU
1	F	217	LYS
1	F	222	LEU
1	F	230	PHE
1	F	274	ILE
1	F	287	ARG
1	F	292	GLU
1	F	295	LYS
1	F	317	HIS
1	F	338	ARG
1	F	349	ARG
1	F	359	ARG
1	F	392	ASP
1	F	401	ASN
1	F	402	GLU
1	F	407	VAL
1	F	420	LEU
1	F	431	ASP
1	F	437	ILE
1	F	464	LEU
1	F	505	LYS
1	F	556	GLU
1	F	573	VAL
1	F	704	GLU
1	F	711	ARG
1	F	730	GLU
1	F	731	ILE
1	F	734	ASP
1	F	745	ARG
1	F	762	LEU
1	G	21	ASN
1	G	22	ARG
1	G	45	LYS
1	G	52	PHE

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Mol	Chain	Res	Type
1	G	78	SER
1	G	79	ASP
1	G	99	VAL
1	G	107	ASP
1	G	113	ARG
1	G	141	GLU
1	G	159	ARG
1	G	162	GLU
1	G	184	CYS
1	G	193	ASP
1	G	211	LYS
1	G	229	LEU
1	G	231	LYS
1	G	236	LYS
1	G	284	SER
1	G	292	GLU
1	G	319	GLU
1	G	322	ARG
1	G	349	ARG
1	G	358	ARG
1	G	359	ARG
1	G	378	LEU
1	G	407	VAL
1	G	414	LEU
1	G	416	SER
1	G	425	LYS
1	G	427	MET
1	G	428	ASP
1	G	435	GLU
1	G	437	ILE
1	G	438	ASP
1	G	442	MET
1	G	456	LEU
1	G	460	ASN
1	G	464	LEU
1	G	551	TRP
1	G	556	GLU
1	G	573	VAL
1	G	651	LYS
1	G	703	ILE
1	G	731	ILE
1	G	734	ASP

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Mol	Chain	Res	Type
1	G	762	LEU
1	H	21	ASN
1	H	45	LYS
1	H	49	LEU
1	H	79	ASP
1	H	99	VAL
1	H	109	LYS
1	H	124	GLU
1	H	184	CYS
1	H	211	LYS
1	H	229	LEU
1	H	235	VAL
1	H	236	LYS
1	H	261	GLU
1	H	274	ILE
1	H	317	HIS
1	H	349	ARG
1	H	407	VAL
1	H	420	LEU
1	H	425	LYS
1	H	429	LEU
1	H	432	LEU
1	H	433	GLU
1	H	445	LEU
1	H	464	LEU
1	H	468	VAL
1	H	487	ARG
1	H	556	GLU
1	H	573	VAL
1	H	668	LYS
1	H	677	LYS
1	H	700	ARG
1	H	711	ARG
1	H	731	ILE
1	H	745	ARG
1	H	762	LEU
1	I	45	LYS
1	I	53	ARG
1	I	80	GLU
1	I	99	VAL
1	I	107	ASP
1	I	109	LYS

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Mol	Chain	Res	Type
1	I	112	LYS
1	I	113	ARG
1	I	130	LEU
1	I	131	PHE
1	I	146	ILE
1	I	173	TYR
1	I	184	CYS
1	I	190	LYS
1	I	229	LEU
1	I	230	PHE
1	I	233	ILE
1	I	236	LYS
1	I	295	LYS
1	I	336	LYS
1	I	349	ARG
1	I	358	ARG
1	I	359	ARG
1	I	392	ASP
1	I	407	VAL
1	I	416	SER
1	I	420	LEU
1	I	427	MET
1	I	433	GLU
1	I	435	GLU
1	I	436	THR
1	I	437	ILE
1	I	442	MET
1	I	445	LEU
1	I	498	GLU
1	I	556	GLU
1	I	573	VAL
1	I	614	LYS
1	I	615	LYS
1	I	675	LEU
1	I	677	LYS
1	I	689	GLU
1	I	712	GLU
1	I	715	THR
1	I	732	ARG
1	I	741	ARG
1	I	742	PHE
1	I	762	LEU

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Mol	Chain	Res	Type
1	J	21	ASN
1	J	45	LYS
1	J	52	PHE
1	J	64	ARG
1	J	79	ASP
1	J	99	VAL
1	J	162	GLU
1	J	184	CYS
1	J	211	LYS
1	J	229	LEU
1	J	230	PHE
1	J	283	GLU
1	J	295	LYS
1	J	335	LEU
1	J	349	ARG
1	J	358	ARG
1	J	359	ARG
1	J	407	VAL
1	J	414	LEU
1	J	416	SER
1	J	425	LYS
1	J	427	MET
1	J	429	LEU
1	J	430	ILE
1	J	432	LEU
1	J	435	GLU
1	J	436	THR
1	J	445	LEU
1	J	450	ASP
1	J	460	ASN
1	J	464	LEU
1	J	487	ARG
1	J	542	ILE
1	J	556	GLU
1	J	573	VAL
1	J	689	GLU
1	J	705	SER
1	J	711	ARG
1	J	715	THR
1	J	730	GLU
1	J	738	GLU
1	J	745	ARG

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Mol	Chain	Res	Type
1	J	762	LEU
1	K	22	ARG
1	K	49	LEU
1	K	64	ARG
1	K	79	ASP
1	K	99	VAL
1	K	109	LYS
1	K	113	ARG
1	K	124	GLU
1	K	127	THR
1	K	131	PHE
1	K	132	GLU
1	K	190	LYS
1	K	191	ARG
1	K	236	LYS
1	K	261	GLU
1	K	313	ARG
1	K	349	ARG
1	K	407	VAL
1	K	416	SER
1	K	420	LEU
1	K	425	LYS
1	K	428	ASP
1	K	429	LEU
1	K	435	GLU
1	K	437	ILE
1	K	445	LEU
1	K	456	LEU
1	K	464	LEU
1	K	468	VAL
1	K	477	GLU
1	K	487	ARG
1	K	509	THR
1	K	556	GLU
1	K	573	VAL
1	K	658	LYS
1	K	669	ASP
1	K	696	LYS
1	K	700	ARG
1	K	707	ILE
1	K	710	GLU
1	K	722	VAL

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Mol	Chain	Res	Type
1	K	723	GLU
1	K	732	ARG
1	K	734	ASP
1	K	745	ARG
1	K	762	LEU
1	K	768	PHE
1	L	22	ARG
1	L	45	LYS
1	L	52	PHE
1	L	53	ARG
1	L	99	VAL
1	L	126	ILE
1	L	131	PHE
1	L	141	GLU
1	L	173	TYR
1	L	184	CYS
1	L	187	GLU
1	L	190	LYS
1	L	222	LEU
1	L	230	PHE
1	L	236	LYS
1	L	274	ILE
1	L	283	GLU
1	L	287	ARG
1	L	317	HIS
1	L	319	GLU
1	L	336	LYS
1	L	338	ARG
1	L	349	ARG
1	L	359	ARG
1	L	401	ASN
1	L	402	GLU
1	L	407	VAL
1	L	420	LEU
1	L	431	ASP
1	L	437	ILE
1	L	442	MET
1	L	464	LEU
1	L	465	ARG
1	L	505	LYS
1	L	556	GLU
1	L	573	VAL

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Mol	Chain	Res	Type
1	L	675	LEU
1	L	703	ILE
1	L	734	ASP
1	L	762	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	A	199	ASN
1	A	270	ASN
1	A	443	ASN
1	A	660	ASN
1	A	680	ASN
1	A	764	GLN
1	B	327	GLN
1	B	401	ASN
1	B	538	ASN
1	B	602	ASN
1	B	660	ASN
1	C	199	ASN
1	C	660	ASN
1	D	90	ASN
1	D	103	GLN
1	D	199	ASN
1	D	270	ASN
1	D	443	ASN
1	D	458	GLN
1	D	490	GLN
1	D	568	GLN
1	D	602	ASN
1	D	680	ASN
1	D	764	GLN
1	E	90	ASN
1	E	406	HIS
1	E	458	GLN
1	F	199	ASN
1	F	270	ASN
1	F	443	ASN
1	F	499	HIS
1	F	602	ASN
1	F	660	ASN

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Mol	Chain	Res	Type
1	G	103	GLN
1	G	490	GLN
1	G	494	GLN
1	G	680	ASN
1	H	103	GLN
1	H	340	HIS
1	H	421	GLN
1	H	602	ASN
1	I	103	GLN
1	I	340	HIS
1	I	494	GLN
1	I	680	ASN
1	J	406	HIS
1	J	490	GLN
1	J	494	GLN
1	J	568	GLN
1	K	103	GLN
1	K	490	GLN
1	K	494	GLN
1	K	538	ASN
1	L	199	ASN
1	L	270	ASN
1	L	327	GLN
1	L	340	HIS
1	L	401	ASN
1	L	494	GLN
1	L	568	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 48 ligands modelled in this entry, 24 are monoatomic - leaving 24 for Mogul analysis.

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	AGS	I	902	3	32,33,33	1.42	5 (15%)	45,52,52	1.96	10 (22%)
2	AGS	J	901	3	32,33,33	1.45	6 (18%)	45,52,52	1.86	10 (22%)
2	AGS	A	901	3	32,33,33	1.48	6 (18%)	45,52,52	1.88	10 (22%)
2	AGS	G	902	3	32,33,33	1.45	5 (15%)	45,52,52	1.92	9 (20%)
2	AGS	A	902	3	32,33,33	1.37	4 (12%)	45,52,52	1.89	9 (20%)
2	AGS	L	902	3	32,33,33	1.43	4 (12%)	45,52,52	1.91	8 (17%)
2	AGS	F	902	3	32,33,33	1.35	6 (18%)	45,52,52	1.96	9 (20%)
2	AGS	J	902	3	32,33,33	1.38	3 (9%)	45,52,52	2.01	8 (17%)
2	AGS	C	901	3	32,33,33	1.46	6 (18%)	45,52,52	2.00	10 (22%)
2	AGS	K	902	3	32,33,33	1.45	5 (15%)	45,52,52	1.97	10 (22%)
2	AGS	I	901	3	32,33,33	1.47	6 (18%)	45,52,52	1.91	10 (22%)
2	AGS	C	902	3	32,33,33	1.46	6 (18%)	45,52,52	1.92	9 (20%)
2	AGS	H	902	3	32,33,33	1.48	5 (15%)	45,52,52	1.94	9 (20%)
2	AGS	D	902	3	32,33,33	1.43	5 (15%)	45,52,52	1.94	9 (20%)
2	AGS	L	901	3	32,33,33	1.47	5 (15%)	45,52,52	1.98	11 (24%)
2	AGS	E	902	3	32,33,33	1.40	4 (12%)	45,52,52	1.86	8 (17%)
2	AGS	B	902	3	32,33,33	1.44	5 (15%)	45,52,52	1.92	11 (24%)
2	AGS	K	901	3	32,33,33	1.42	6 (18%)	45,52,52	1.91	9 (20%)
2	AGS	F	901	3	32,33,33	1.44	6 (18%)	45,52,52	1.92	10 (22%)
2	AGS	D	901	3	32,33,33	1.41	5 (15%)	45,52,52	1.95	8 (17%)
2	AGS	H	901	3	32,33,33	1.49	7 (21%)	45,52,52	1.99	10 (22%)
2	AGS	G	901	3	32,33,33	1.43	6 (18%)	45,52,52	1.93	10 (22%)
2	AGS	E	901	3	32,33,33	1.59	8 (25%)	45,52,52	1.93	11 (24%)
2	AGS	B	901	3	32,33,33	1.46	5 (15%)	45,52,52	1.98	9 (20%)

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	AGS	I	902	3	-	5/21/38/38	0/3/3/3
2	AGS	J	901	3	-	3/21/38/38	0/3/3/3
2	AGS	A	901	3	-	2/21/38/38	0/3/3/3
2	AGS	G	902	3	-	10/21/38/38	0/3/3/3
2	AGS	A	902	3	-	8/21/38/38	0/3/3/3
2	AGS	L	902	3	-	8/21/38/38	0/3/3/3
2	AGS	F	902	3	-	7/21/38/38	0/3/3/3
2	AGS	J	902	3	-	4/21/38/38	0/3/3/3
2	AGS	C	901	3	-	5/21/38/38	0/3/3/3
2	AGS	K	902	3	-	6/21/38/38	0/3/3/3
2	AGS	I	901	3	-	3/21/38/38	0/3/3/3
2	AGS	C	902	3	-	6/21/38/38	0/3/3/3
2	AGS	H	902	3	-	4/21/38/38	0/3/3/3
2	AGS	D	902	3	-	4/21/38/38	0/3/3/3
2	AGS	L	901	3	-	4/21/38/38	0/3/3/3
2	AGS	E	902	3	-	6/21/38/38	0/3/3/3
2	AGS	B	902	3	-	3/21/38/38	0/3/3/3
2	AGS	K	901	3	-	2/21/38/38	0/3/3/3
2	AGS	F	901	3	-	2/21/38/38	0/3/3/3
2	AGS	D	901	3	-	0/21/38/38	0/3/3/3
2	AGS	H	901	3	-	4/21/38/38	0/3/3/3
2	AGS	G	901	3	-	2/21/38/38	0/3/3/3
2	AGS	E	901	3	-	1/21/38/38	0/3/3/3
2	AGS	B	901	3	-	1/21/38/38	0/3/3/3

All (129) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	902	AGS	C6-N6	4.25	1.45	1.34
2	H	902	AGS	C6-N6	4.21	1.45	1.34
2	I	902	AGS	C6-N6	4.19	1.44	1.34
2	G	902	AGS	C6-N6	4.19	1.44	1.34
2	B	902	AGS	C6-N6	4.15	1.44	1.34
2	C	902	AGS	C6-N6	4.13	1.44	1.34
2	A	902	AGS	C6-N6	4.11	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	901	AGS	C6-N6	4.10	1.44	1.34
2	E	902	AGS	C6-N6	4.10	1.44	1.34
2	L	902	AGS	C6-N6	4.09	1.44	1.34
2	F	902	AGS	C6-N6	4.08	1.44	1.34
2	L	901	AGS	C6-N6	4.03	1.44	1.34
2	H	901	AGS	C6-N6	4.01	1.44	1.34
2	E	901	AGS	C6-N6	3.97	1.44	1.34
2	K	901	AGS	C6-N6	3.97	1.44	1.34
2	K	902	AGS	C6-N6	3.96	1.44	1.34
2	J	902	AGS	C6-N6	3.96	1.44	1.34
2	C	901	AGS	C6-N6	3.94	1.44	1.34
2	G	901	AGS	C6-N6	3.92	1.44	1.34
2	F	901	AGS	C6-N6	3.90	1.44	1.34
2	B	901	AGS	C6-N6	3.83	1.44	1.34
2	A	901	AGS	C6-N6	3.82	1.44	1.34
2	J	901	AGS	C6-N6	3.78	1.43	1.34
2	I	901	AGS	C6-N6	3.72	1.43	1.34
2	L	901	AGS	C5-N7	-3.09	1.33	1.39
2	E	901	AGS	PB-O3A	-3.05	1.56	1.59
2	C	901	AGS	C5-N7	-2.89	1.33	1.39
2	B	901	AGS	C5-N7	-2.87	1.33	1.39
2	F	901	AGS	C5-N7	-2.85	1.33	1.39
2	K	901	AGS	C5-N7	-2.76	1.34	1.39
2	G	901	AGS	C5-N7	-2.72	1.34	1.39
2	D	901	AGS	C5-N7	-2.67	1.34	1.39
2	I	901	AGS	PB-O3A	-2.63	1.56	1.59
2	J	901	AGS	C5-N7	-2.62	1.34	1.39
2	B	902	AGS	C5-N7	-2.59	1.34	1.39
2	H	901	AGS	C5-N7	-2.59	1.34	1.39
2	H	902	AGS	PB-O3A	-2.56	1.56	1.59
2	K	902	AGS	C5-N7	-2.53	1.34	1.39
2	J	902	AGS	C5-N7	-2.52	1.34	1.39
2	A	901	AGS	C5-N7	-2.52	1.34	1.39
2	J	901	AGS	O2'-C2'	-2.51	1.36	1.43
2	E	901	AGS	PG-S1G	2.50	1.96	1.90
2	A	902	AGS	C5-N7	-2.47	1.34	1.39
2	E	901	AGS	C5-N7	-2.47	1.34	1.39
2	I	901	AGS	C5-N7	-2.45	1.34	1.39
2	K	902	AGS	C2'-C3'	-2.43	1.46	1.53
2	E	902	AGS	PG-S1G	2.43	1.95	1.90
2	H	901	AGS	PB-O3A	-2.41	1.56	1.59
2	G	902	AGS	C5-N7	-2.41	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	902	AGS	C2'-C3'	-2.40	1.46	1.53
2	E	901	AGS	O2'-C2'	-2.39	1.37	1.43
2	I	901	AGS	PG-S1G	2.38	1.95	1.90
2	D	902	AGS	C5-N7	-2.38	1.34	1.39
2	A	901	AGS	O2'-C2'	-2.37	1.37	1.43
2	H	902	AGS	C5-N7	-2.35	1.34	1.39
2	F	901	AGS	O2'-C2'	-2.34	1.37	1.43
2	L	902	AGS	C5-N7	-2.34	1.34	1.39
2	I	902	AGS	O2'-C2'	-2.33	1.37	1.43
2	K	902	AGS	O2'-C2'	-2.32	1.37	1.43
2	G	901	AGS	PG-S1G	2.32	1.95	1.90
2	C	901	AGS	PG-S1G	2.31	1.95	1.90
2	E	902	AGS	C5-N7	-2.30	1.34	1.39
2	I	902	AGS	C5-N7	-2.30	1.34	1.39
2	B	902	AGS	O2'-C2'	-2.27	1.37	1.43
2	C	902	AGS	PB-O3A	-2.27	1.57	1.59
2	L	902	AGS	O2'-C2'	-2.27	1.37	1.43
2	A	902	AGS	O2'-C2'	-2.25	1.37	1.43
2	A	901	AGS	PG-S1G	2.24	1.95	1.90
2	G	902	AGS	C2'-C3'	-2.23	1.47	1.53
2	G	902	AGS	O2'-C2'	-2.23	1.37	1.43
2	H	901	AGS	PG-S1G	2.23	1.95	1.90
2	C	902	AGS	C2'-C3'	-2.23	1.47	1.53
2	E	901	AGS	C2'-C3'	-2.22	1.47	1.53
2	J	901	AGS	C2'-C3'	-2.22	1.47	1.53
2	C	901	AGS	O2'-C2'	-2.22	1.37	1.43
2	D	901	AGS	PG-S1G	2.22	1.95	1.90
2	F	902	AGS	PG-S1G	2.21	1.95	1.90
2	C	902	AGS	O2'-C2'	-2.21	1.37	1.43
2	C	901	AGS	C2'-C3'	-2.20	1.47	1.53
2	D	901	AGS	O2'-C2'	-2.20	1.37	1.43
2	L	901	AGS	O2'-C2'	-2.20	1.37	1.43
2	G	901	AGS	O2'-C2'	-2.20	1.37	1.43
2	B	901	AGS	O2'-C2'	-2.20	1.37	1.43
2	K	901	AGS	PG-S1G	2.19	1.95	1.90
2	H	901	AGS	O2'-C2'	-2.18	1.37	1.43
2	C	902	AGS	C5-N7	-2.18	1.35	1.39
2	I	901	AGS	O2'-C2'	-2.18	1.37	1.43
2	J	901	AGS	PG-S1G	2.18	1.95	1.90
2	I	902	AGS	C2-N3	2.17	1.37	1.33
2	B	901	AGS	PG-S1G	2.17	1.95	1.90
2	K	901	AGS	O2'-C2'	-2.17	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	902	AGS	C2-N3	2.15	1.37	1.33
2	L	902	AGS	C2'-C3'	-2.15	1.47	1.53
2	F	902	AGS	C5-N7	-2.15	1.35	1.39
2	A	901	AGS	O3'-C3'	-2.15	1.37	1.43
2	D	902	AGS	O2'-C2'	-2.13	1.37	1.43
2	H	901	AGS	O3'-C3'	-2.12	1.37	1.43
2	G	902	AGS	PG-S1G	2.12	1.95	1.90
2	L	901	AGS	C2'-C3'	-2.12	1.47	1.53
2	G	901	AGS	C2'-C3'	-2.12	1.47	1.53
2	F	902	AGS	C2'-C3'	-2.12	1.47	1.53
2	H	901	AGS	C2'-C3'	-2.12	1.47	1.53
2	D	901	AGS	C2'-C3'	-2.11	1.47	1.53
2	H	902	AGS	C2'-C3'	-2.11	1.47	1.53
2	E	901	AGS	O3'-C3'	-2.11	1.37	1.43
2	F	902	AGS	O2'-C2'	-2.10	1.37	1.43
2	H	902	AGS	O2'-C2'	-2.09	1.37	1.43
2	L	901	AGS	O3'-C3'	-2.09	1.37	1.43
2	D	902	AGS	C2-N3	2.09	1.37	1.33
2	K	901	AGS	O3'-C3'	-2.09	1.37	1.43
2	K	902	AGS	O3'-C3'	-2.09	1.37	1.43
2	I	901	AGS	C2'-C3'	-2.08	1.47	1.53
2	G	901	AGS	O3'-C3'	-2.08	1.37	1.43
2	C	901	AGS	PB-O3A	-2.07	1.57	1.59
2	F	901	AGS	C2'-C3'	-2.07	1.47	1.53
2	K	901	AGS	C8-N9	-2.06	1.34	1.37
2	F	902	AGS	C2-N3	2.05	1.37	1.33
2	D	902	AGS	PG-S1G	2.05	1.95	1.90
2	I	902	AGS	PG-S1G	2.05	1.95	1.90
2	C	902	AGS	C2-N3	2.05	1.37	1.33
2	F	901	AGS	O3'-C3'	-2.04	1.37	1.43
2	J	902	AGS	PG-S1G	2.04	1.95	1.90
2	B	902	AGS	O3'-C3'	-2.04	1.37	1.43
2	B	901	AGS	O3'-C3'	-2.03	1.37	1.43
2	A	902	AGS	C3'-C4'	-2.02	1.47	1.53
2	A	901	AGS	C2'-C3'	-2.02	1.47	1.53
2	F	901	AGS	PB-O3A	-2.02	1.57	1.59
2	J	901	AGS	C8-N9	-2.01	1.34	1.37
2	E	901	AGS	C8-N9	-2.00	1.34	1.37

All (227) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	902	AGS	N3-C2-N1	-5.87	119.70	128.58
2	B	901	AGS	C5-C4-N3	-5.84	118.68	126.72
2	J	902	AGS	N3-C2-N1	-5.81	119.79	128.58
2	L	901	AGS	N3-C2-N1	-5.75	119.88	128.58
2	B	902	AGS	N3-C2-N1	-5.69	119.96	128.58
2	G	901	AGS	N3-C2-N1	-5.68	119.98	128.58
2	H	901	AGS	C5-C4-N3	-5.65	118.94	126.72
2	L	902	AGS	N3-C2-N1	-5.63	120.06	128.58
2	H	902	AGS	N3-C2-N1	-5.62	120.07	128.58
2	J	902	AGS	C5-C4-N3	-5.60	119.01	126.72
2	C	902	AGS	N3-C2-N1	-5.58	120.13	128.58
2	G	902	AGS	N3-C2-N1	-5.58	120.14	128.58
2	A	902	AGS	N3-C2-N1	-5.58	120.14	128.58
2	I	902	AGS	N3-C2-N1	-5.57	120.15	128.58
2	E	902	AGS	C5-C4-N3	-5.56	119.06	126.72
2	K	902	AGS	N3-C2-N1	-5.55	120.18	128.58
2	I	902	AGS	C5-C4-N3	-5.55	119.08	126.72
2	A	901	AGS	N3-C2-N1	-5.54	120.20	128.58
2	E	901	AGS	N3-C2-N1	-5.52	120.22	128.58
2	D	901	AGS	N3-C2-N1	-5.52	120.22	128.58
2	K	901	AGS	N3-C2-N1	-5.47	120.31	128.58
2	D	902	AGS	N3-C2-N1	-5.46	120.32	128.58
2	J	901	AGS	N3-C2-N1	-5.44	120.35	128.58
2	C	901	AGS	C5-C4-N3	-5.44	119.23	126.72
2	D	901	AGS	C5-C4-N3	-5.41	119.27	126.72
2	F	901	AGS	N3-C2-N1	-5.40	120.41	128.58
2	L	901	AGS	C5-C4-N3	-5.37	119.32	126.72
2	D	902	AGS	C5-C4-N3	-5.37	119.32	126.72
2	C	901	AGS	N3-C2-N1	-5.36	120.47	128.58
2	H	902	AGS	C5-C4-N3	-5.35	119.35	126.72
2	G	902	AGS	C5-C4-N3	-5.33	119.38	126.72
2	I	901	AGS	N3-C2-N1	-5.32	120.53	128.58
2	C	902	AGS	C5-C4-N3	-5.27	119.46	126.72
2	E	902	AGS	N3-C2-N1	-5.26	120.62	128.58
2	I	901	AGS	C5-C4-N3	-5.24	119.50	126.72
2	H	901	AGS	N3-C2-N1	-5.22	120.68	128.58
2	F	902	AGS	C5-C4-N3	-5.21	119.54	126.72
2	K	901	AGS	C5-C4-N3	-5.18	119.58	126.72
2	K	902	AGS	C5-C4-N3	-5.11	119.67	126.72
2	B	901	AGS	N3-C2-N1	-5.10	120.86	128.58
2	E	901	AGS	C5-C4-N3	-5.05	119.76	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	902	AGS	C5-C4-N3	-5.05	119.77	126.72
2	A	902	AGS	C5-C4-N3	-5.01	119.81	126.72
2	G	901	AGS	C5-C4-N3	-5.00	119.83	126.72
2	B	902	AGS	C5-C4-N3	-4.94	119.92	126.72
2	F	901	AGS	C5-C4-N3	-4.88	119.99	126.72
2	A	901	AGS	C5-C4-N3	-4.86	120.02	126.72
2	J	901	AGS	C5-C4-N3	-4.84	120.05	126.72
2	J	902	AGS	N3-C4-N9	4.64	135.06	127.17
2	B	901	AGS	N3-C4-N9	4.63	135.04	127.17
2	I	902	AGS	N3-C4-N9	4.58	134.96	127.17
2	C	901	AGS	N3-C4-N9	4.55	134.91	127.17
2	J	902	AGS	PB-O3B-PG	-4.53	116.60	133.17
2	C	902	AGS	N3-C4-N9	4.48	134.79	127.17
2	L	901	AGS	N3-C4-N9	4.47	134.78	127.17
2	E	901	AGS	N3-C4-N9	4.46	134.75	127.17
2	D	902	AGS	N3-C4-N9	4.45	134.74	127.17
2	I	901	AGS	N3-C4-N9	4.36	134.58	127.17
2	A	901	AGS	N3-C4-N9	4.36	134.58	127.17
2	H	901	AGS	N3-C4-N9	4.36	134.58	127.17
2	F	902	AGS	N3-C4-N9	4.35	134.56	127.17
2	K	901	AGS	N3-C4-N9	4.33	134.53	127.17
2	H	902	AGS	N3-C4-N9	4.33	134.53	127.17
2	G	901	AGS	N3-C4-N9	4.31	134.50	127.17
2	E	902	AGS	N3-C4-N9	4.29	134.47	127.17
2	D	901	AGS	N3-C4-N9	4.29	134.47	127.17
2	G	902	AGS	N3-C4-N9	4.29	134.46	127.17
2	F	901	AGS	N3-C4-N9	4.19	134.29	127.17
2	K	902	AGS	N3-C4-N9	4.15	134.22	127.17
2	L	902	AGS	N3-C4-N9	4.07	134.09	127.17
2	A	902	AGS	N3-C4-N9	4.03	134.03	127.17
2	J	901	AGS	N3-C4-N9	4.00	133.97	127.17
2	L	902	AGS	C5-N7-C8	3.94	109.64	103.45
2	B	901	AGS	PB-O3B-PG	-3.92	118.84	133.17
2	B	902	AGS	N3-C4-N9	3.91	133.82	127.17
2	L	901	AGS	PB-O3B-PG	-3.88	118.97	133.17
2	K	902	AGS	C5-N7-C8	3.88	109.55	103.45
2	C	901	AGS	PB-O3B-PG	-3.88	118.98	133.17
2	J	902	AGS	C2-N3-C4	3.88	121.30	111.83
2	A	902	AGS	C5-N7-C8	3.86	109.52	103.45
2	F	902	AGS	C5-N7-C8	3.86	109.52	103.45
2	H	901	AGS	C5-N7-C8	3.85	109.49	103.45
2	D	902	AGS	C5-N7-C8	3.83	109.47	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	901	AGS	C5-N7-C8	3.83	109.47	103.45
2	H	901	AGS	PB-O3B-PG	-3.81	119.24	133.17
2	H	902	AGS	C5-N7-C8	3.79	109.41	103.45
2	F	902	AGS	C2-N3-C4	3.78	121.06	111.83
2	B	902	AGS	PB-O3B-PG	-3.77	119.37	133.17
2	G	902	AGS	PB-O3B-PG	-3.76	119.39	133.17
2	I	902	AGS	C5-N7-C8	3.76	109.36	103.45
2	E	902	AGS	C5-N7-C8	3.76	109.36	103.45
2	I	902	AGS	C2-N3-C4	3.75	120.98	111.83
2	C	902	AGS	C5-N7-C8	3.74	109.33	103.45
2	K	901	AGS	C5-N7-C8	3.74	109.32	103.45
2	E	901	AGS	C5-N7-C8	3.70	109.27	103.45
2	B	901	AGS	C2-N3-C4	3.70	120.86	111.83
2	H	901	AGS	C2-N3-C4	3.69	120.85	111.83
2	C	902	AGS	C2-N3-C4	3.69	120.84	111.83
2	B	902	AGS	C5-N7-C8	3.67	109.22	103.45
2	H	902	AGS	C2-N3-C4	3.67	120.79	111.83
2	L	901	AGS	C2-N3-C4	3.66	120.78	111.83
2	G	901	AGS	C5-N7-C8	3.66	109.20	103.45
2	G	902	AGS	C5-N7-C8	3.66	109.19	103.45
2	G	902	AGS	C2-N3-C4	3.65	120.75	111.83
2	I	901	AGS	C5-N7-C8	3.65	109.18	103.45
2	D	901	AGS	C2-N3-C4	3.64	120.71	111.83
2	F	901	AGS	C5-N7-C8	3.63	109.16	103.45
2	B	901	AGS	C5-N7-C8	3.63	109.15	103.45
2	J	901	AGS	C5-N7-C8	3.63	109.15	103.45
2	K	902	AGS	PB-O3B-PG	-3.63	119.90	133.17
2	G	901	AGS	C2-N3-C4	3.62	120.68	111.83
2	E	902	AGS	C2-N3-C4	3.61	120.66	111.83
2	H	902	AGS	PB-O3B-PG	-3.61	119.94	133.17
2	L	902	AGS	PB-O3B-PG	-3.60	119.98	133.17
2	A	902	AGS	C2-N3-C4	3.59	120.59	111.83
2	C	901	AGS	C5-N7-C8	3.58	109.08	103.45
2	I	901	AGS	C2-N3-C4	3.58	120.57	111.83
2	D	902	AGS	C2-N3-C4	3.58	120.56	111.83
2	C	901	AGS	C2-N3-C4	3.57	120.54	111.83
2	J	902	AGS	C5-N7-C8	3.57	109.05	103.45
2	B	902	AGS	C2-N3-C4	3.56	120.52	111.83
2	L	902	AGS	C2-N3-C4	3.55	120.50	111.83
2	A	901	AGS	C2-N3-C4	3.55	120.49	111.83
2	K	902	AGS	C2-N3-C4	3.54	120.48	111.83
2	L	901	AGS	C5-N7-C8	3.54	109.01	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	902	AGS	PB-O3B-PG	-3.53	120.24	133.17
2	K	901	AGS	C2-N3-C4	3.52	120.43	111.83
2	E	901	AGS	C2-N3-C4	3.52	120.42	111.83
2	G	901	AGS	PB-O3B-PG	-3.46	120.50	133.17
2	A	901	AGS	C5-N7-C8	3.46	108.89	103.45
2	J	901	AGS	C2-N3-C4	3.44	120.23	111.83
2	F	901	AGS	PB-O3B-PG	-3.39	120.78	133.17
2	A	901	AGS	PB-O3B-PG	-3.39	120.78	133.17
2	F	901	AGS	C2-N3-C4	3.31	119.91	111.83
2	K	901	AGS	PB-O3B-PG	-3.28	121.18	133.17
2	H	901	AGS	C4-C5-N7	-3.18	106.94	110.58
2	L	902	AGS	C4-C5-N7	-3.15	106.98	110.58
2	D	901	AGS	PB-O3B-PG	-3.12	121.76	133.17
2	E	902	AGS	C4-C5-N7	-3.12	107.02	110.58
2	G	901	AGS	N9-C8-N7	-3.10	109.54	113.94
2	A	902	AGS	C4-C5-N7	-3.06	107.08	110.58
2	E	901	AGS	N9-C8-N7	-3.05	109.61	113.94
2	K	902	AGS	C4-C5-N7	-3.05	107.10	110.58
2	D	901	AGS	C4-C5-N7	-2.99	107.16	110.58
2	I	901	AGS	PB-O3B-PG	-2.98	122.26	133.17
2	E	901	AGS	PB-O3B-PG	-2.95	122.38	133.17
2	F	902	AGS	N9-C8-N7	-2.94	109.77	113.94
2	H	902	AGS	C4-C5-N7	-2.94	107.22	110.58
2	B	902	AGS	C4-C5-N7	-2.93	107.23	110.58
2	K	902	AGS	N9-C8-N7	-2.93	109.78	113.94
2	F	901	AGS	N9-C8-N7	-2.93	109.78	113.94
2	A	901	AGS	N9-C8-N7	-2.90	109.83	113.94
2	J	901	AGS	N9-C8-N7	-2.89	109.83	113.94
2	D	902	AGS	C4-C5-N7	-2.89	107.28	110.58
2	K	901	AGS	C4-C5-N7	-2.89	107.28	110.58
2	J	901	AGS	C4-C5-N7	-2.87	107.30	110.58
2	F	902	AGS	PB-O3B-PG	-2.87	122.66	133.17
2	A	902	AGS	N9-C8-N7	-2.85	109.89	113.94
2	I	902	AGS	C4-C5-N7	-2.85	107.32	110.58
2	A	902	AGS	PB-O3B-PG	-2.84	122.76	133.17
2	L	902	AGS	N9-C8-N7	-2.84	109.90	113.94
2	B	901	AGS	C4-C5-N7	-2.83	107.35	110.58
2	J	901	AGS	PB-O3B-PG	-2.83	122.83	133.17
2	I	901	AGS	N9-C8-N7	-2.82	109.94	113.94
2	G	902	AGS	C4-C5-N7	-2.81	107.37	110.58
2	I	902	AGS	PB-O3B-PG	-2.80	122.91	133.17
2	I	901	AGS	C4-C5-N7	-2.79	107.39	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	902	AGS	C4-C5-N7	-2.78	107.40	110.58
2	K	901	AGS	N9-C8-N7	-2.77	110.00	113.94
2	F	902	AGS	C4-C5-N7	-2.76	107.42	110.58
2	C	902	AGS	N9-C8-N7	-2.75	110.04	113.94
2	E	902	AGS	PB-O3B-PG	-2.74	123.15	133.17
2	E	901	AGS	O4'-C4'-C3'	2.72	110.56	105.15
2	E	901	AGS	C4-C5-N7	-2.72	107.48	110.58
2	H	901	AGS	N9-C8-N7	-2.70	110.11	113.94
2	H	901	AGS	C3'-C2'-C1'	2.69	106.55	101.46
2	C	902	AGS	PB-O3B-PG	-2.68	123.36	133.17
2	B	902	AGS	N9-C8-N7	-2.67	110.14	113.94
2	D	901	AGS	N9-C8-N7	-2.66	110.16	113.94
2	I	901	AGS	O4'-C4'-C3'	2.63	110.37	105.15
2	H	902	AGS	N9-C8-N7	-2.62	110.21	113.94
2	J	901	AGS	O4'-C4'-C3'	2.61	110.34	105.15
2	D	902	AGS	N9-C8-N7	-2.61	110.23	113.94
2	C	901	AGS	N9-C8-N7	-2.59	110.27	113.94
2	G	901	AGS	C4-C5-N7	-2.55	107.66	110.58
2	I	902	AGS	N9-C8-N7	-2.55	110.32	113.94
2	L	901	AGS	N9-C8-N7	-2.54	110.34	113.94
2	F	901	AGS	C4-C5-N7	-2.54	107.68	110.58
2	C	901	AGS	C3'-C2'-C1'	2.51	106.22	101.46
2	C	901	AGS	C4-C5-N7	-2.50	107.72	110.58
2	B	901	AGS	C3'-C2'-C1'	2.48	106.16	101.46
2	G	902	AGS	N9-C8-N7	-2.47	110.42	113.94
2	B	901	AGS	N9-C8-N7	-2.47	110.43	113.94
2	J	902	AGS	N9-C8-N7	-2.47	110.43	113.94
2	G	901	AGS	O4'-C4'-C3'	2.46	110.05	105.15
2	F	901	AGS	O4'-C4'-C3'	2.44	110.00	105.15
2	L	901	AGS	C4-C5-N7	-2.43	107.80	110.58
2	J	902	AGS	C4-C5-N7	-2.43	107.81	110.58
2	A	901	AGS	C4-C5-N7	-2.41	107.83	110.58
2	L	901	AGS	O4'-C4'-C3'	2.41	109.93	105.15
2	A	901	AGS	O4'-C4'-C3'	2.38	109.87	105.15
2	H	901	AGS	O4'-C4'-C3'	2.35	109.81	105.15
2	K	902	AGS	O4'-C4'-C3'	2.33	109.78	105.15
2	C	901	AGS	O4'-C4'-C3'	2.33	109.78	105.15
2	E	902	AGS	N9-C8-N7	-2.33	110.63	113.94
2	E	901	AGS	C4-N9-C8	2.30	108.15	105.74
2	I	902	AGS	C3'-C2'-C1'	2.28	105.77	101.46
2	L	901	AGS	C3'-C2'-C1'	2.26	105.75	101.46
2	E	901	AGS	C3'-C2'-C1'	2.24	105.71	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	902	AGS	O2B-PB-O3A	2.23	113.30	107.27
2	C	902	AGS	O3G-PG-O3B	2.22	112.07	104.64
2	F	902	AGS	O4'-C4'-C3'	2.22	109.55	105.15
2	A	901	AGS	C4-N9-C8	2.20	108.05	105.74
2	J	901	AGS	C3'-C2'-C1'	2.20	105.62	101.46
2	F	901	AGS	C3'-C2'-C1'	2.19	105.61	101.46
2	I	902	AGS	O4'-C4'-C3'	2.17	109.46	105.15
2	G	902	AGS	O4'-C4'-C3'	2.16	109.44	105.15
2	L	901	AGS	O4'-C1'-N9	2.16	112.23	108.09
2	B	902	AGS	O4'-C4'-C3'	2.15	109.42	105.15
2	I	901	AGS	C3'-C2'-C1'	2.13	105.48	101.46
2	A	902	AGS	O4'-C4'-C3'	2.12	109.35	105.15
2	K	901	AGS	O4'-C4'-C3'	2.12	109.35	105.15
2	B	902	AGS	C3'-C2'-C1'	2.10	105.44	101.46
2	H	902	AGS	O4'-C4'-C3'	2.09	109.30	105.15
2	G	901	AGS	C4-N9-C8	2.08	107.93	105.74
2	B	902	AGS	C2-N1-C6	2.08	122.15	118.73
2	D	902	AGS	O3G-PG-O3B	2.05	111.47	104.64

There are no chirality outliers.

All (100) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	902	AGS	PB-O3B-PG-O2G
2	A	902	AGS	PB-O3B-PG-O3G
2	A	902	AGS	C5'-O5'-PA-O1A
2	A	902	AGS	C5'-O5'-PA-O2A
2	A	902	AGS	C5'-O5'-PA-O3A
2	B	902	AGS	PB-O3B-PG-O2G
2	B	902	AGS	PB-O3B-PG-O3G
2	C	901	AGS	PB-O3B-PG-O2G
2	C	901	AGS	C5'-O5'-PA-O1A
2	C	901	AGS	C5'-O5'-PA-O2A
2	C	901	AGS	C5'-O5'-PA-O3A
2	C	902	AGS	C5'-O5'-PA-O1A
2	C	902	AGS	C5'-O5'-PA-O2A
2	C	902	AGS	C5'-O5'-PA-O3A
2	D	902	AGS	C5'-O5'-PA-O1A
2	D	902	AGS	C5'-O5'-PA-O2A
2	D	902	AGS	C5'-O5'-PA-O3A
2	E	902	AGS	PB-O3B-PG-O2G
2	E	902	AGS	PB-O3B-PG-O3G

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Mol	Chain	Res	Type	Atoms
2	E	902	AGS	C5'-O5'-PA-O1A
2	E	902	AGS	C5'-O5'-PA-O2A
2	E	902	AGS	C5'-O5'-PA-O3A
2	F	901	AGS	C5'-O5'-PA-O2A
2	F	901	AGS	C5'-O5'-PA-O3A
2	F	902	AGS	PB-O3B-PG-O2G
2	F	902	AGS	C5'-O5'-PA-O1A
2	F	902	AGS	C5'-O5'-PA-O2A
2	F	902	AGS	C5'-O5'-PA-O3A
2	G	902	AGS	PB-O3B-PG-O2G
2	G	902	AGS	PB-O3B-PG-O3G
2	G	902	AGS	C5'-O5'-PA-O1A
2	G	902	AGS	C5'-O5'-PA-O2A
2	G	902	AGS	C5'-O5'-PA-O3A
2	H	902	AGS	PB-O3B-PG-O2G
2	H	902	AGS	PB-O3B-PG-O3G
2	I	901	AGS	PB-O3B-PG-O2G
2	I	902	AGS	C5'-O5'-PA-O3A
2	J	902	AGS	C5'-O5'-PA-O3A
2	K	902	AGS	PB-O3B-PG-O2G
2	K	902	AGS	PB-O3B-PG-O3G
2	L	901	AGS	C5'-O5'-PA-O1A
2	L	901	AGS	C5'-O5'-PA-O2A
2	L	901	AGS	C5'-O5'-PA-O3A
2	L	902	AGS	PB-O3B-PG-O2G
2	L	902	AGS	PB-O3B-PG-O3G
2	L	902	AGS	C5'-O5'-PA-O1A
2	L	902	AGS	C5'-O5'-PA-O2A
2	L	902	AGS	C5'-O5'-PA-O3A
2	I	902	AGS	O4'-C4'-C5'-O5'
2	I	902	AGS	C3'-C4'-C5'-O5'
2	L	902	AGS	PG-O3B-PB-O1B
2	H	902	AGS	O4'-C4'-C5'-O5'
2	K	902	AGS	O4'-C4'-C5'-O5'
2	H	901	AGS	O4'-C4'-C5'-O5'
2	A	901	AGS	PG-O3B-PB-O1B
2	A	902	AGS	PB-O3A-PA-O1A
2	C	902	AGS	PB-O3A-PA-O2A
2	G	902	AGS	PB-O3A-PA-O1A
2	H	902	AGS	PA-O3A-PB-O2B
2	J	902	AGS	PA-O3A-PB-O2B
2	L	902	AGS	PB-O3A-PA-O1A

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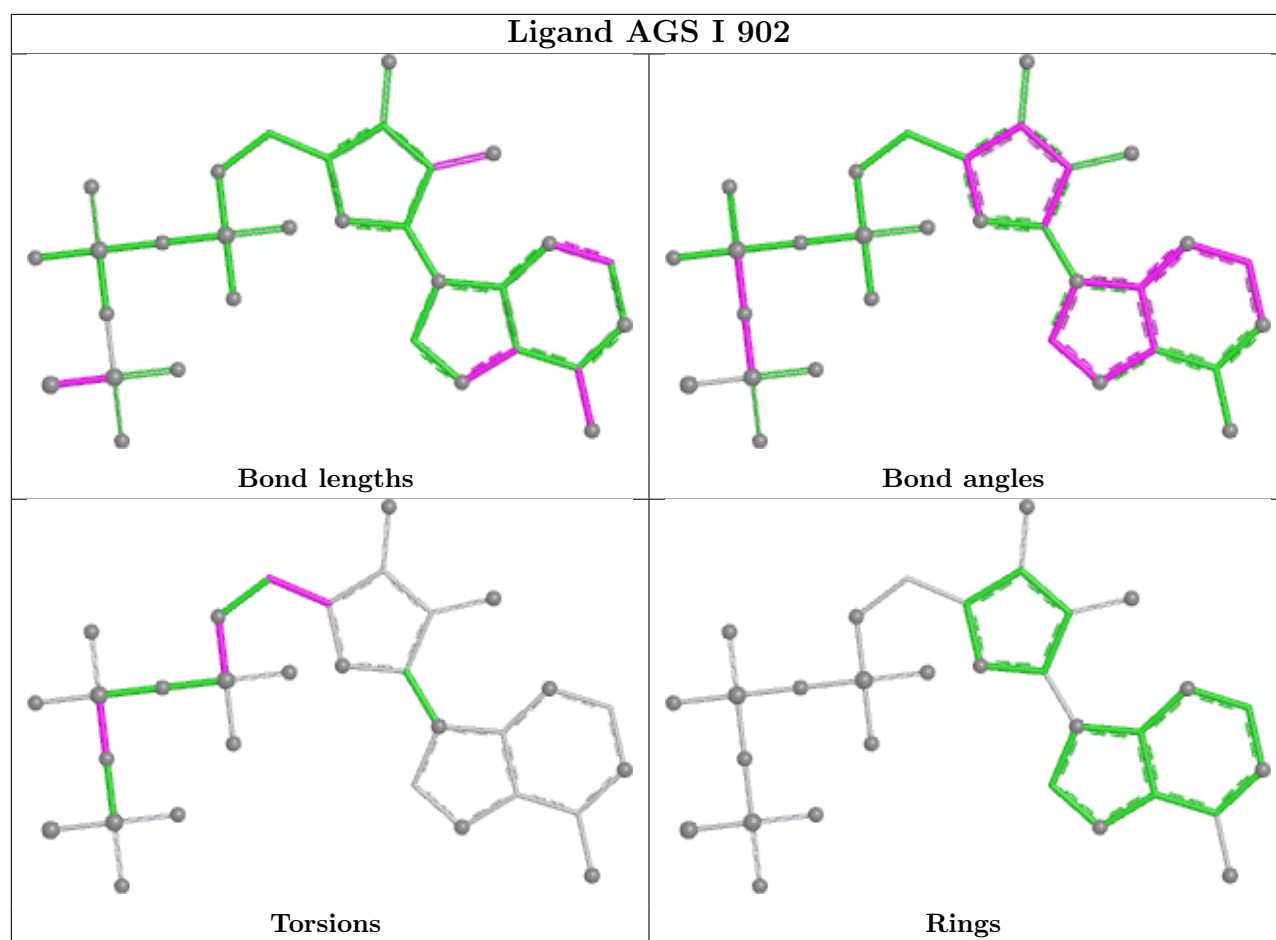
Mol	Chain	Res	Type	Atoms
2	B	901	AGS	C5'-O5'-PA-O1A
2	I	902	AGS	C5'-O5'-PA-O1A
2	J	902	AGS	C5'-O5'-PA-O1A
2	J	902	AGS	C5'-O5'-PA-O2A
2	G	901	AGS	PG-O3B-PB-O2B
2	G	901	AGS	O4'-C4'-C5'-O5'
2	H	901	AGS	PA-O3A-PB-O2B
2	J	901	AGS	PA-O3A-PB-O2B
2	K	902	AGS	PA-O3A-PB-O2B
2	K	902	AGS	C3'-C4'-C5'-O5'
2	G	902	AGS	PG-O3B-PB-O2B
2	H	901	AGS	PG-O3B-PB-O2B
2	I	902	AGS	PG-O3B-PB-O2B
2	G	902	AGS	O4'-C4'-C5'-O5'
2	I	901	AGS	PA-O3A-PB-O1B
2	K	901	AGS	PA-O3A-PB-O1B
2	K	901	AGS	PA-O3A-PB-O2B
2	F	902	AGS	PB-O3B-PG-O3G
2	I	901	AGS	PB-O3B-PG-O3G
2	L	901	AGS	PB-O3B-PG-O2G
2	G	902	AGS	C3'-C4'-C5'-O5'
2	C	902	AGS	C2'-C1'-N9-C8
2	A	901	AGS	PG-O3B-PB-O2B
2	C	902	AGS	PG-O3B-PB-O2B
2	F	902	AGS	PG-O3B-PB-O2B
2	J	901	AGS	PG-O3B-PB-O2B
2	L	902	AGS	PG-O3B-PB-O2B
2	C	901	AGS	PB-O3A-PA-O2A
2	D	902	AGS	PA-O3A-PB-O2B
2	H	901	AGS	PA-O3A-PB-O1B
2	J	901	AGS	PA-O3A-PB-O1B
2	K	902	AGS	PA-O3A-PB-O1B
2	E	901	AGS	O4'-C4'-C5'-O5'
2	A	902	AGS	PB-O3A-PA-O2A
2	B	902	AGS	PA-O3A-PB-O2B
2	E	902	AGS	PB-O3A-PA-O2A
2	F	902	AGS	PB-O3A-PA-O2A
2	G	902	AGS	PB-O3A-PA-O2A
2	A	902	AGS	O4'-C4'-C5'-O5'

There are no ring outliers.

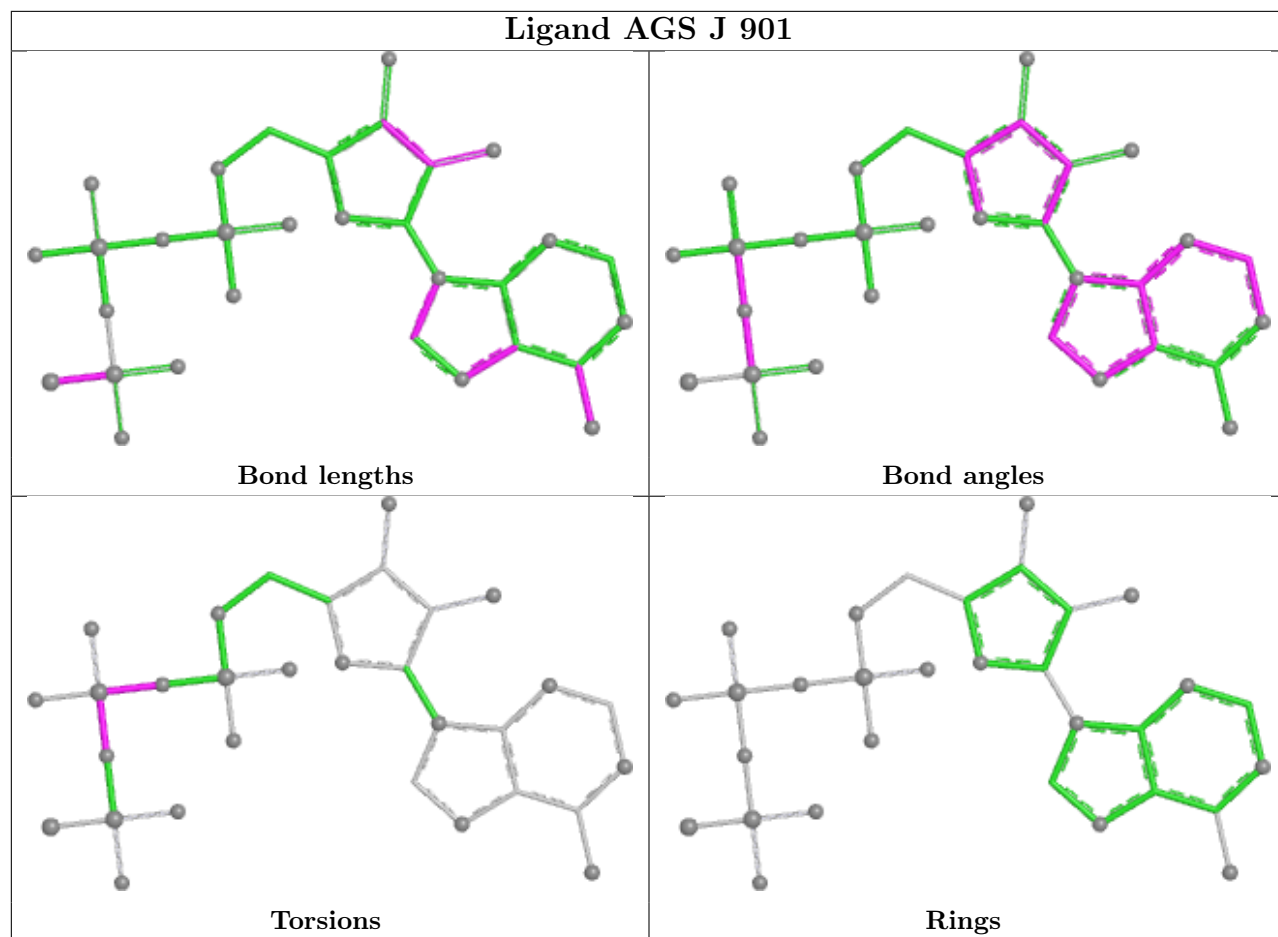
19 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	902	AGS	2	0
2	J	901	AGS	2	0
2	G	902	AGS	1	0
2	L	902	AGS	2	0
2	F	902	AGS	1	0
2	J	902	AGS	2	0
2	C	901	AGS	2	0
2	K	902	AGS	1	0
2	I	901	AGS	2	0
2	C	902	AGS	1	0
2	L	901	AGS	2	0
2	E	902	AGS	1	0
2	B	902	AGS	1	0
2	K	901	AGS	1	0
2	F	901	AGS	5	0
2	H	901	AGS	1	0
2	G	901	AGS	1	0
2	E	901	AGS	2	0
2	B	901	AGS	3	0

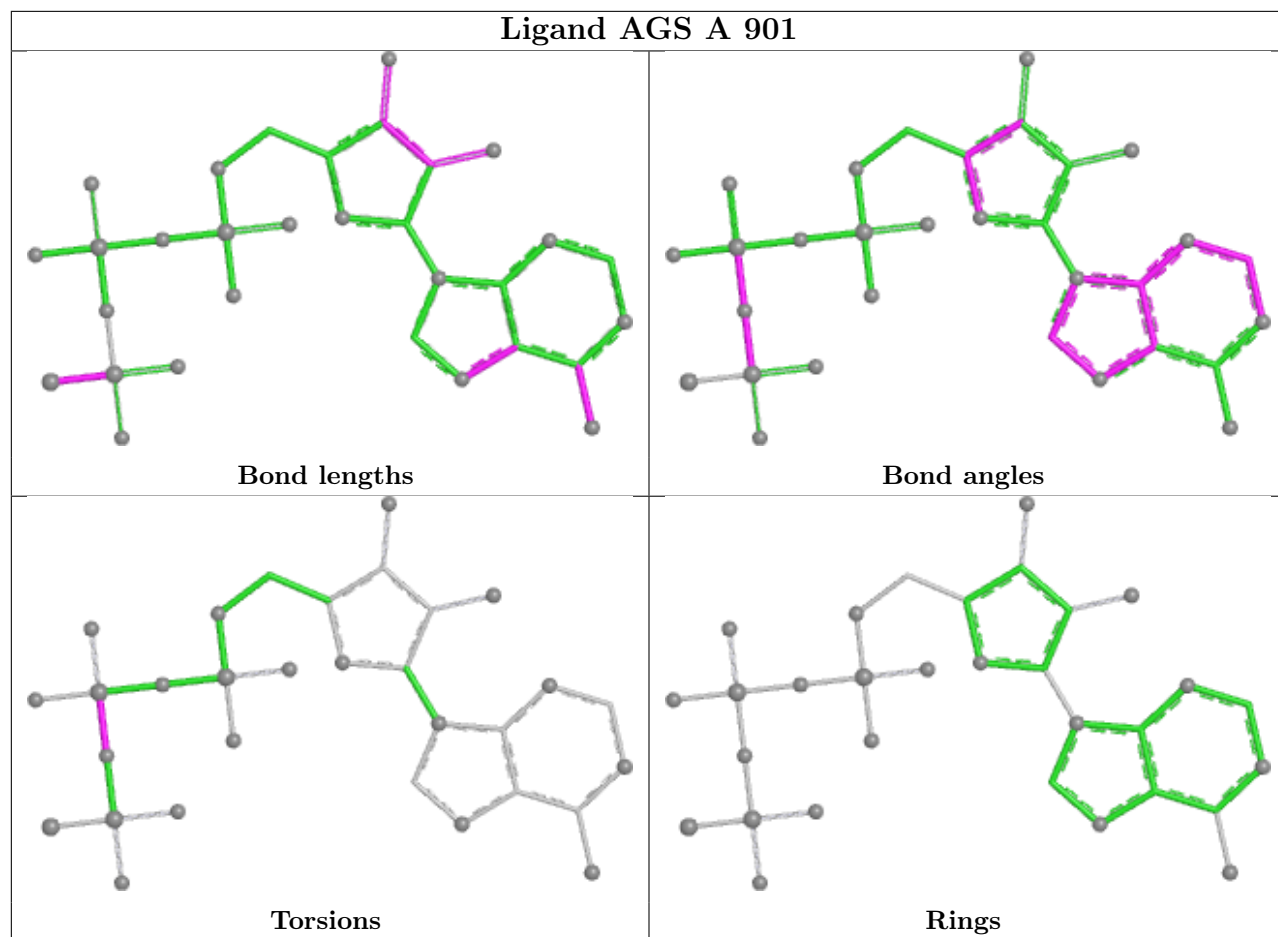
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

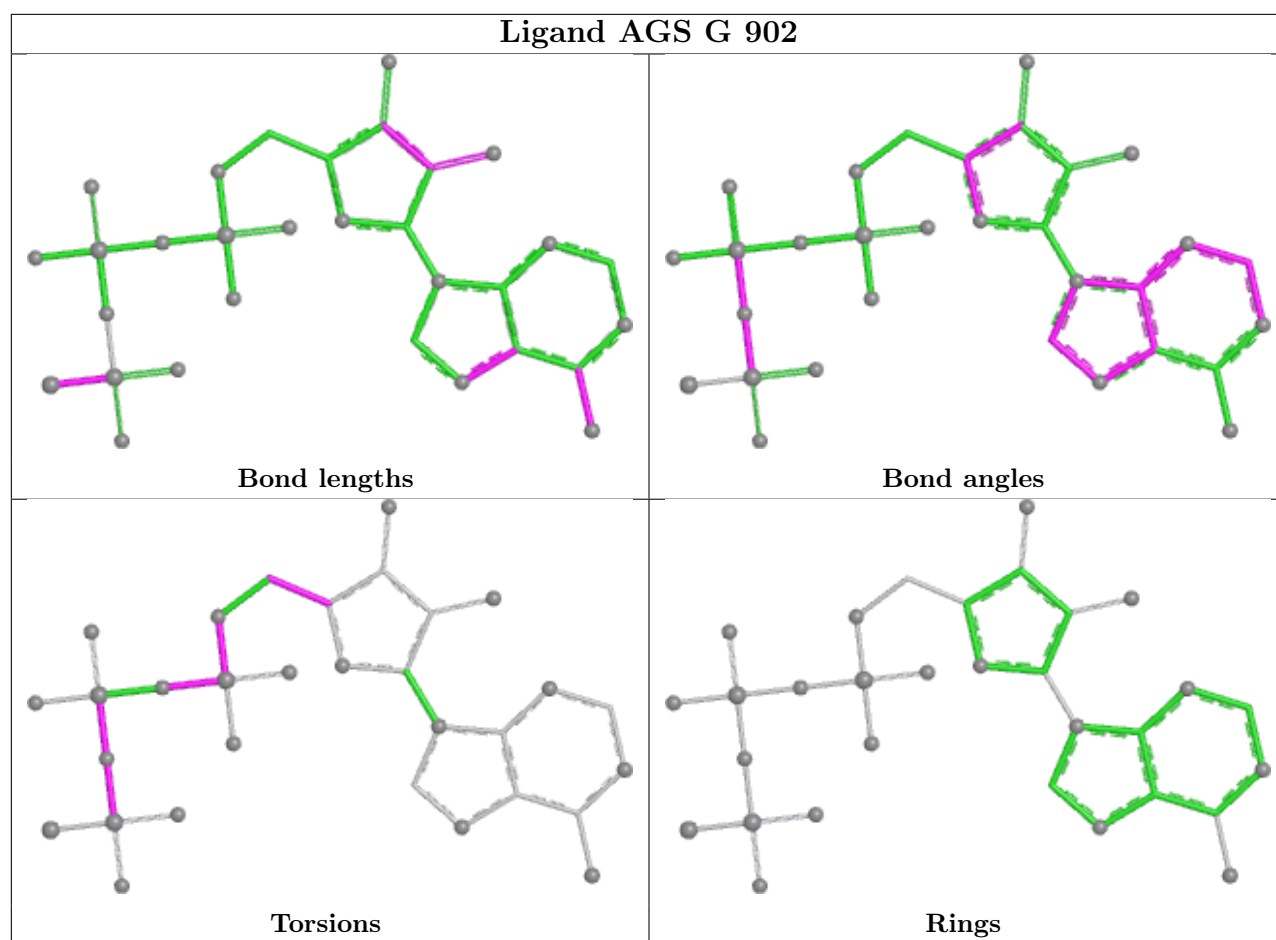


Ligand AGS J 901

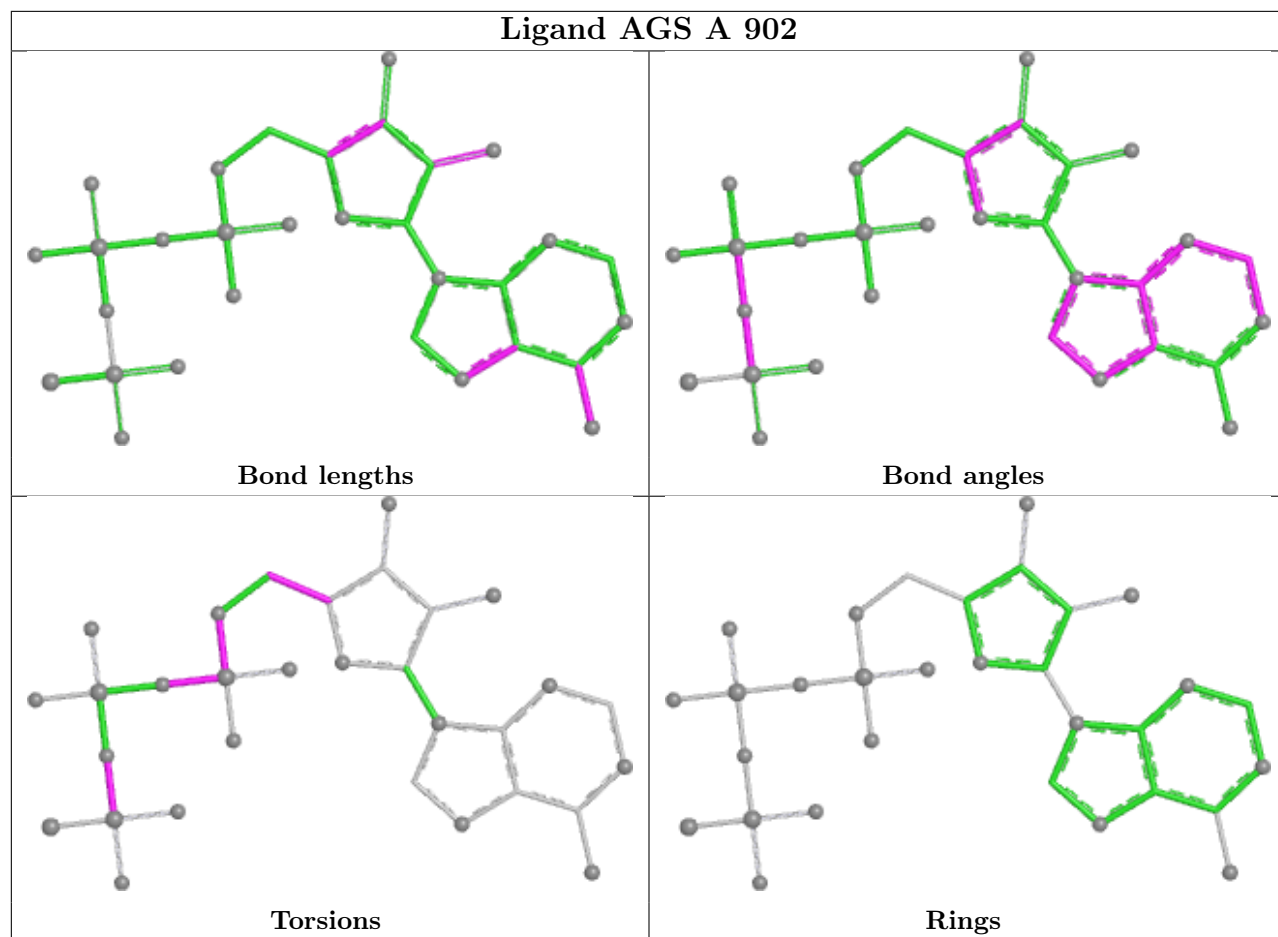


Ligand AGS A 901

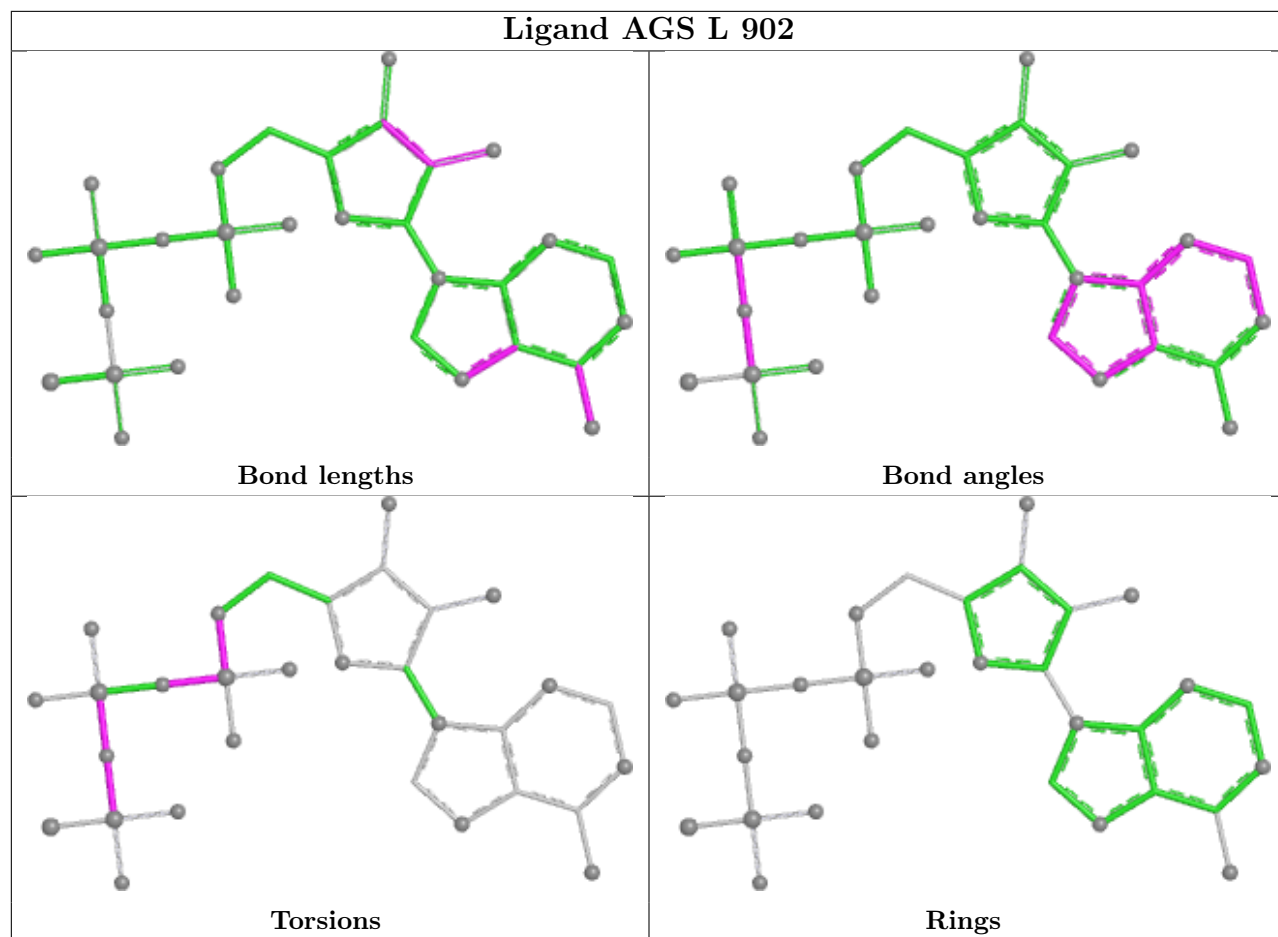




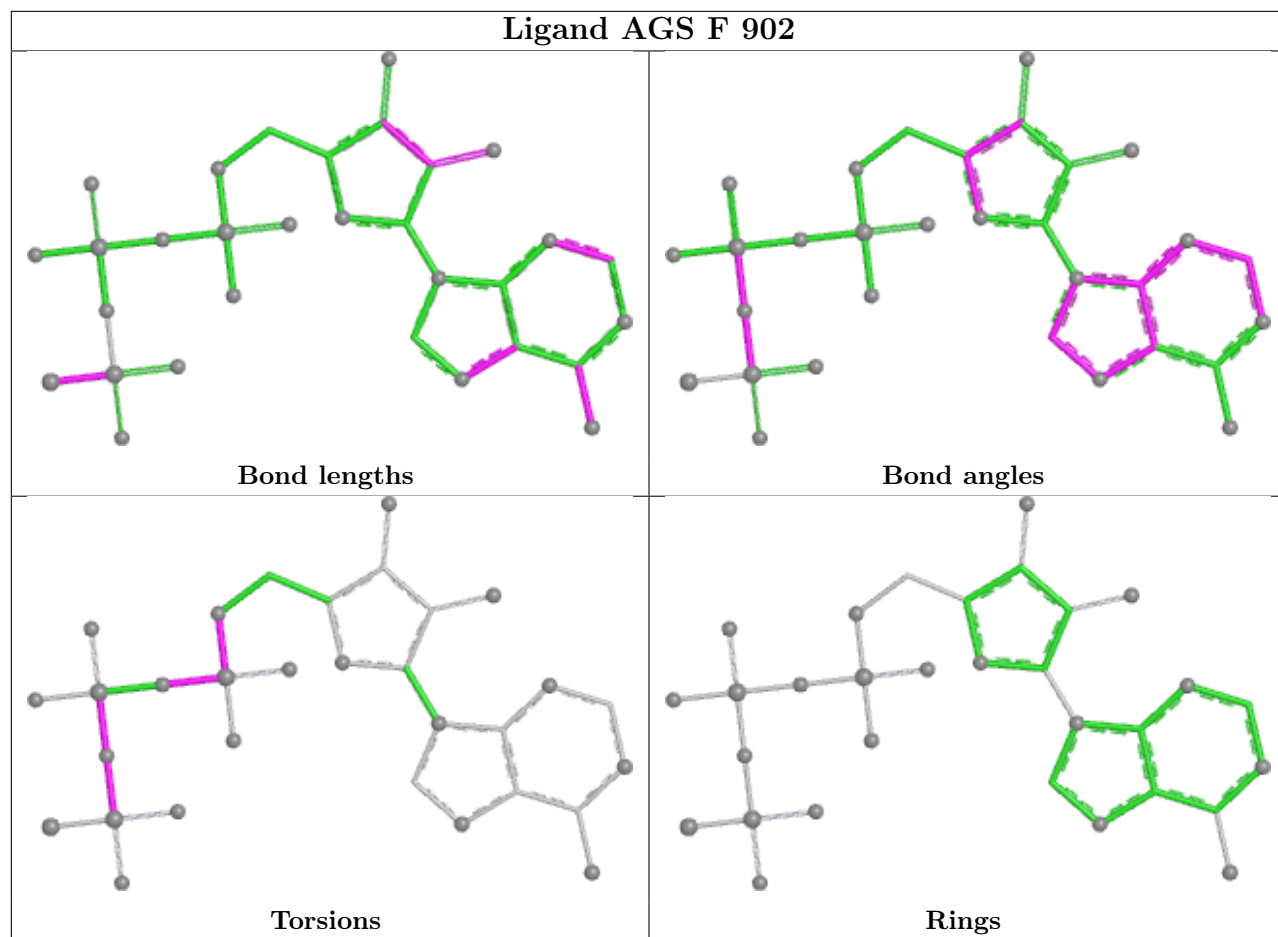
Ligand AGS A 902



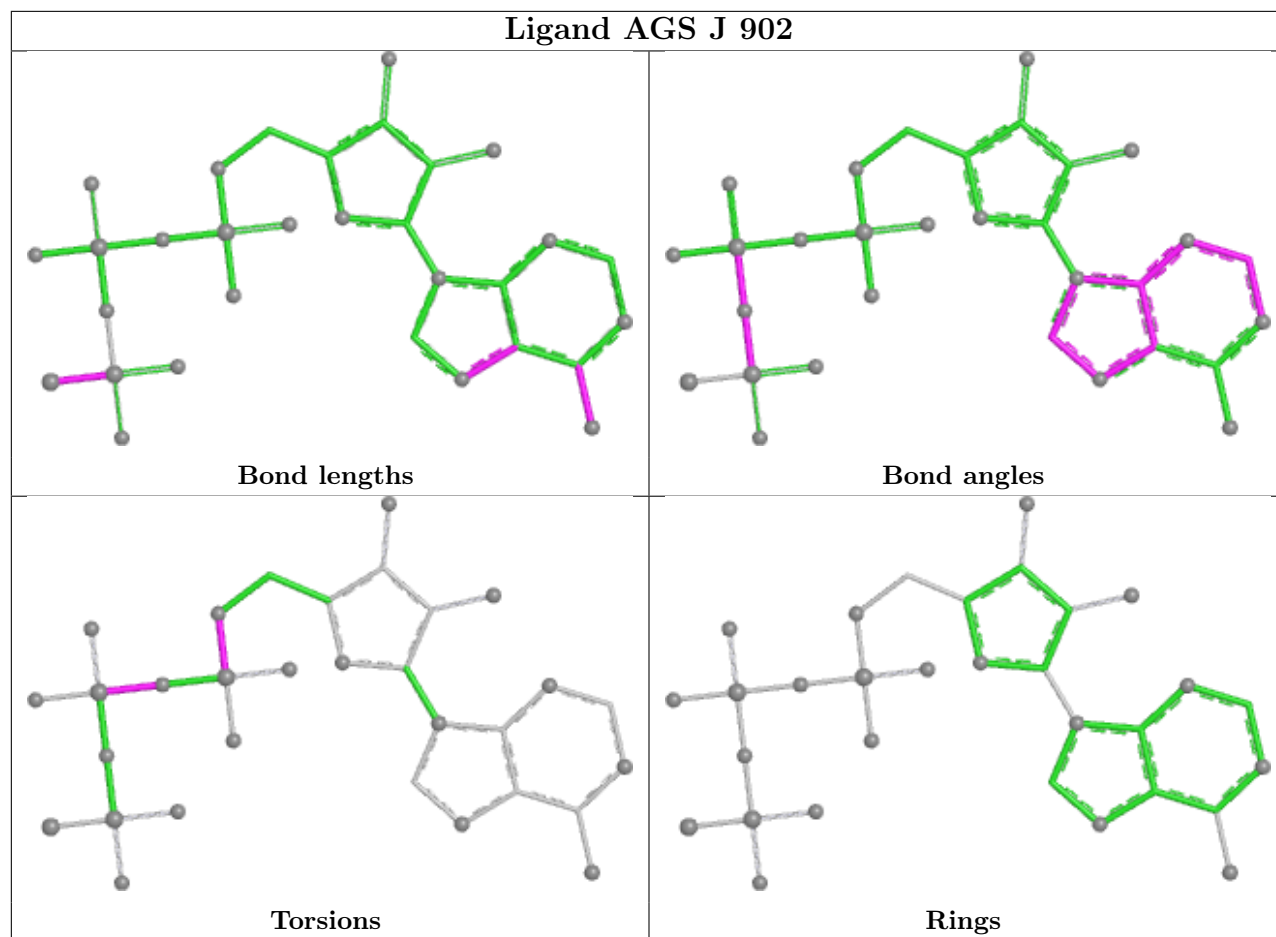
Ligand AGS L 902

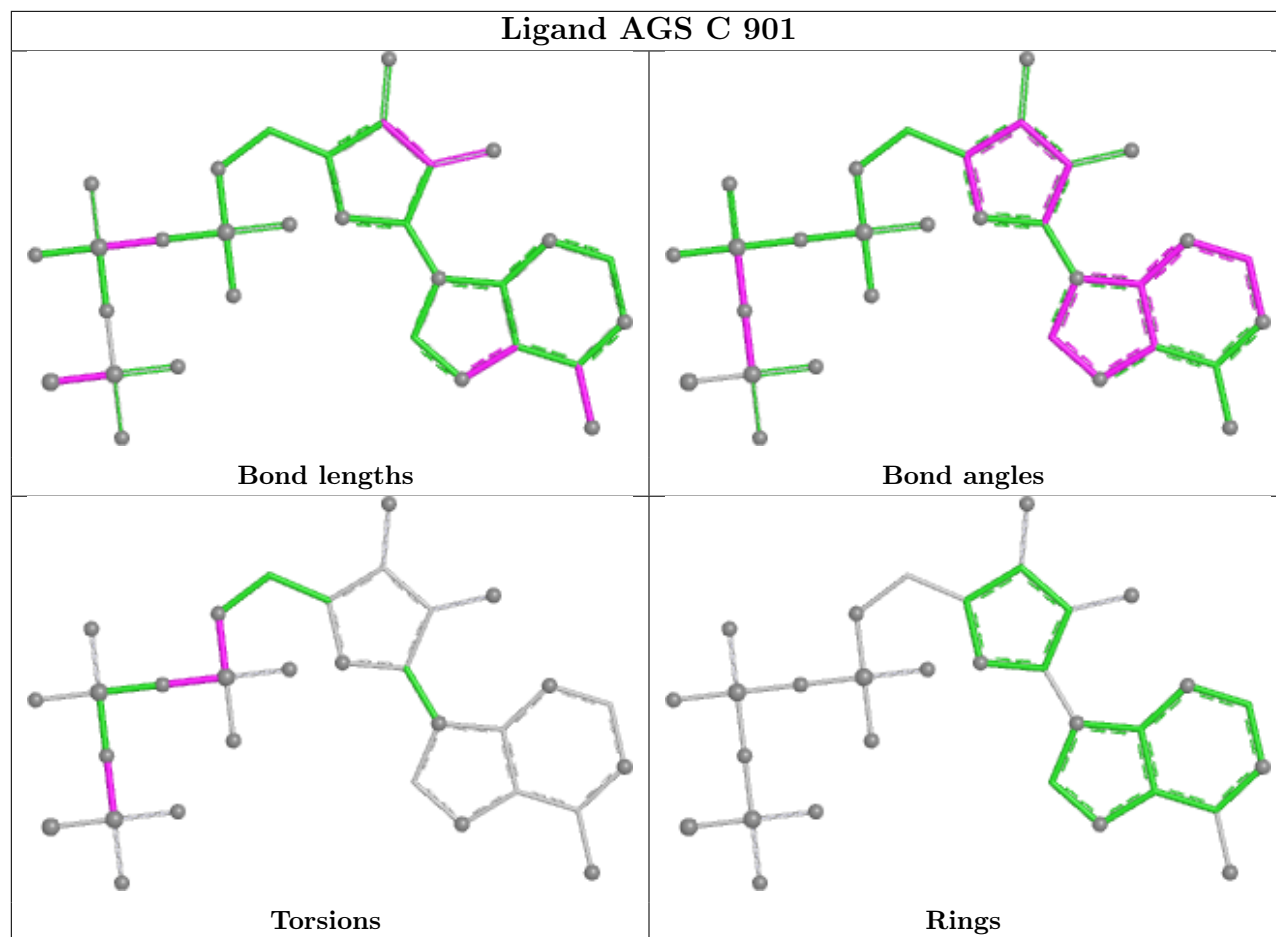


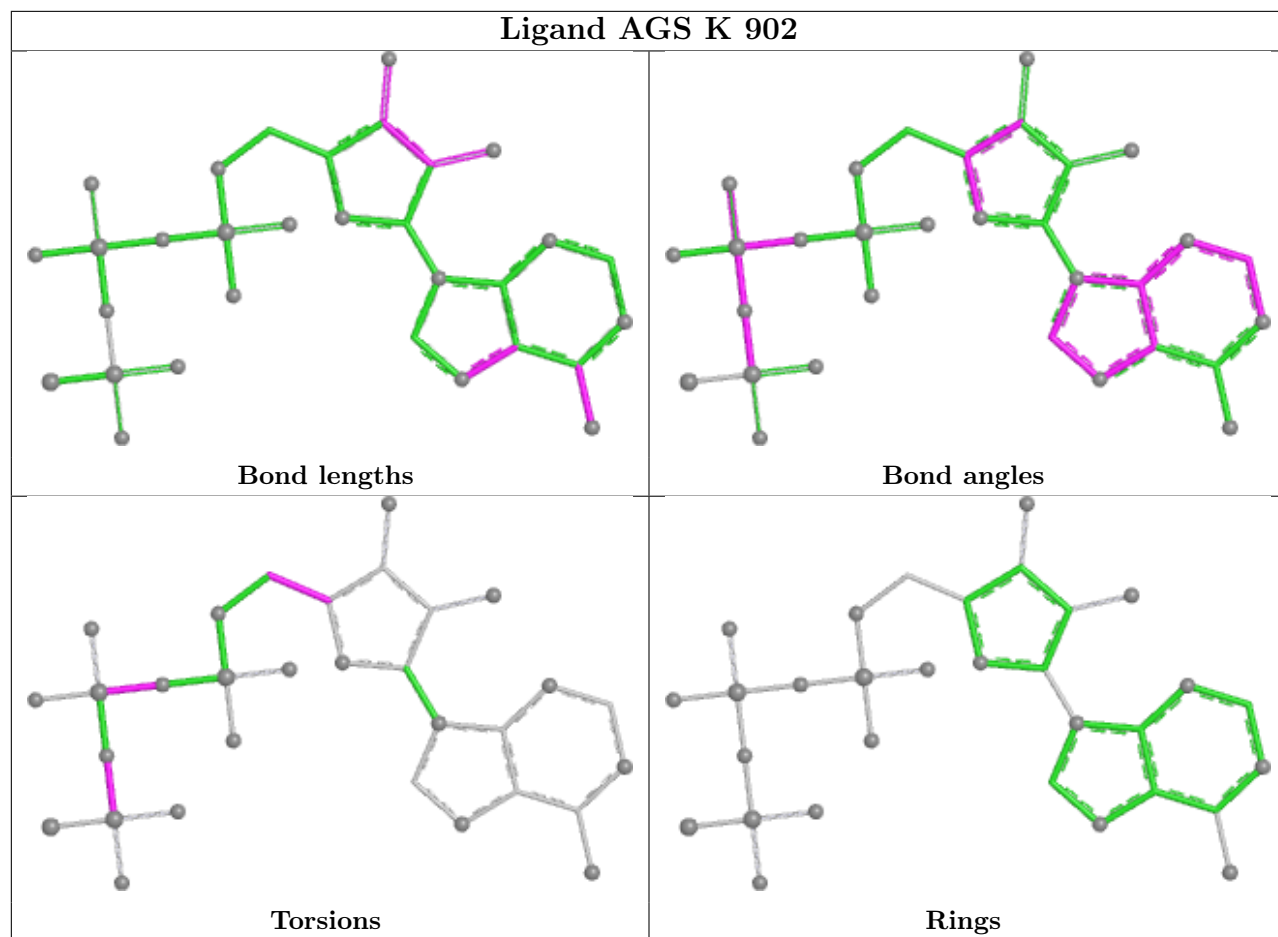
Ligand AGS F 902



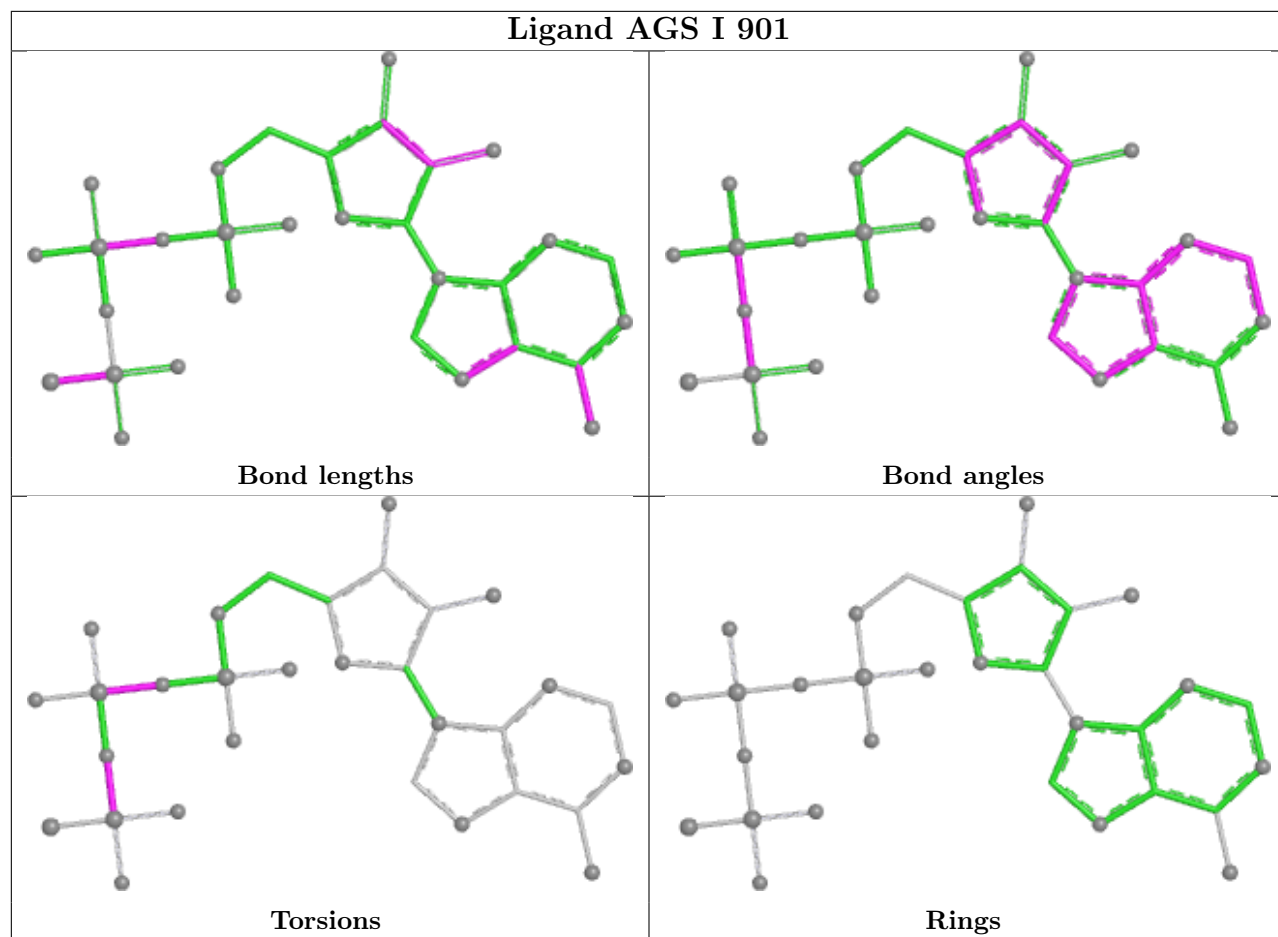
Ligand AGS J 902



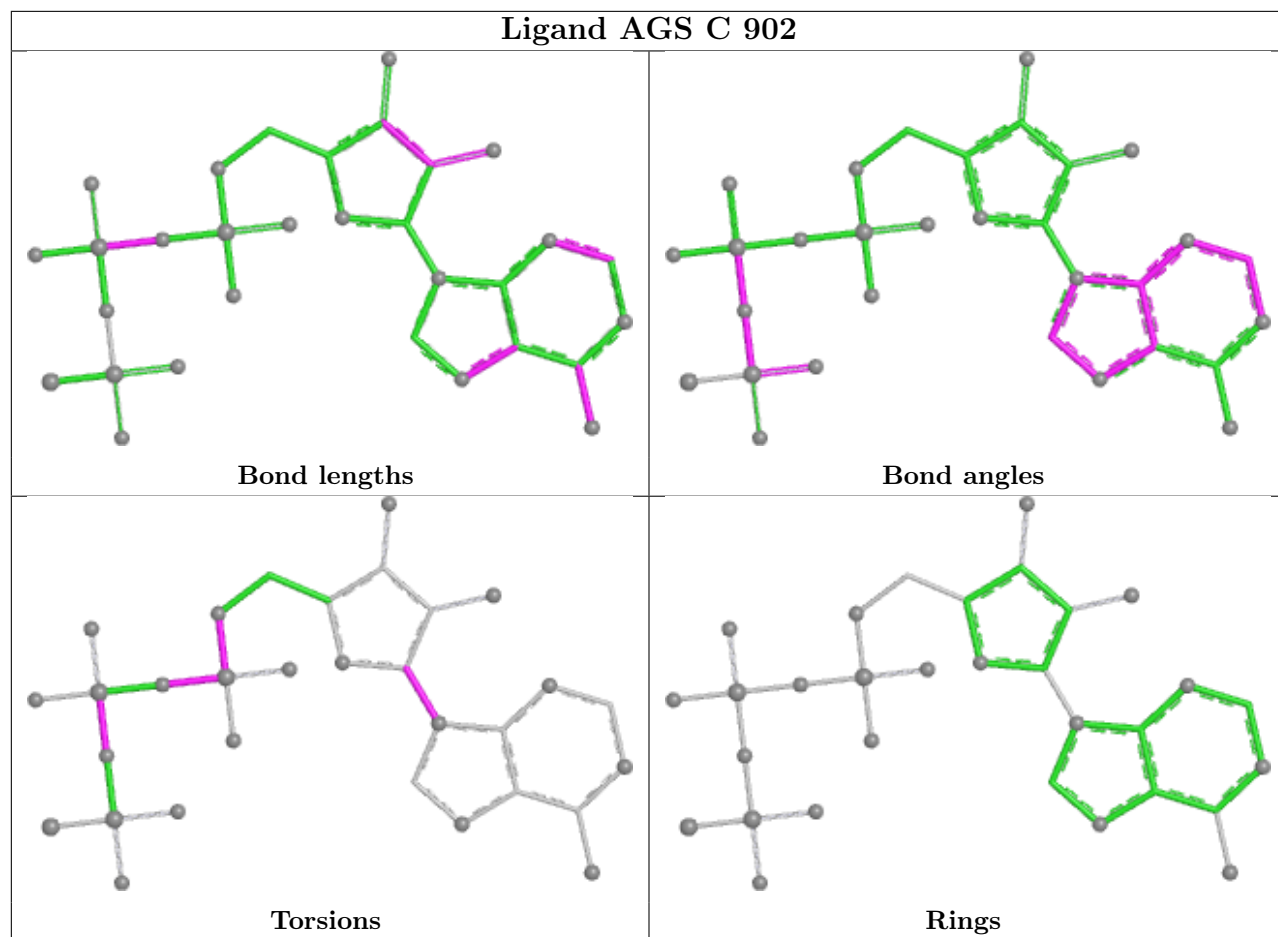


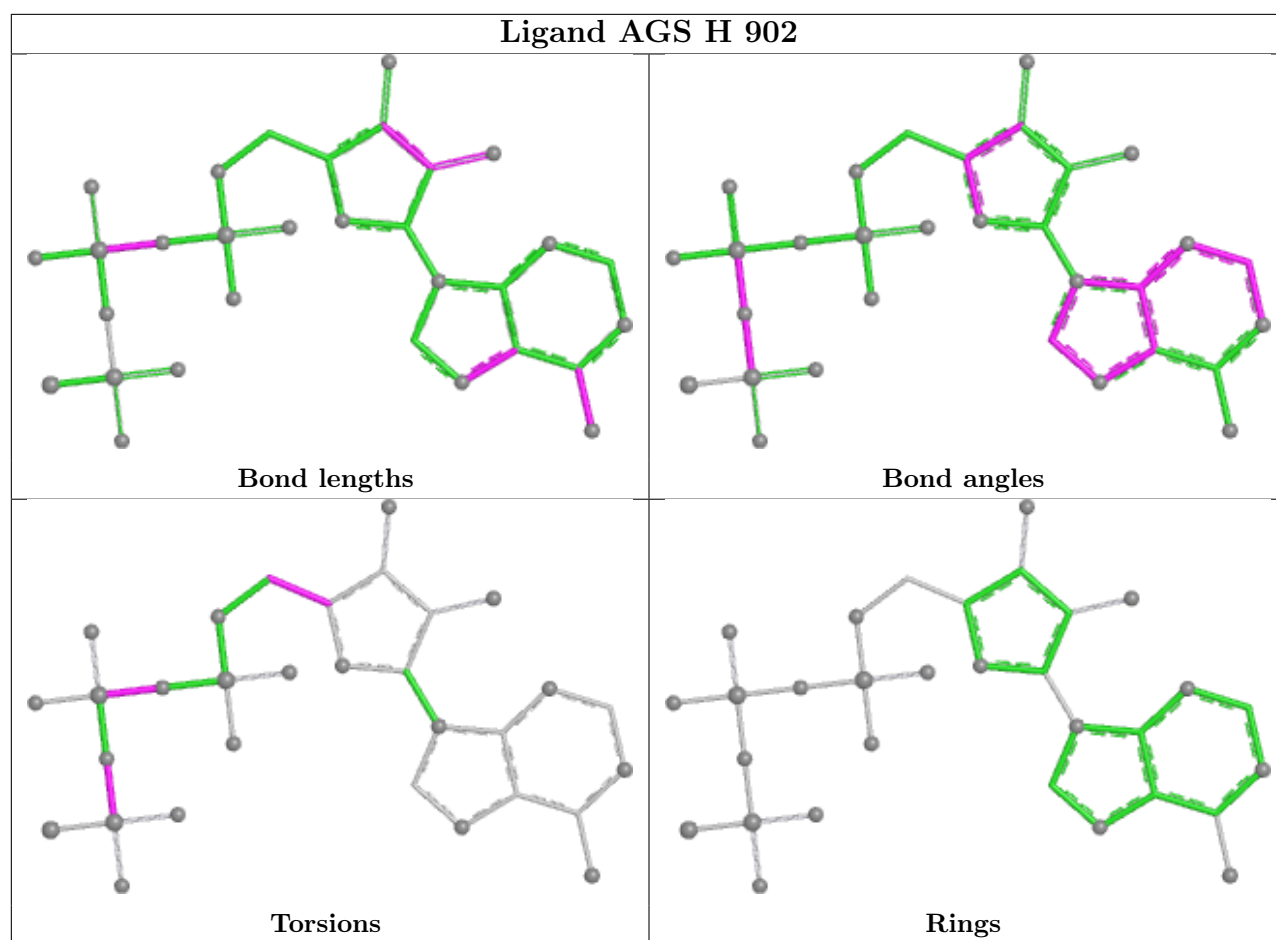


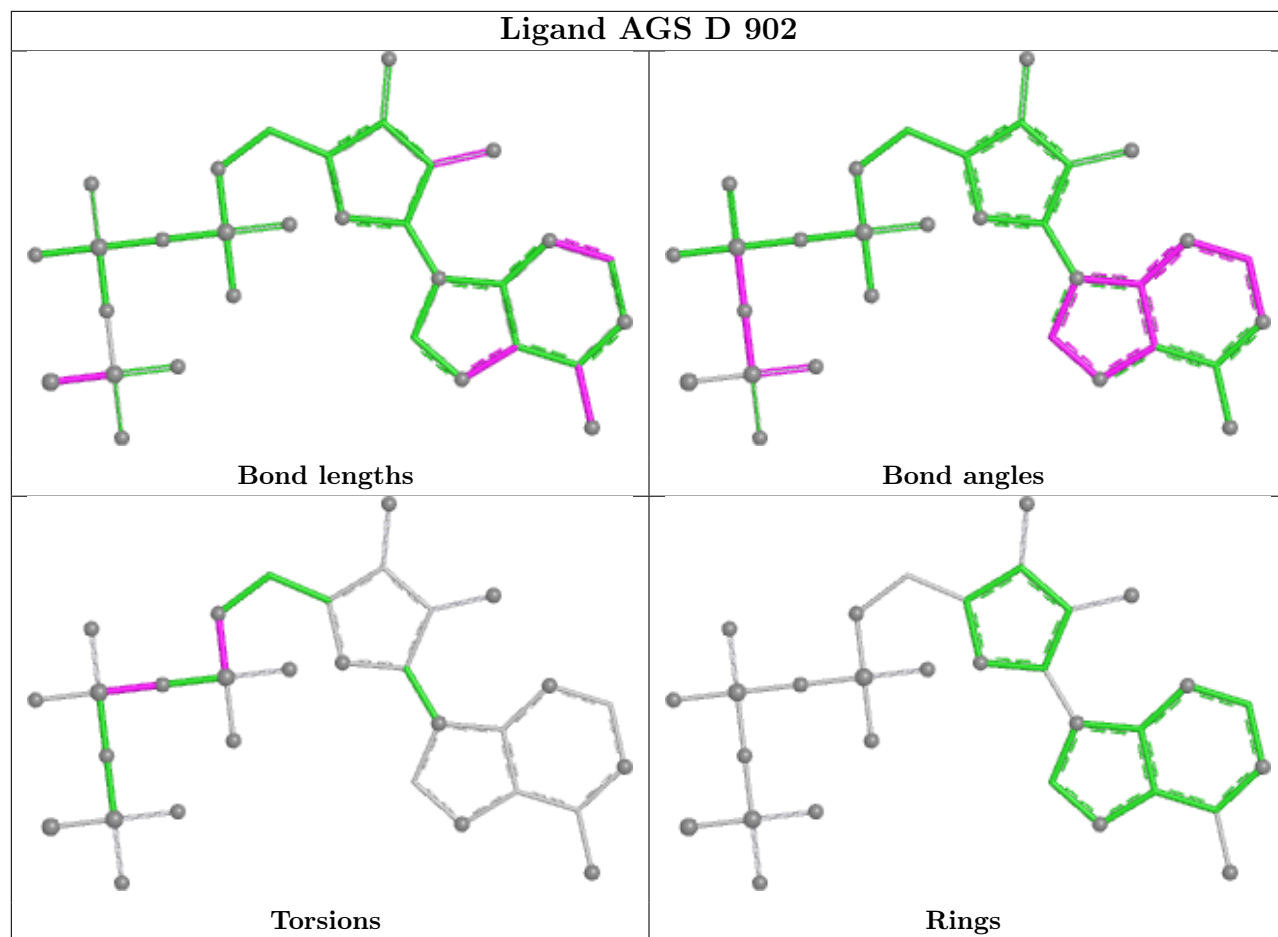
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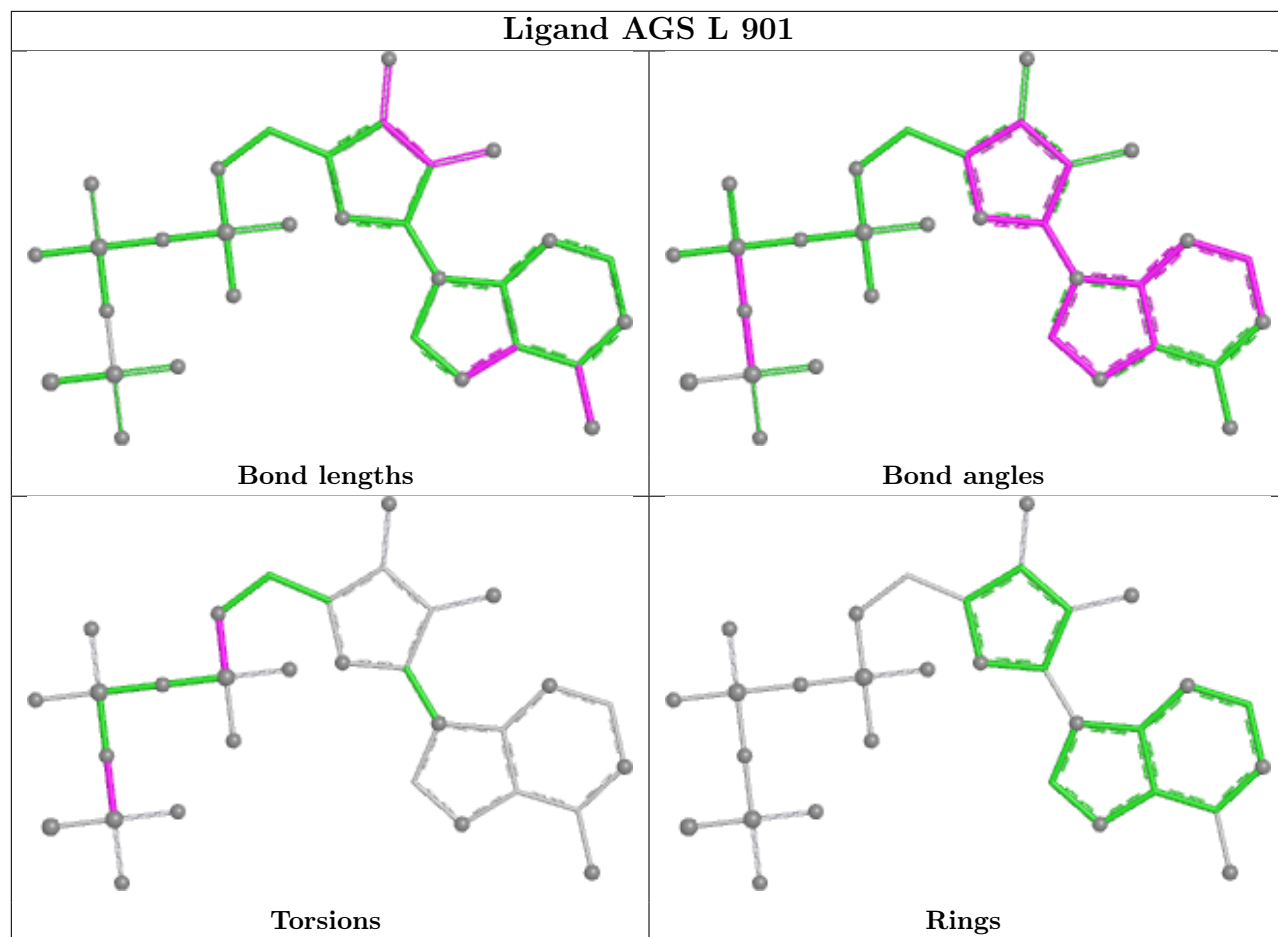
Ligand AGS C 902



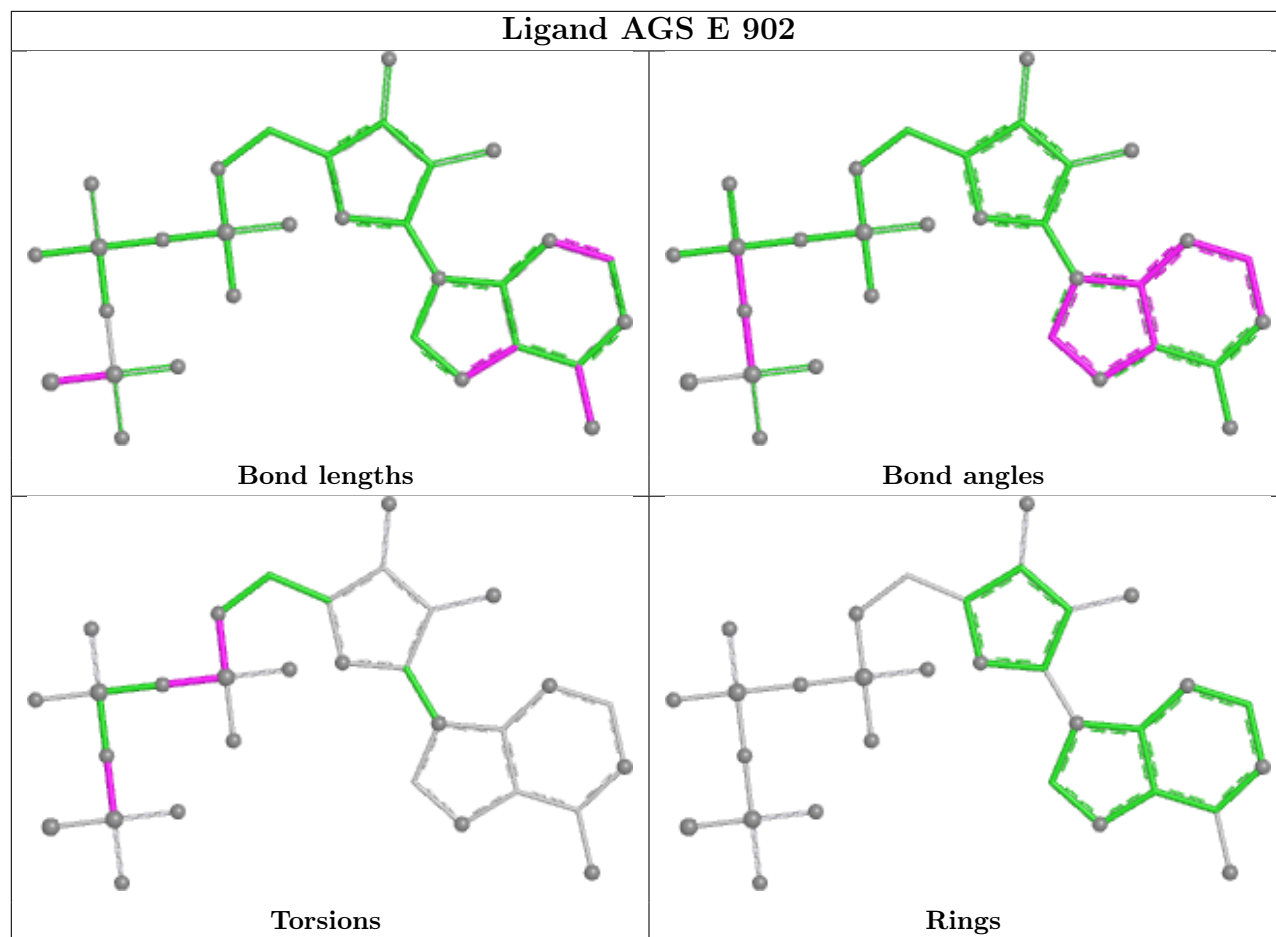




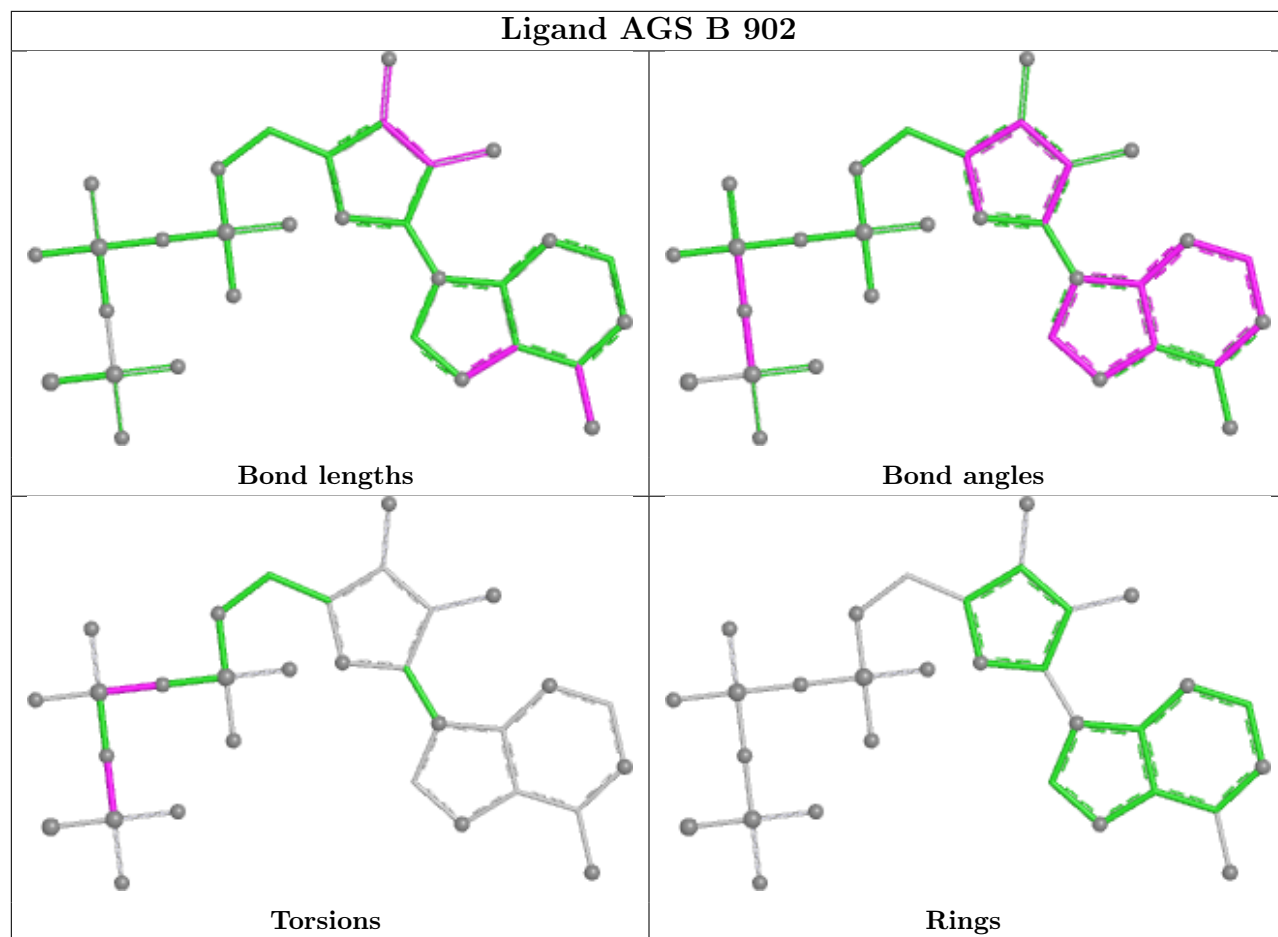
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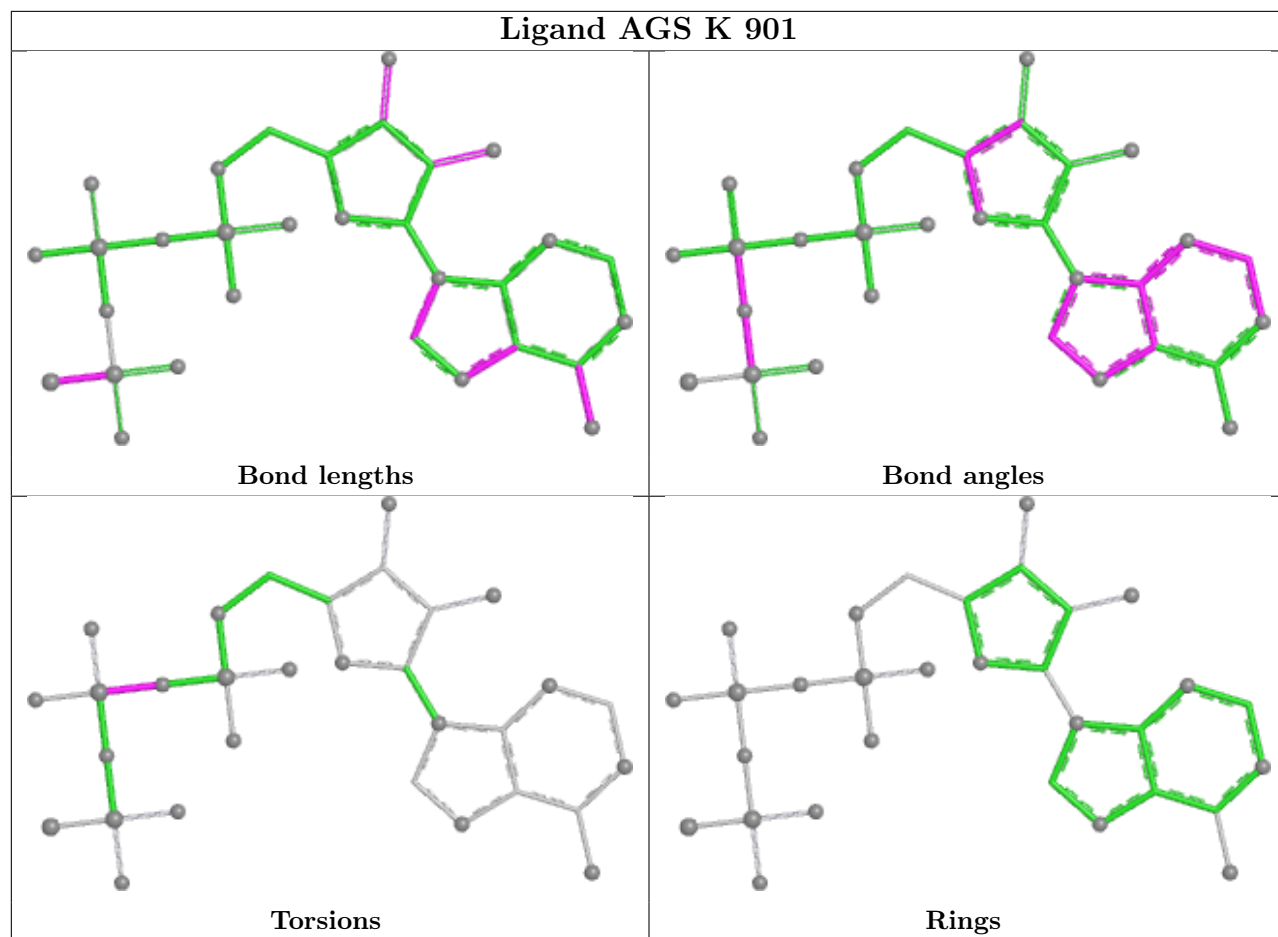
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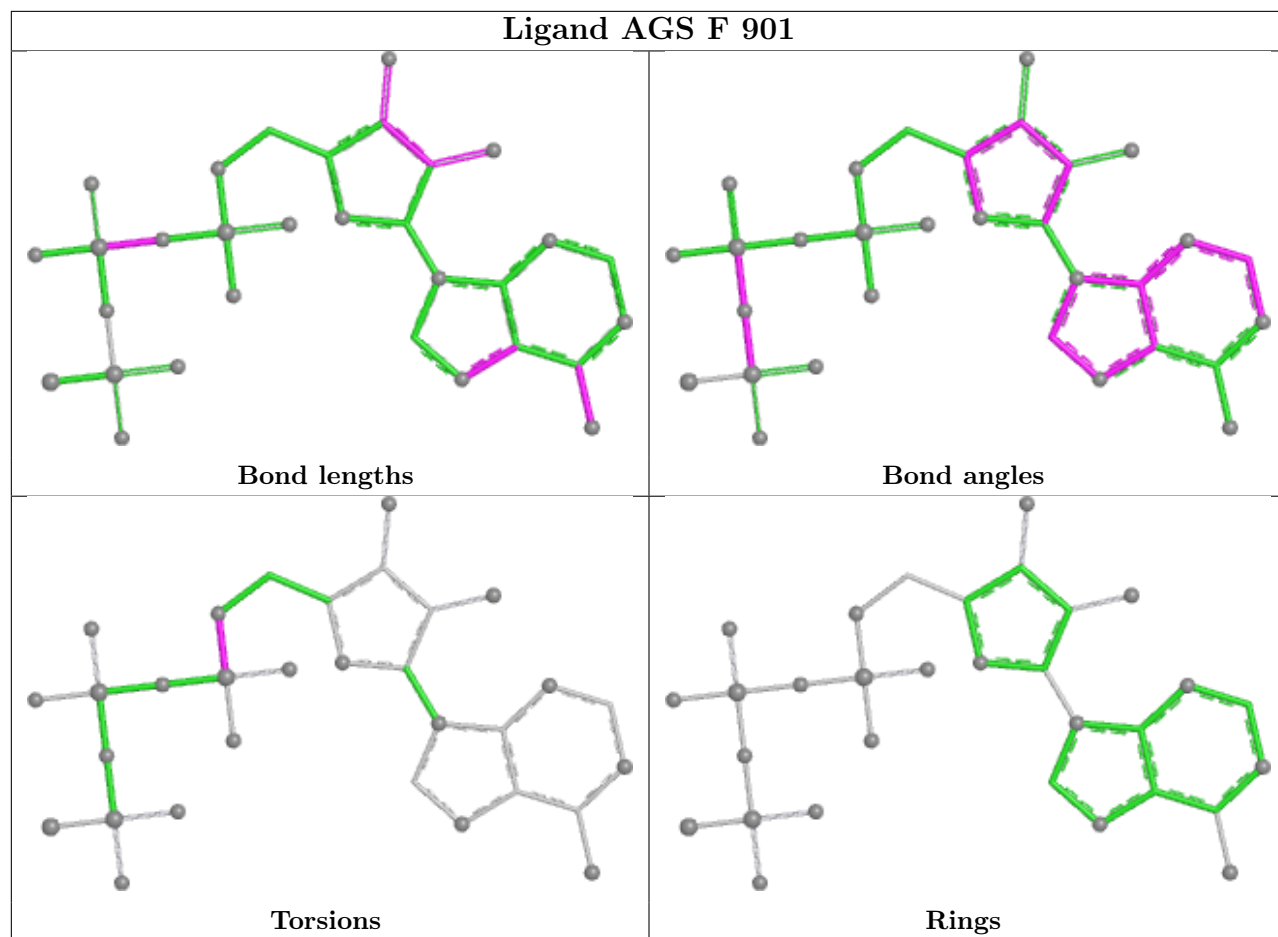
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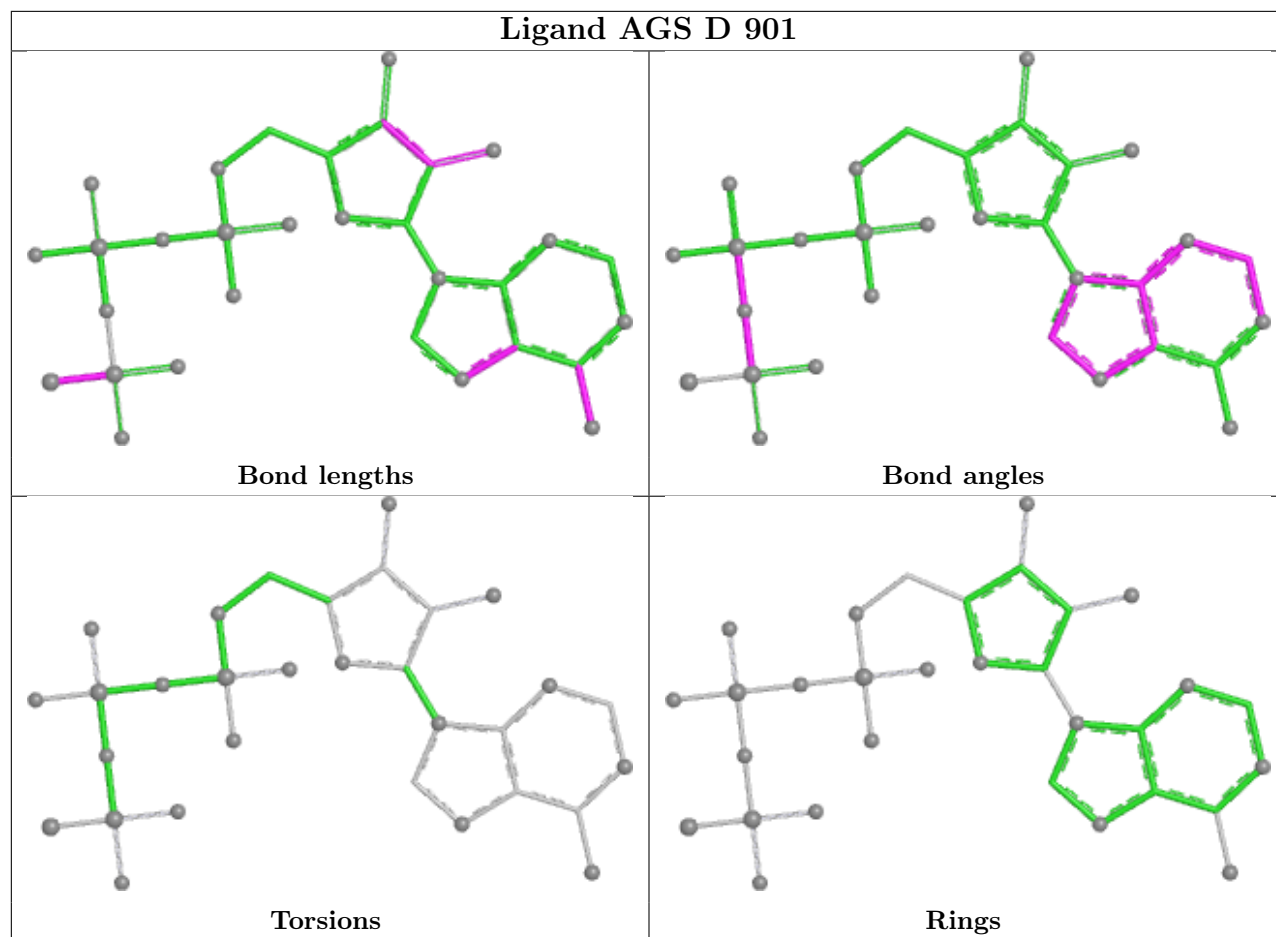


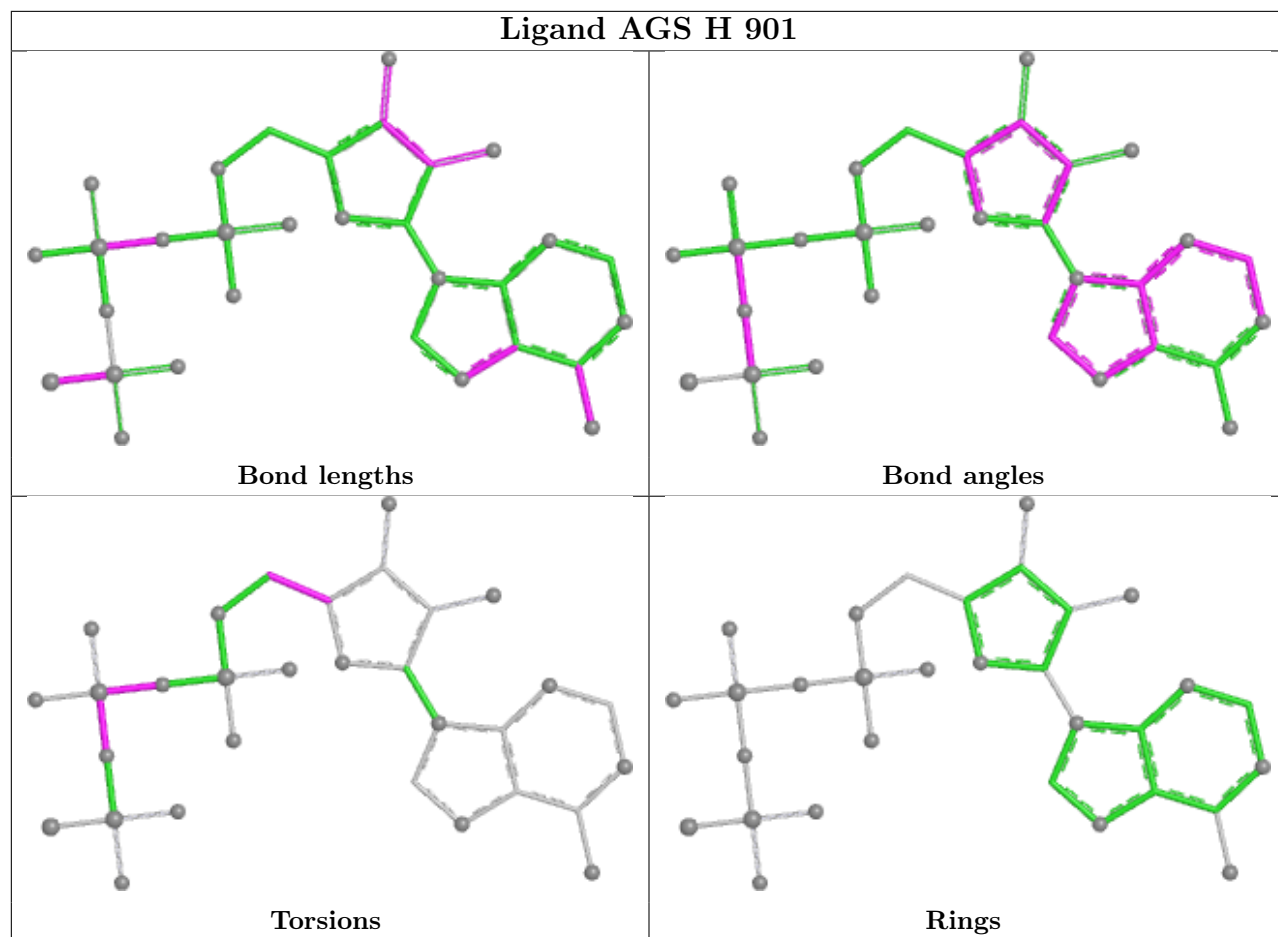
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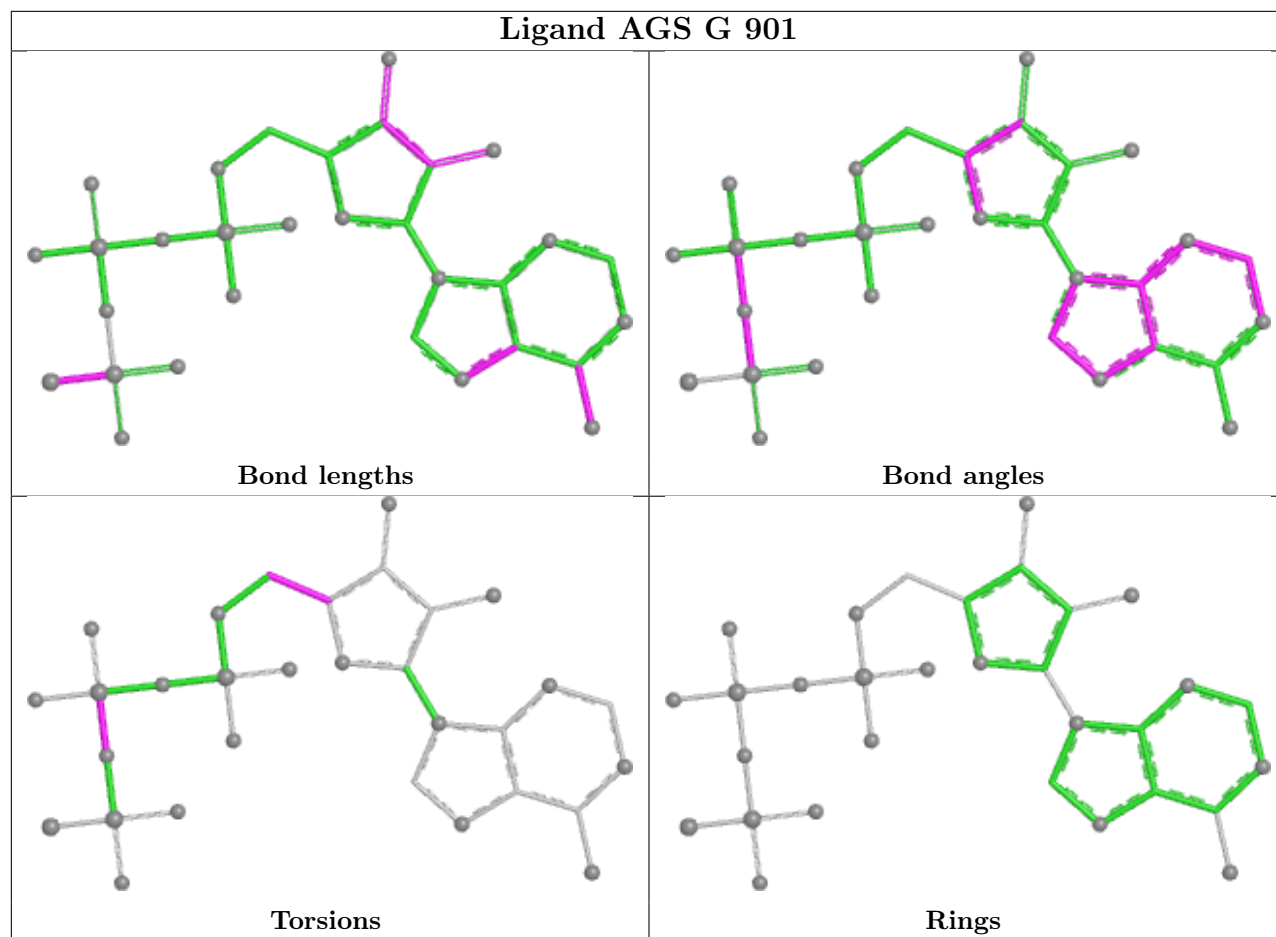


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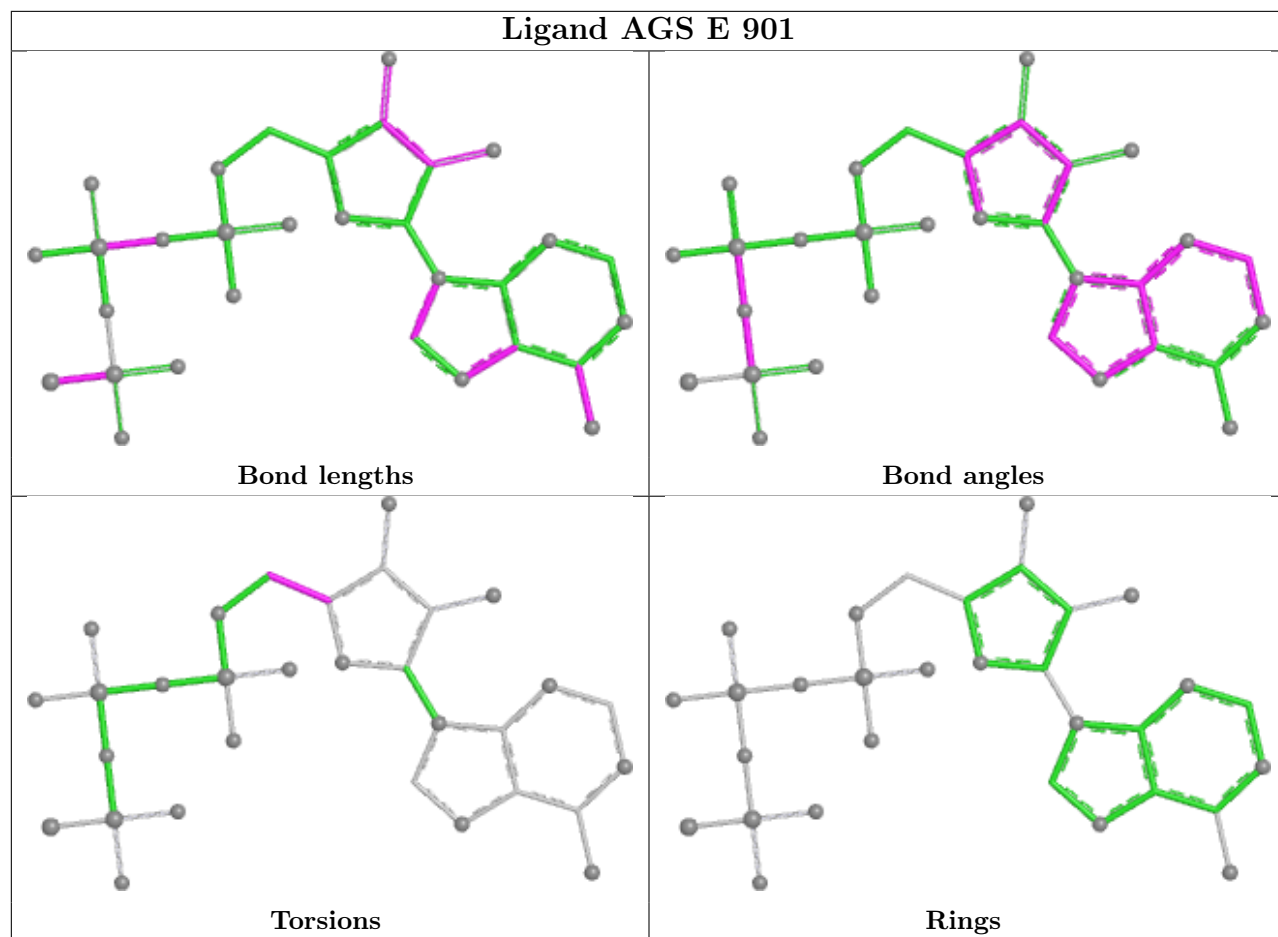


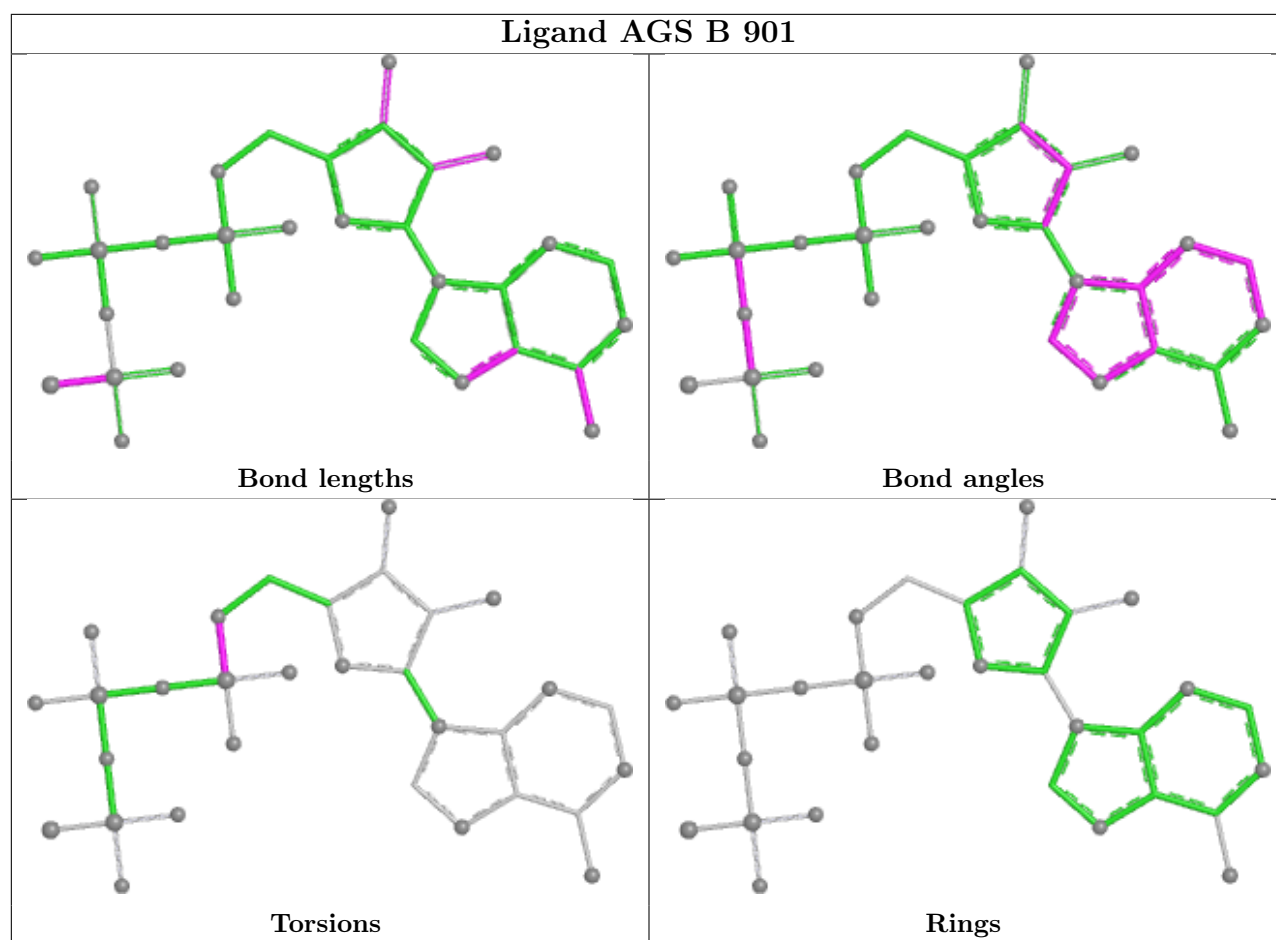






Ligand AGS E 901





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	728:VAL	C	729:PRO	N	3.06

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	735/805 (91%)	-0.84	0 100 100	113, 194, 259, 355	0
1	B	735/805 (91%)	-0.79	1 (0%) 92 87	106, 186, 267, 411	0
1	C	735/805 (91%)	-0.81	0 100 100	124, 198, 272, 350	0
1	D	735/805 (91%)	-0.86	0 100 100	131, 213, 287, 373	0
1	E	735/805 (91%)	-0.81	0 100 100	114, 191, 278, 374	0
1	F	735/805 (91%)	-0.80	0 100 100	109, 186, 276, 359	0
1	G	735/805 (91%)	-0.83	0 100 100	114, 190, 268, 337	0
1	H	735/805 (91%)	-0.81	0 100 100	116, 195, 270, 331	0
1	I	735/805 (91%)	-0.82	1 (0%) 92 87	126, 203, 288, 379	0
1	J	735/805 (91%)	-0.85	1 (0%) 92 87	120, 197, 263, 464	0
1	K	744/805 (92%)	-0.83	0 100 100	110, 189, 279, 406	0
1	L	735/805 (91%)	-0.82	0 100 100	111, 186, 264, 369	0
All	All	8829/9660 (91%)	-0.82	3 (0%) 100 100	106, 195, 275, 464	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	126	ILE	2.5
1	I	423	ILE	2.2
1	B	482	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
3	MG	D	903	1/1	0.88	0.07	122,122,122,122	0
3	MG	D	904	1/1	0.90	0.04	127,127,127,127	0
3	MG	J	903	1/1	0.92	0.06	105,105,105,105	0
3	MG	C	904	1/1	0.93	0.04	137,137,137,137	0
2	AGS	E	902	31/31	0.93	0.06	102,148,179,184	0
2	AGS	D	902	31/31	0.94	0.05	111,144,182,204	0
3	MG	A	903	1/1	0.94	0.06	110,110,110,110	0
3	MG	B	903	1/1	0.94	0.06	113,113,113,113	0
3	MG	G	903	1/1	0.94	0.07	113,113,113,113	0
3	MG	B	904	1/1	0.94	0.05	114,114,114,114	0
3	MG	F	904	1/1	0.95	0.03	149,149,149,149	0
3	MG	E	904	1/1	0.95	0.06	151,151,151,151	0
3	MG	I	903	1/1	0.95	0.06	138,138,138,138	0
3	MG	F	903	1/1	0.95	0.08	94,94,94,94	0
2	AGS	B	902	31/31	0.96	0.05	101,128,152,156	0
2	AGS	C	901	31/31	0.96	0.04	105,138,166,177	0
2	AGS	C	902	31/31	0.96	0.05	105,140,172,196	0
2	AGS	D	901	31/31	0.96	0.05	103,137,166,208	0
2	AGS	A	901	31/31	0.96	0.06	102,125,153,197	0
2	AGS	B	901	31/31	0.96	0.05	102,131,160,170	0
3	MG	E	903	1/1	0.96	0.04	113,113,113,113	0
2	AGS	F	902	31/31	0.96	0.05	122,150,185,190	0
2	AGS	G	901	31/31	0.96	0.05	104,134,164,210	0
2	AGS	I	901	31/31	0.96	0.05	105,131,158,186	0
2	AGS	I	902	31/31	0.96	0.05	125,150,180,187	0
3	MG	H	903	1/1	0.96	0.06	132,132,132,132	0
3	MG	H	904	1/1	0.96	0.03	134,134,134,134	0
2	AGS	K	901	31/31	0.96	0.05	100,132,164,172	0
2	AGS	L	901	31/31	0.96	0.05	102,132,160,173	0
3	MG	L	903	1/1	0.96	0.07	117,117,117,117	0
3	MG	L	904	1/1	0.96	0.06	115,115,115,115	0
2	AGS	J	902	31/31	0.97	0.04	99,140,168,181	0

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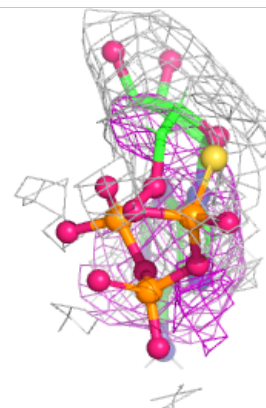
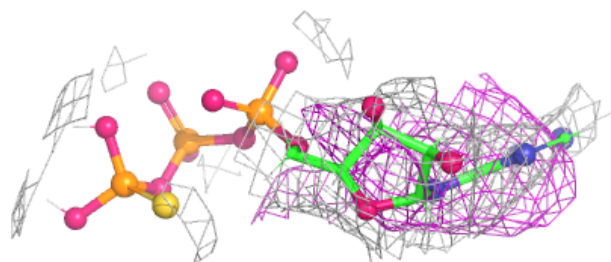
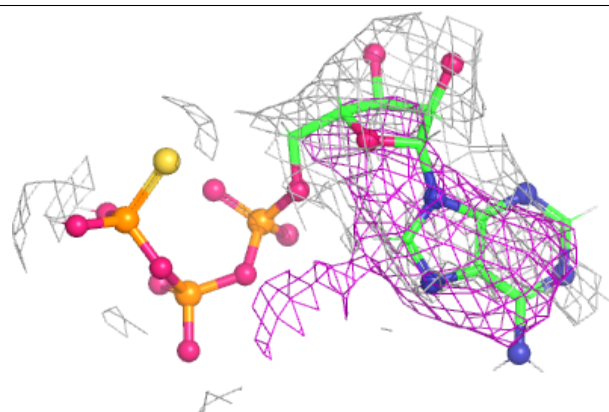
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	G	904	1/1	0.97	0.05	119,119,119,119	0
2	AGS	H	901	31/31	0.97	0.05	105,133,162,165	0
2	AGS	H	902	31/31	0.97	0.04	110,139,165,169	0
2	AGS	E	901	31/31	0.97	0.05	105,131,164,179	0
2	AGS	G	902	31/31	0.97	0.05	112,139,179,187	0
2	AGS	J	901	31/31	0.97	0.04	111,139,167,210	0
3	MG	C	903	1/1	0.97	0.06	94,94,94,94	0
2	AGS	F	901	31/31	0.98	0.05	94,131,160,160	0
3	MG	A	904	1/1	0.98	0.05	128,128,128,128	0
3	MG	I	904	1/1	0.98	0.02	145,145,145,145	0
2	AGS	K	902	31/31	0.98	0.05	96,121,149,154	0
3	MG	J	904	1/1	0.98	0.04	112,112,112,112	0
3	MG	K	903	1/1	0.98	0.07	112,112,112,112	0
3	MG	K	904	1/1	0.98	0.06	99,99,99,99	0
2	AGS	A	902	31/31	0.98	0.03	120,142,172,177	0
2	AGS	L	902	31/31	0.98	0.04	112,136,166,169	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.

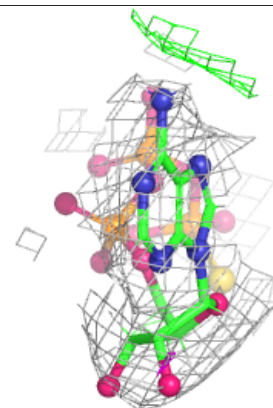
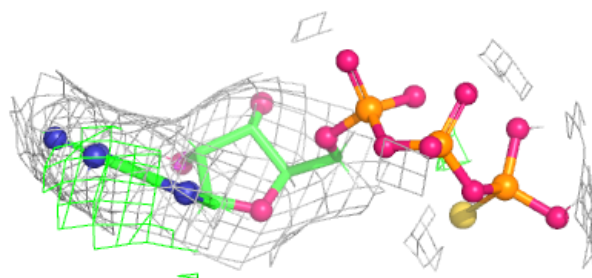
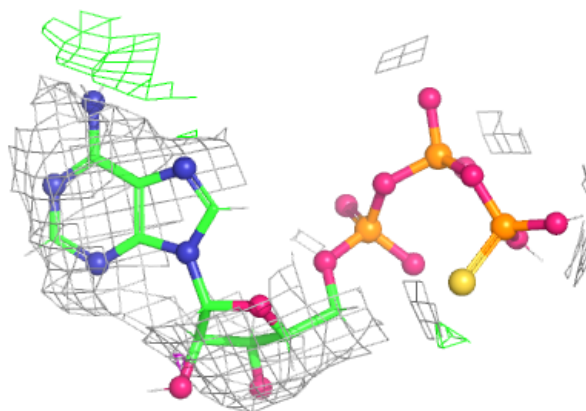
Electron density around AGS E 902:

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



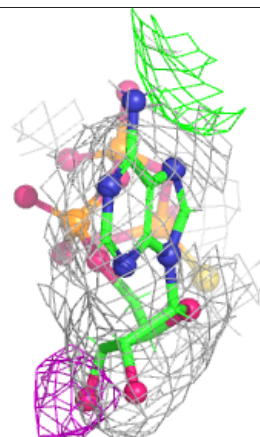
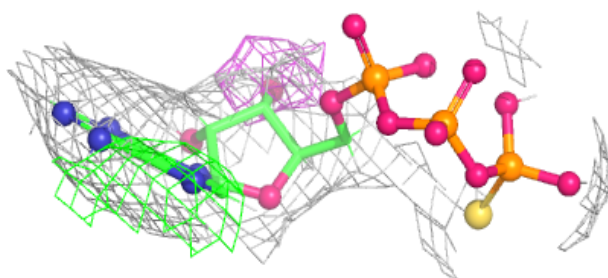
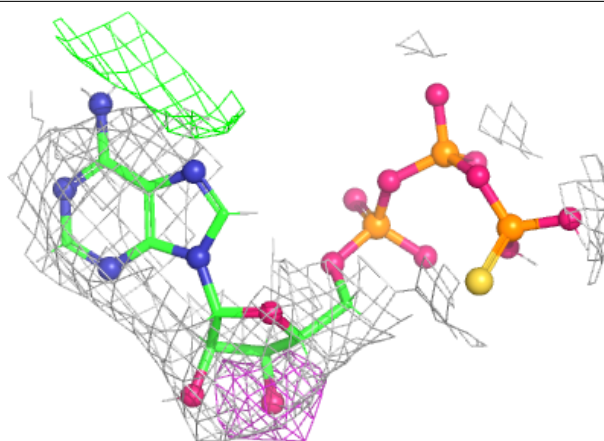
Electron density around AGS D 902:

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and green (positive)

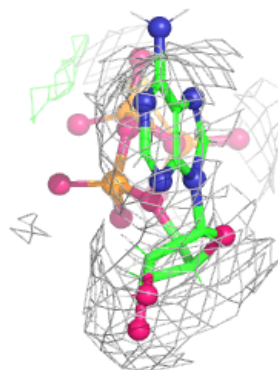
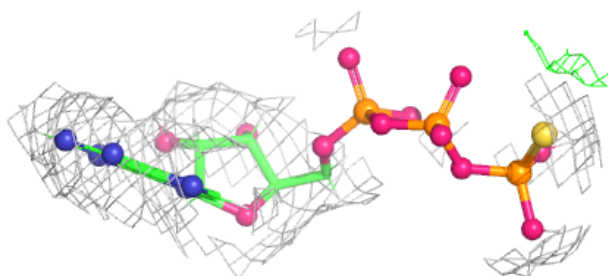
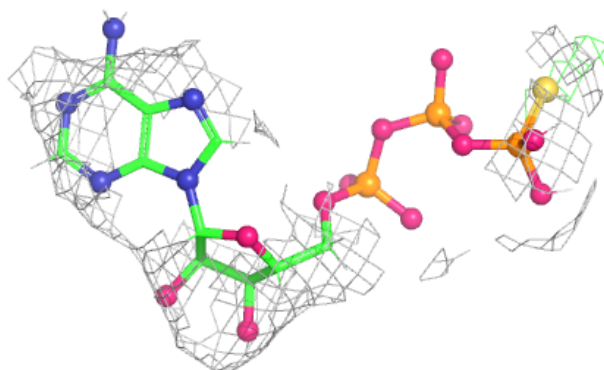


Electron density around AGS B 902:

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and green (positive)

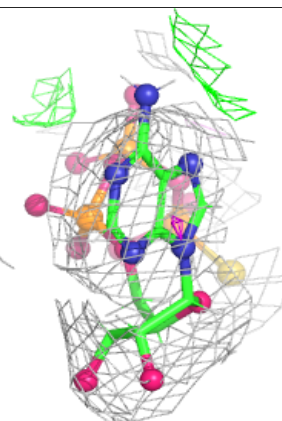
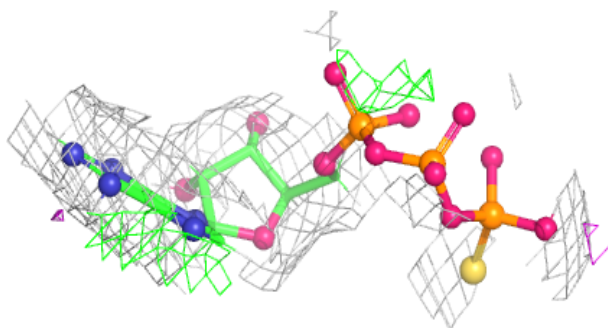
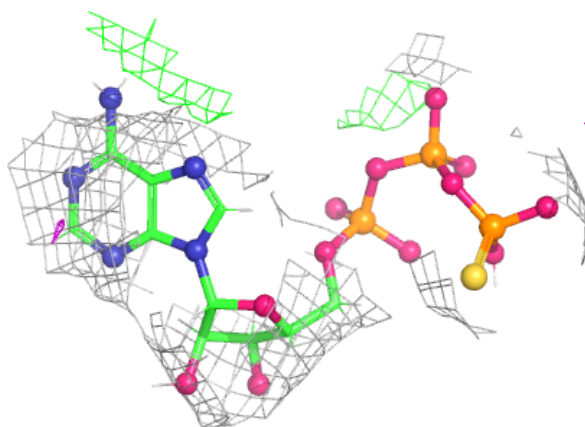
**Electron density around AGS C 901:**

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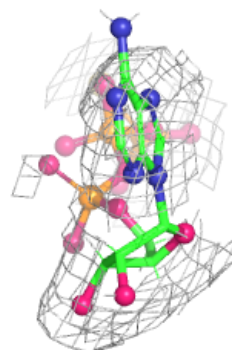
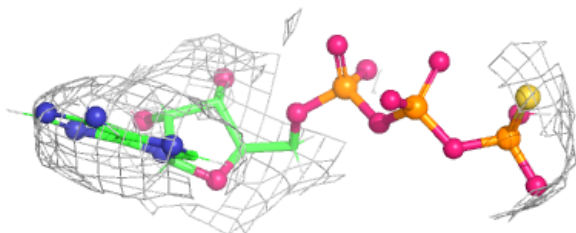
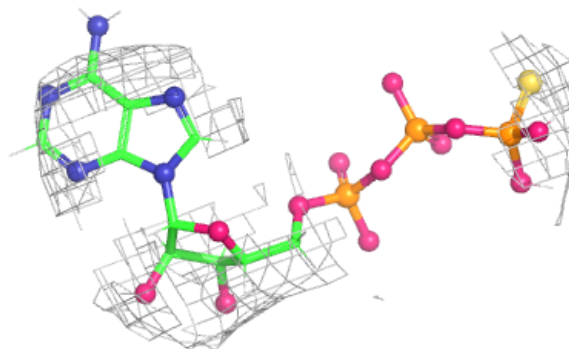


Electron density around AGS C 902:

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

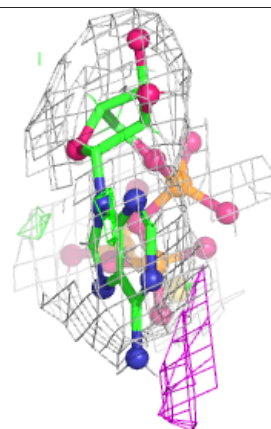
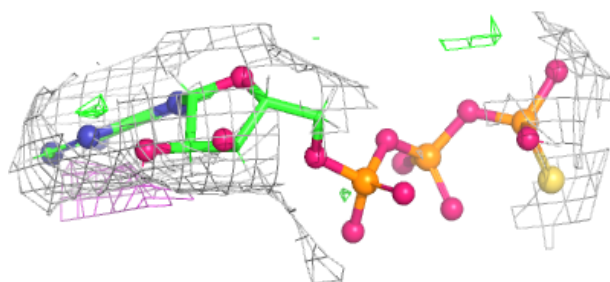
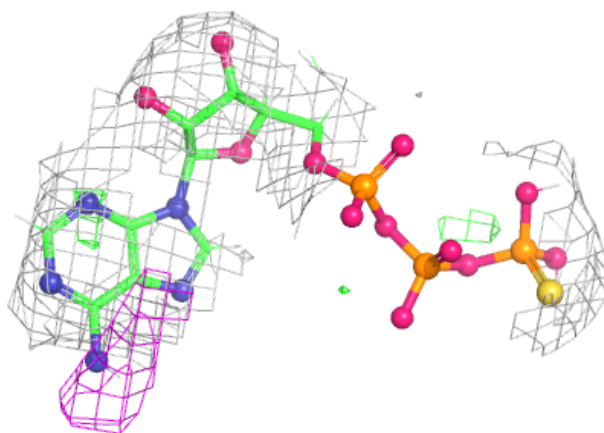
**Electron density around AGS D 901:**

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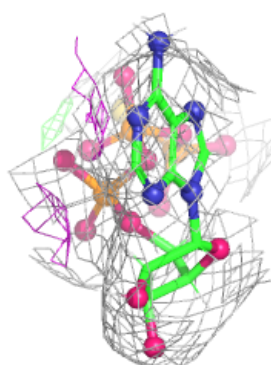
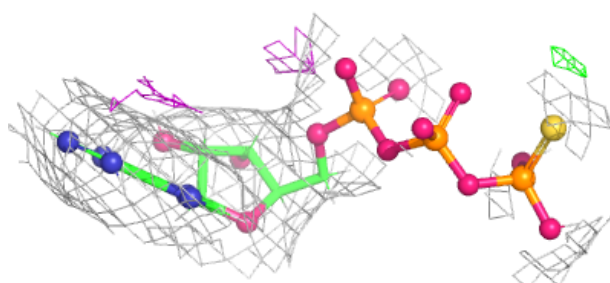
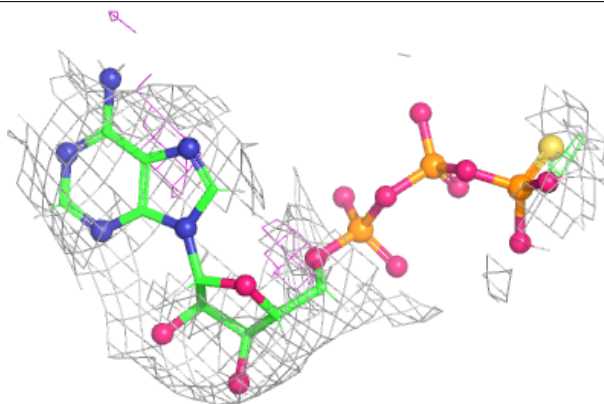


Electron density around AGS A 901:

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and green (positive)

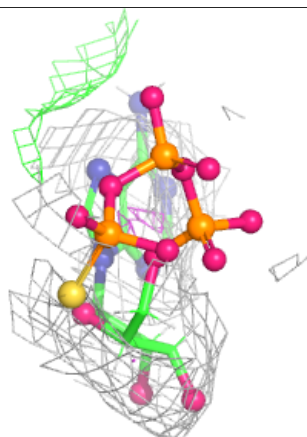
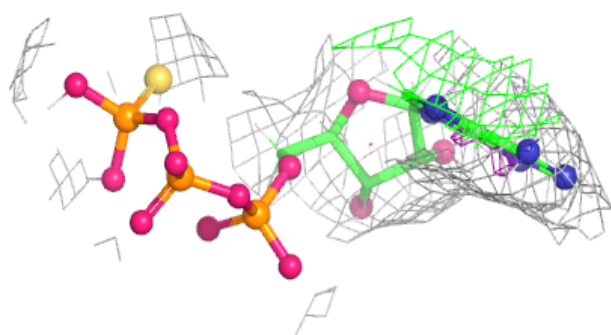
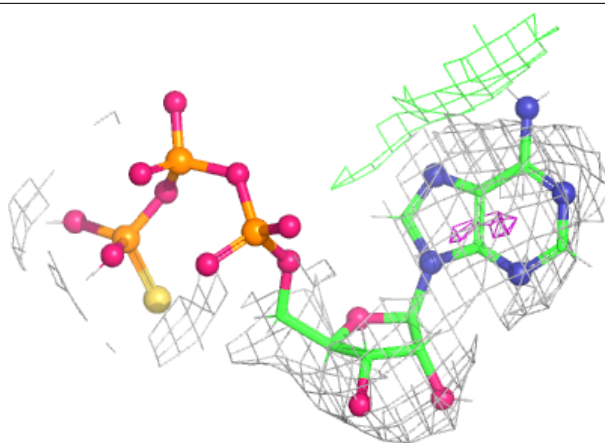
**Electron density around AGS B 901:**

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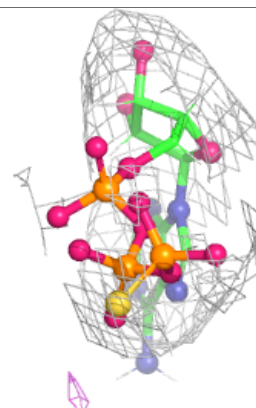
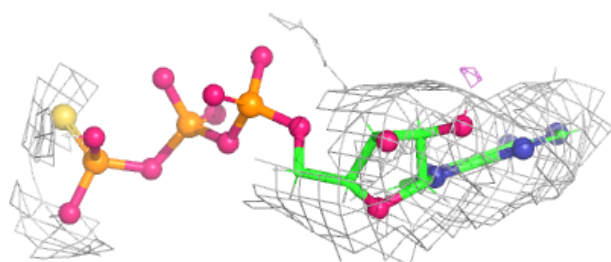
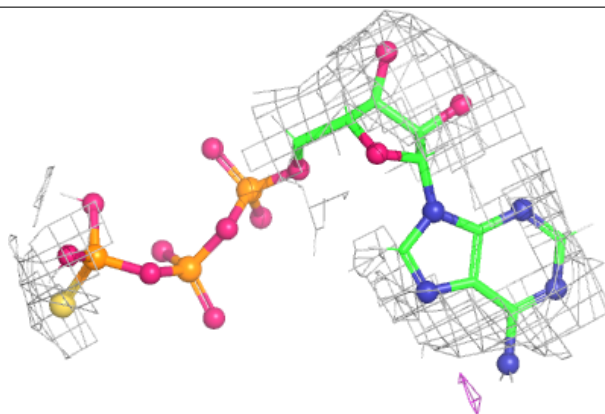


Electron density around AGS F 902:

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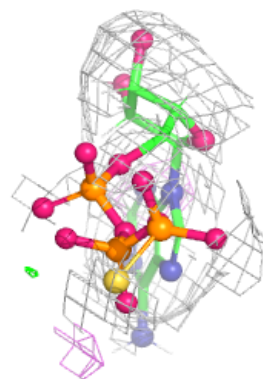
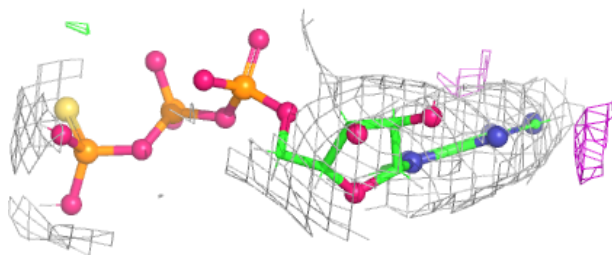
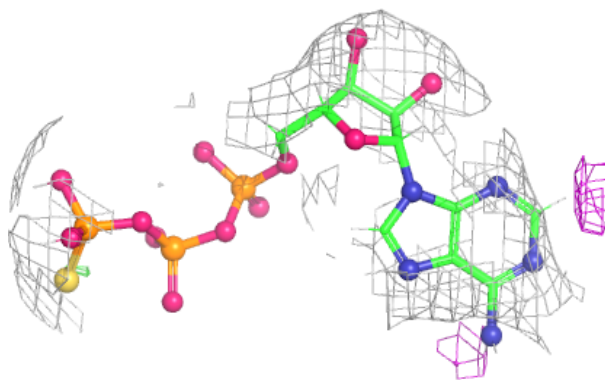
**Electron density around AGS G 901:**

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and green (positive)

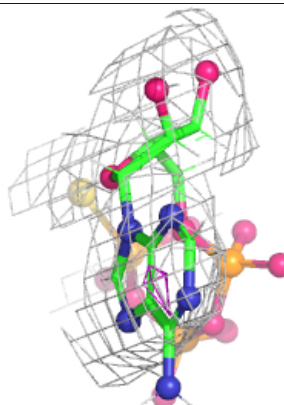
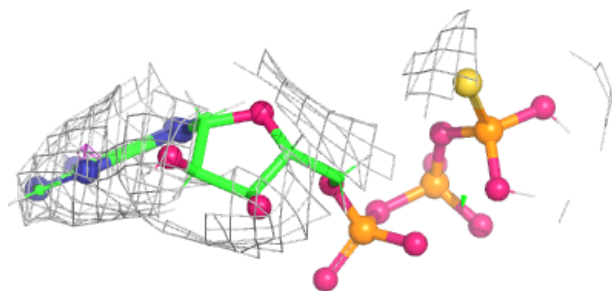
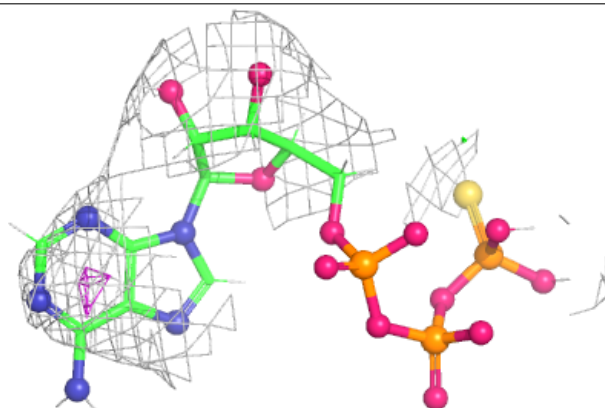


Electron density around AGS I 901:

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and green (positive)

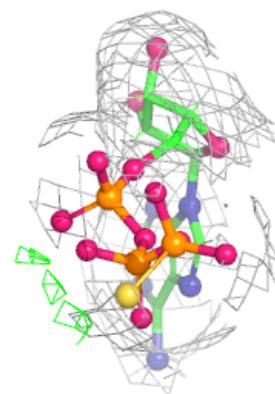
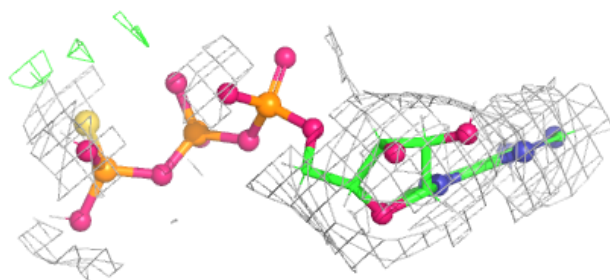
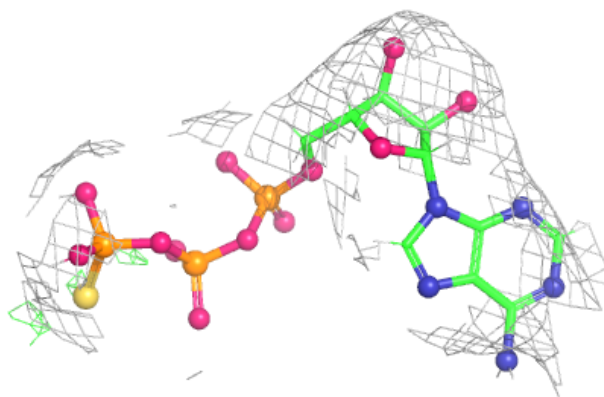
**Electron density around AGS I 902:**

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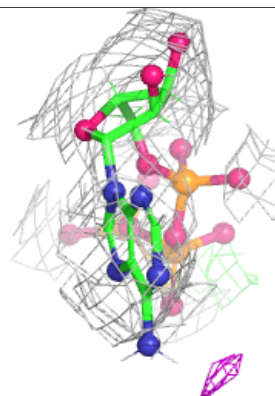
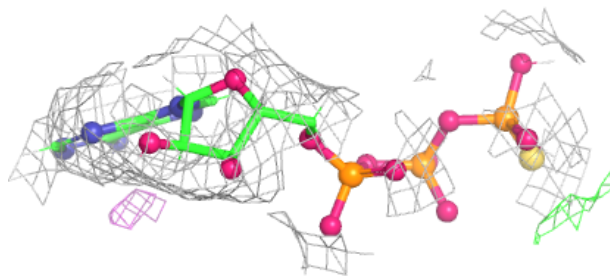
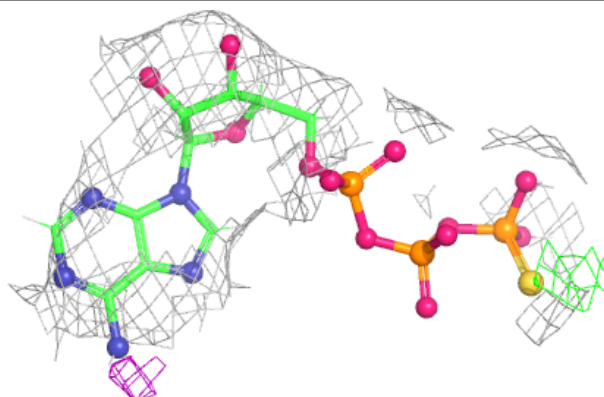


Electron density around AGS K 901:

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and green (positive)

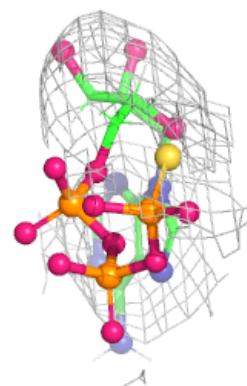
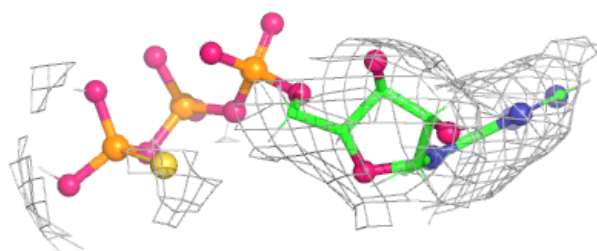
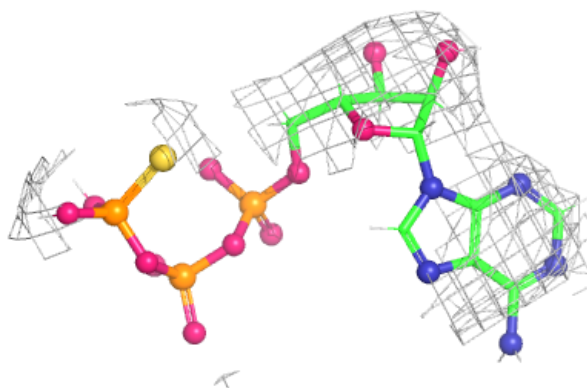
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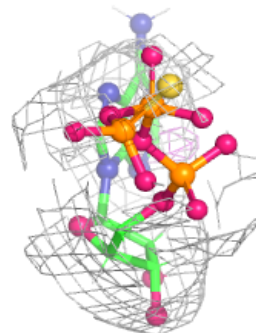
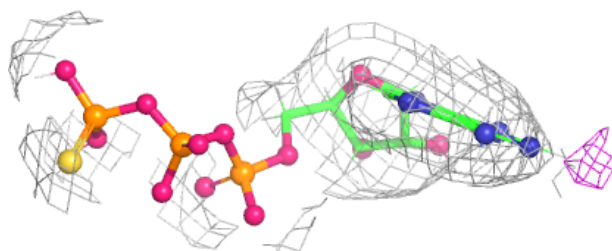
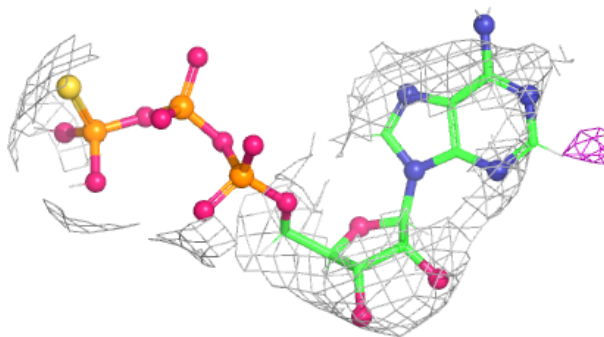


Electron density around AGS J 902:

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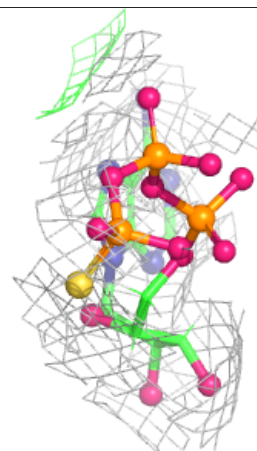
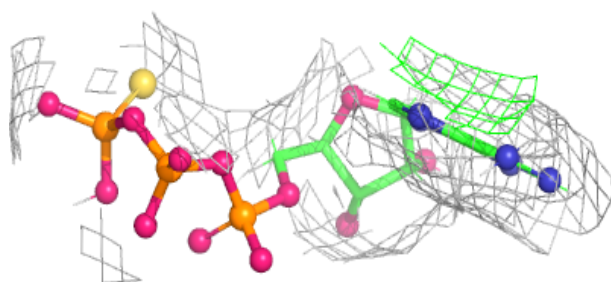
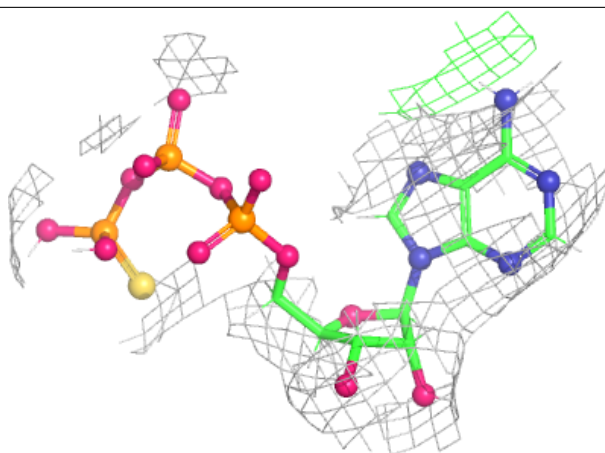
**Electron density around AGS H 901:**

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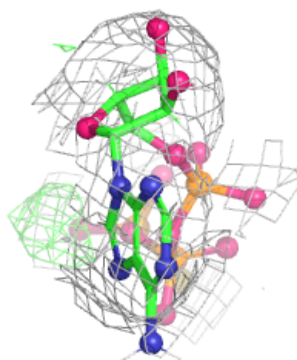
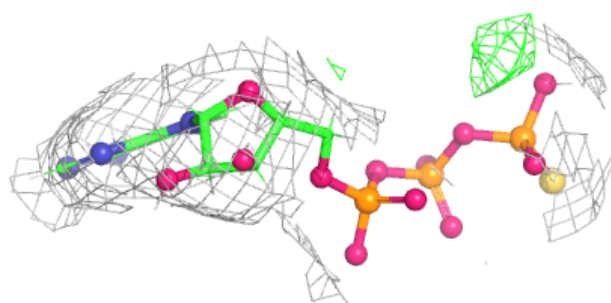
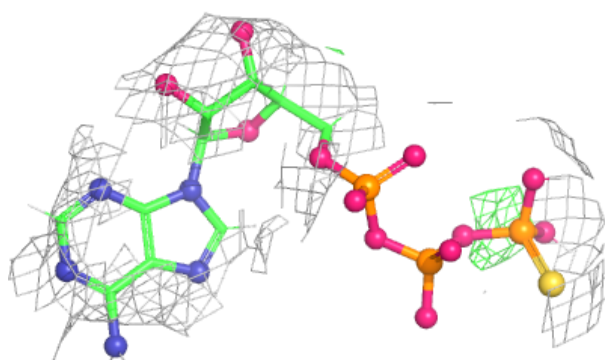


Electron density around AGS H 902:

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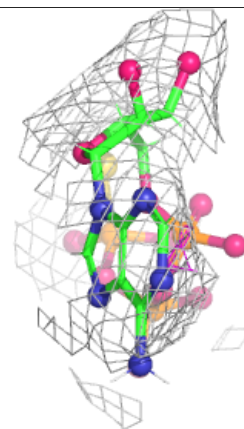
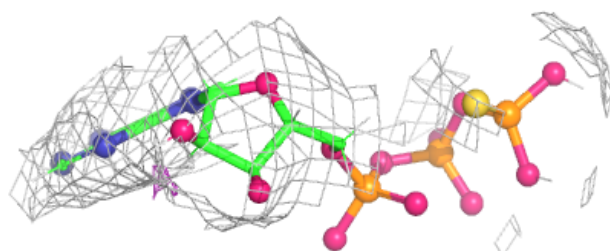
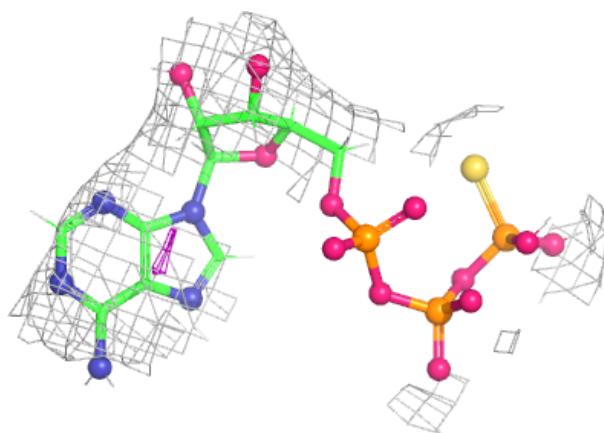
**Electron density around AGS E 901:**

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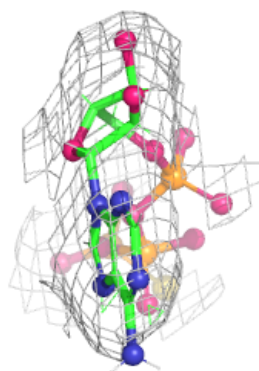
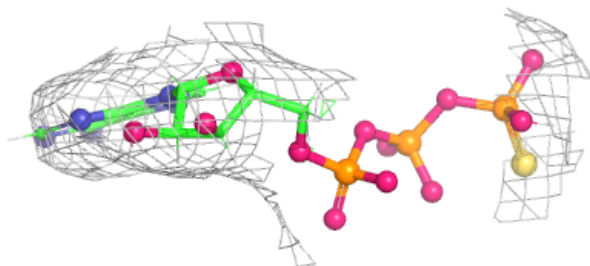
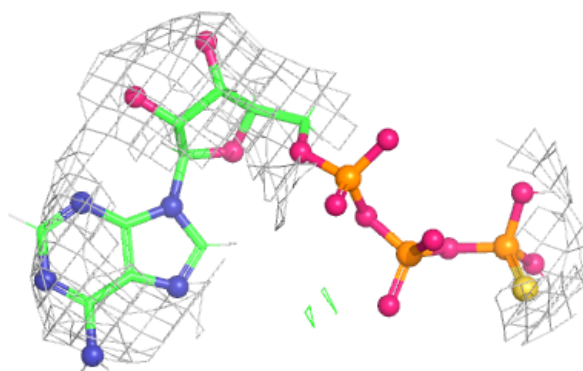


Electron density around AGS G 902:

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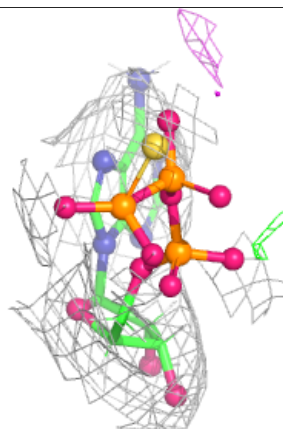
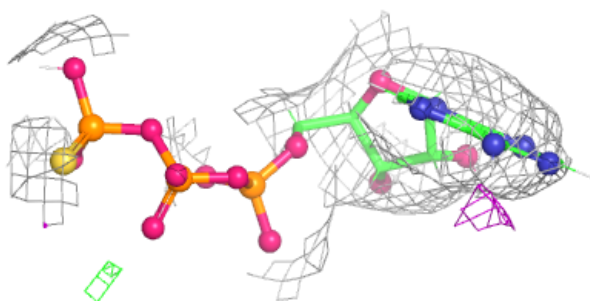
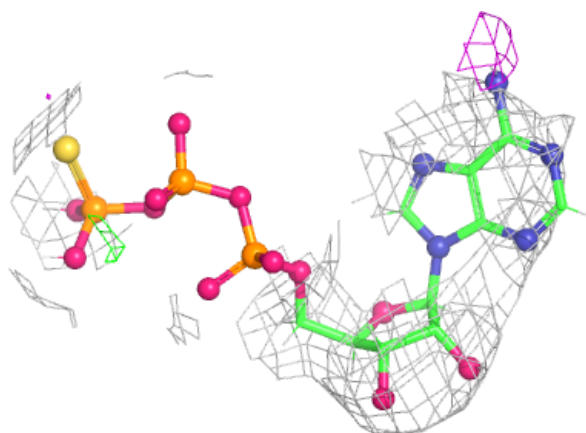
**Electron density around AGS J 901:**

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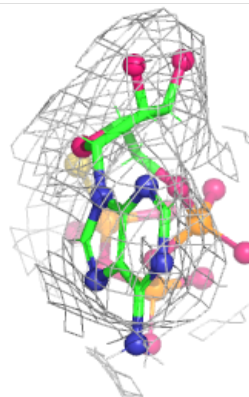
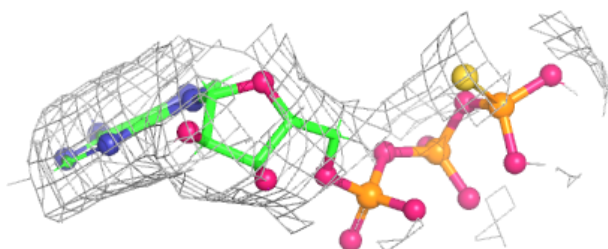
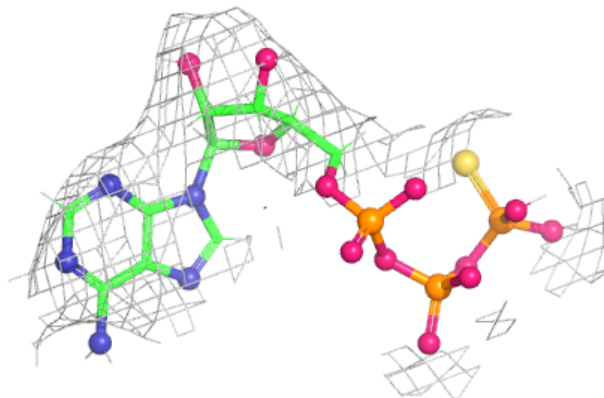


Electron density around AGS F 901:

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and green (positive)

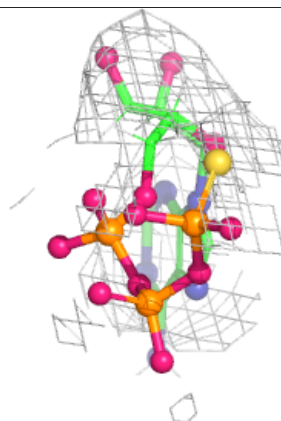
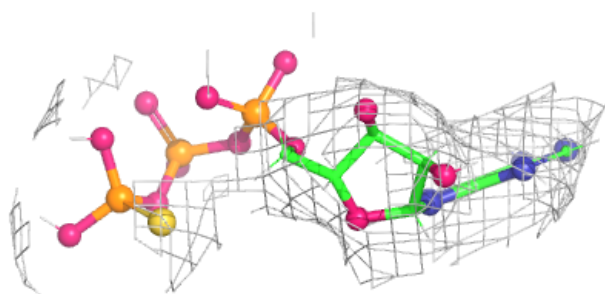
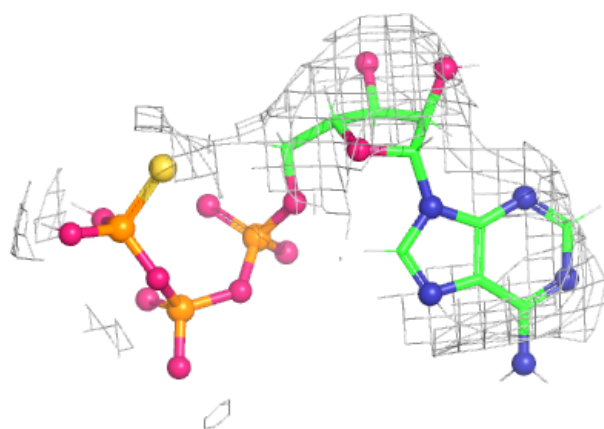
**Electron density around AGS K 902:**

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

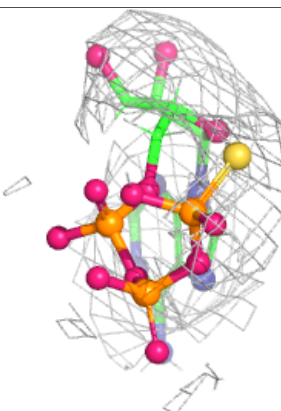
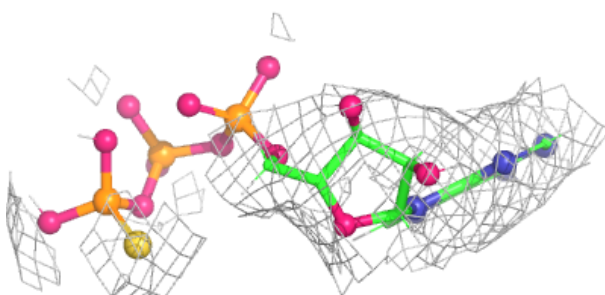
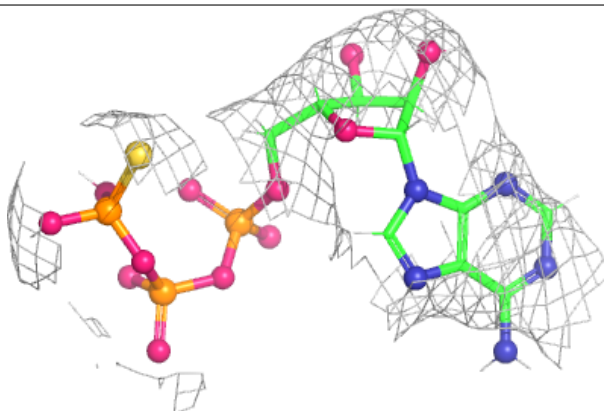


Electron density around AGS A 902:

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

**Electron density around AGS L 902:**

$2mF_o-DF_c$ (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.