Full wwPDB X-ray Structure Validation Report (i)

Jan 5, 2024 – 12:38 am GMT

PDB ID	:	5C1A
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 (i) 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 (i)) were used in the production of this report:

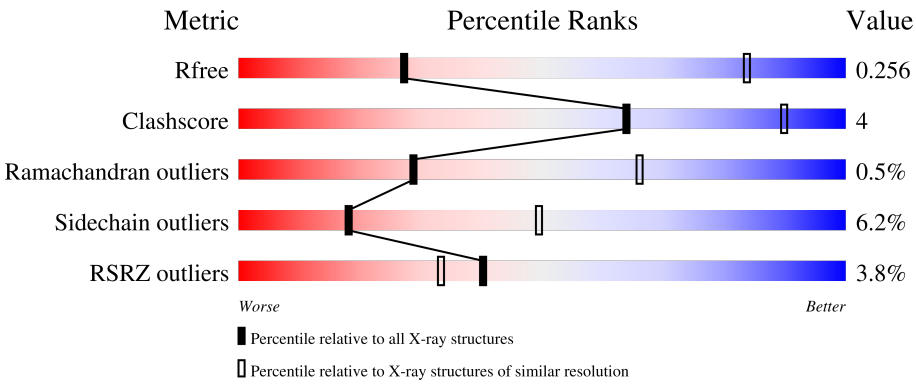
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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 <=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	3% 78% 13% • 9%
1	B	805	2% 77% 13% • 9%
1	C	805	4% 79% 12% 9%
1	D	805	7% 79% 12% • 9%
1	E	805	2% 77% 13% • 9%

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Mol	Chain	Length	Quality of chain
1	F	805	2% 79% 11% • 9%
1	G	805	2% 78% 13% • 9%
1	H	805	3% 77% 12% • 9%
1	I	805	4% 77% 13% • 9%
1	J	805	4% 77% 13% • 9%
1	K	805	5% 76% 15% • 8%
1	L	805	3% 78% 13% • 9%

2 Entry composition (i)

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

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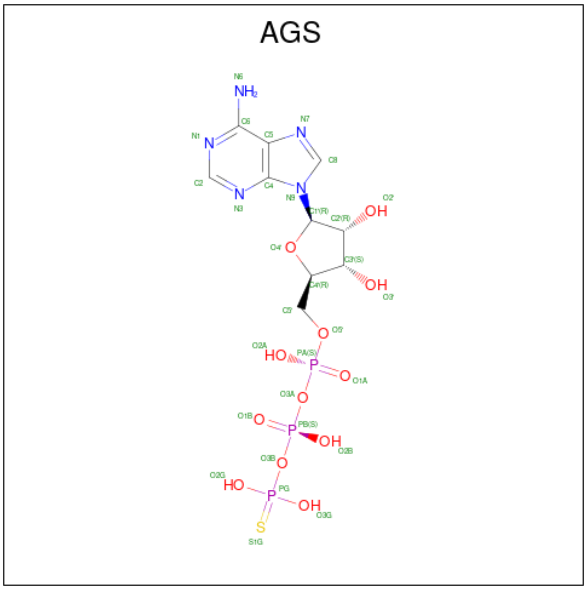
Chain	Residue	Modelled	Actual	Comment	Reference
L	760	ASP	GLN	engineered mutation	UNP P55072

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



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

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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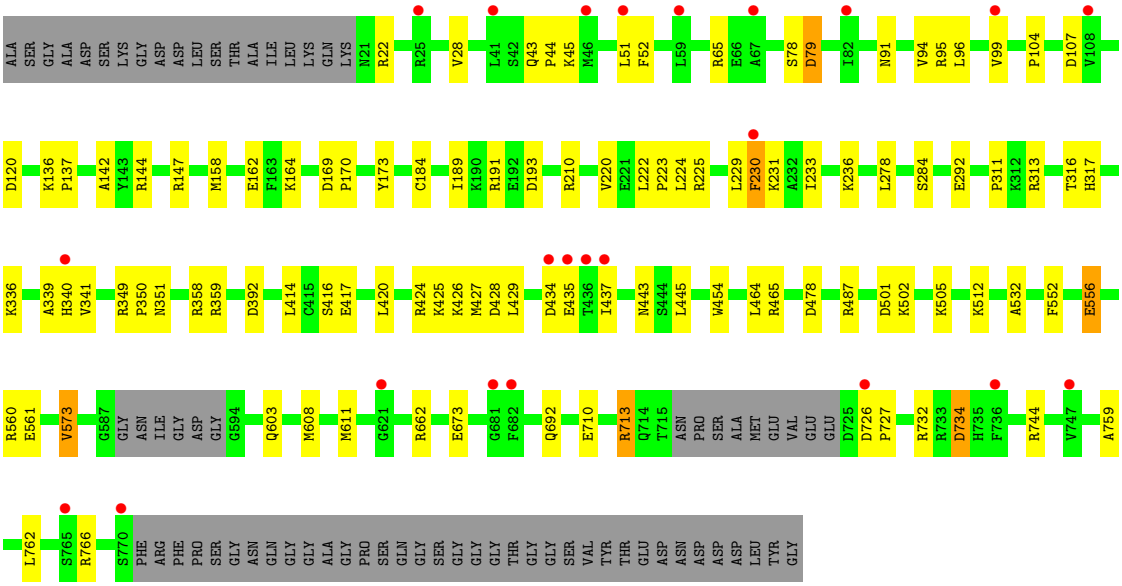
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	F	2	2	2	0	0
3	G	2	2	2	0	0
3	H	2	2	2	0	0
3	I	2	2	2	0	0
3	J	2	2	2	0	0
3	K	2	2	2	0	0
3	L	2	2	2	0	0

3 Residue-property plots (i)

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

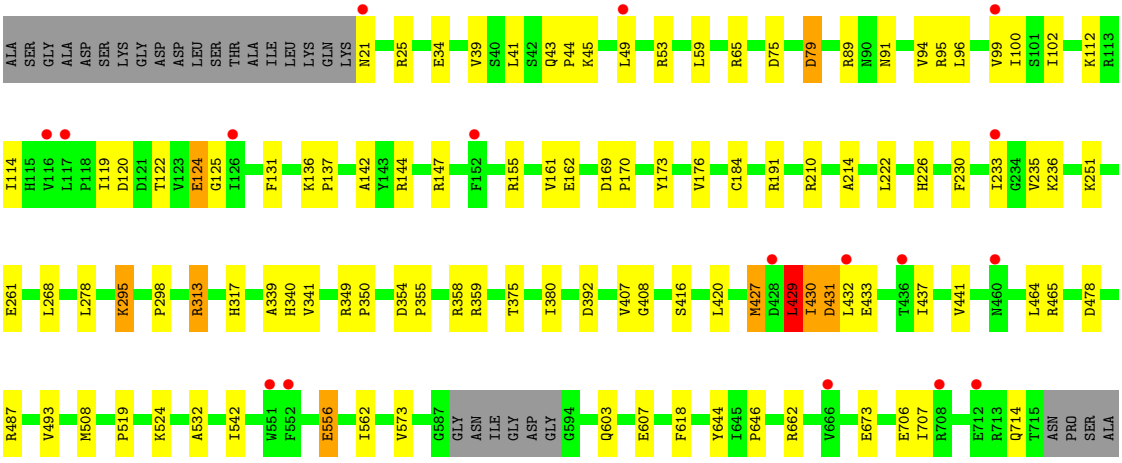
• Molecule 1: Transitional endoplasmic reticulum ATPase

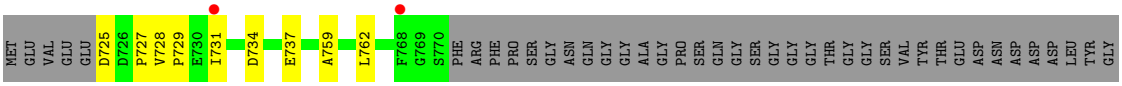
Chain A:



• Molecule 1: Transitional endoplasmic reticulum ATPase

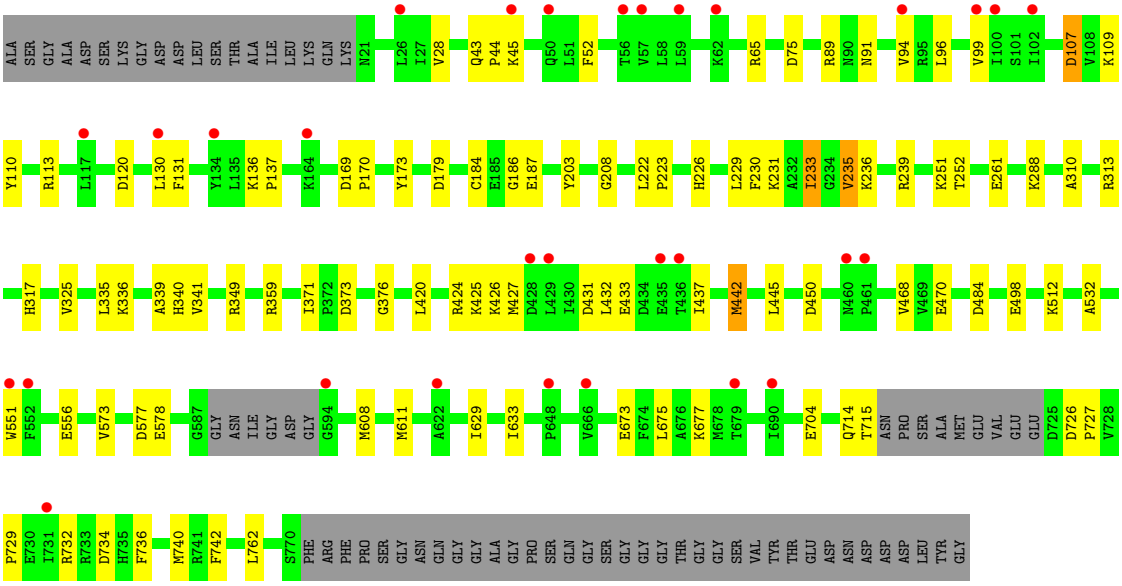
Chain B:





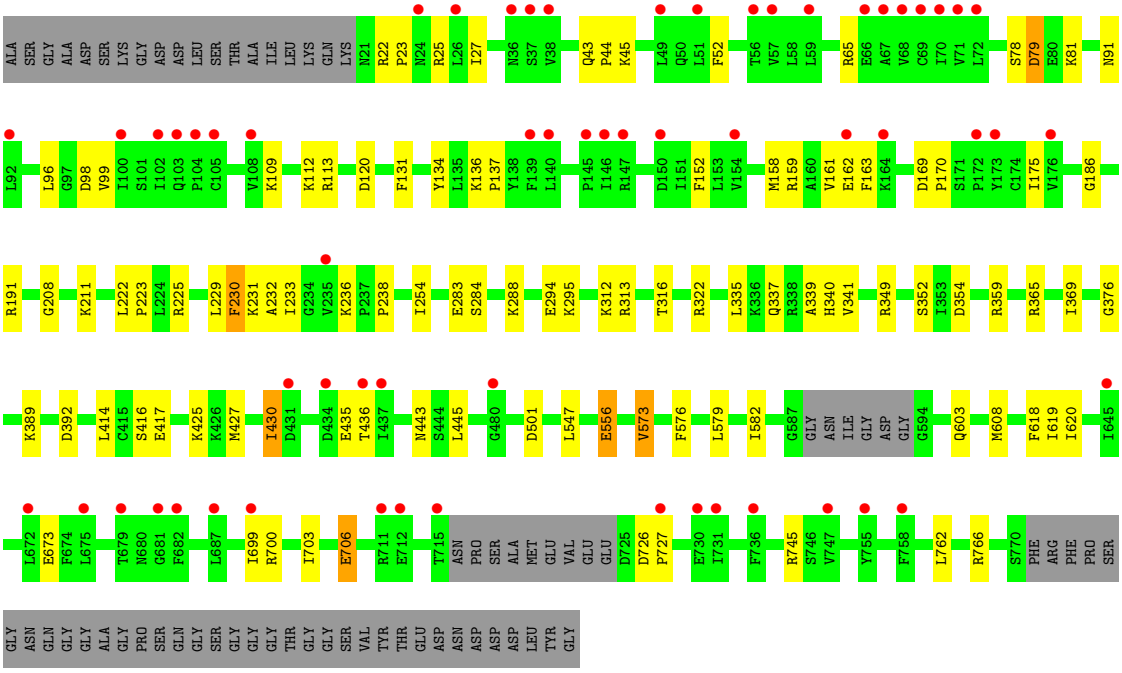
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain C:



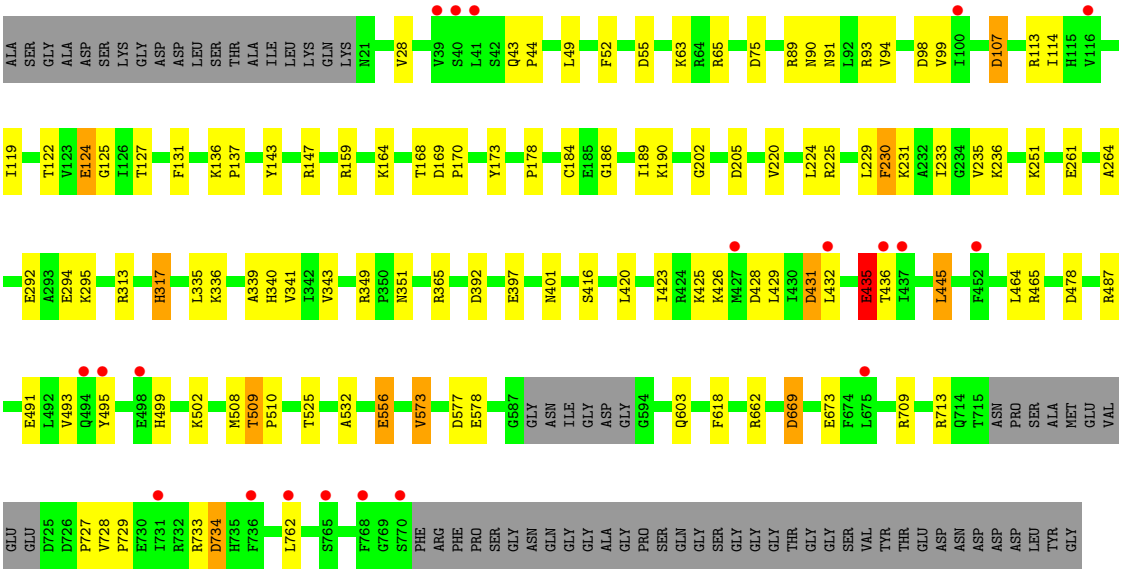
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain D:



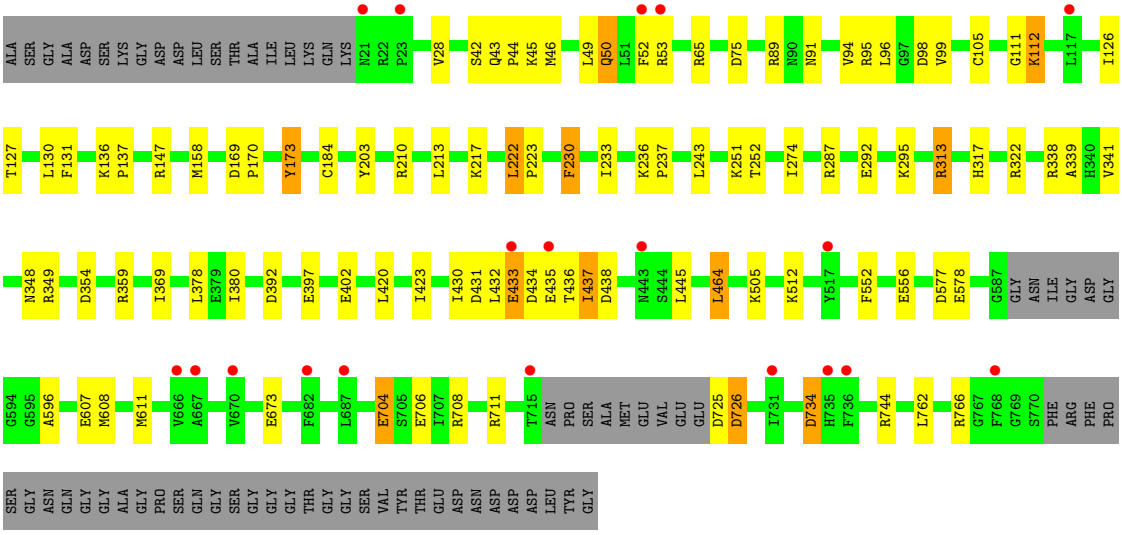
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain E:



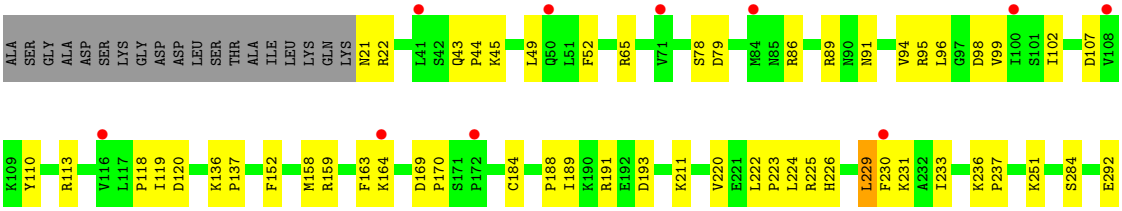
- Molecule 1: Transitional endoplasmic reticulum ATPase

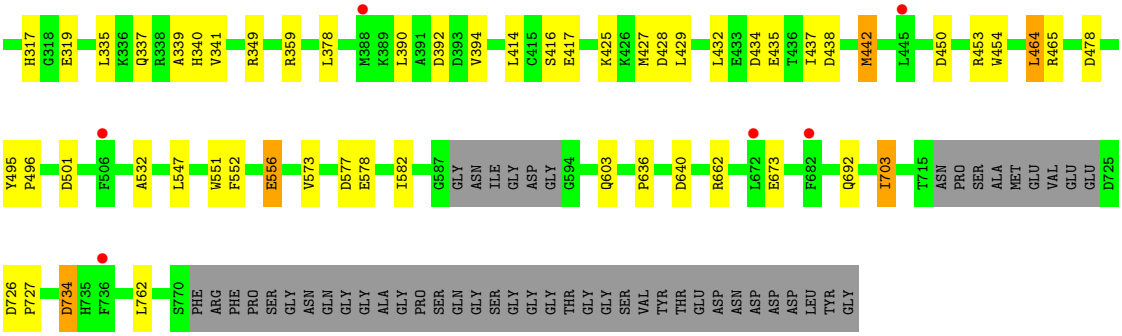
Chain F:



- Molecule 1: Transitional endoplasmic reticulum ATPase

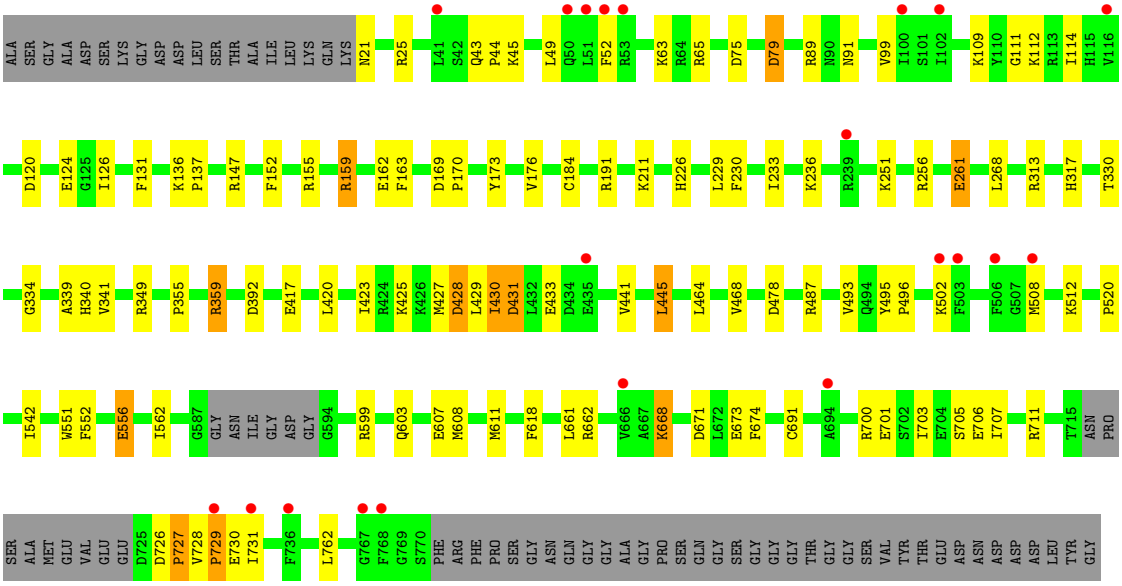
Chain G:





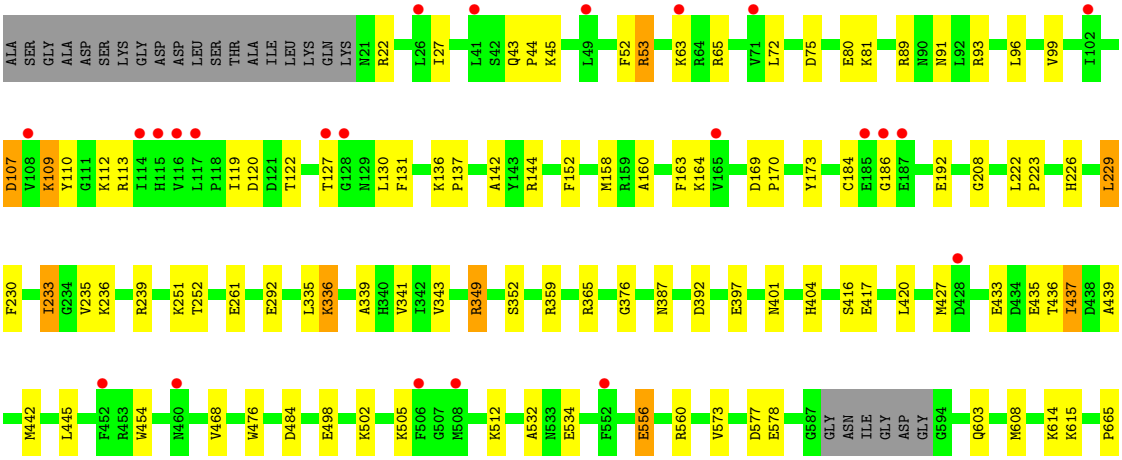
- Molecule 1: Transitional endoplasmic reticulum ATPase

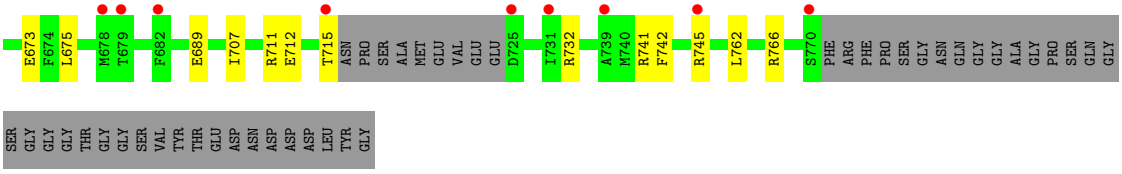
Chain H:



- Molecule 1: Transitional endoplasmic reticulum ATPase

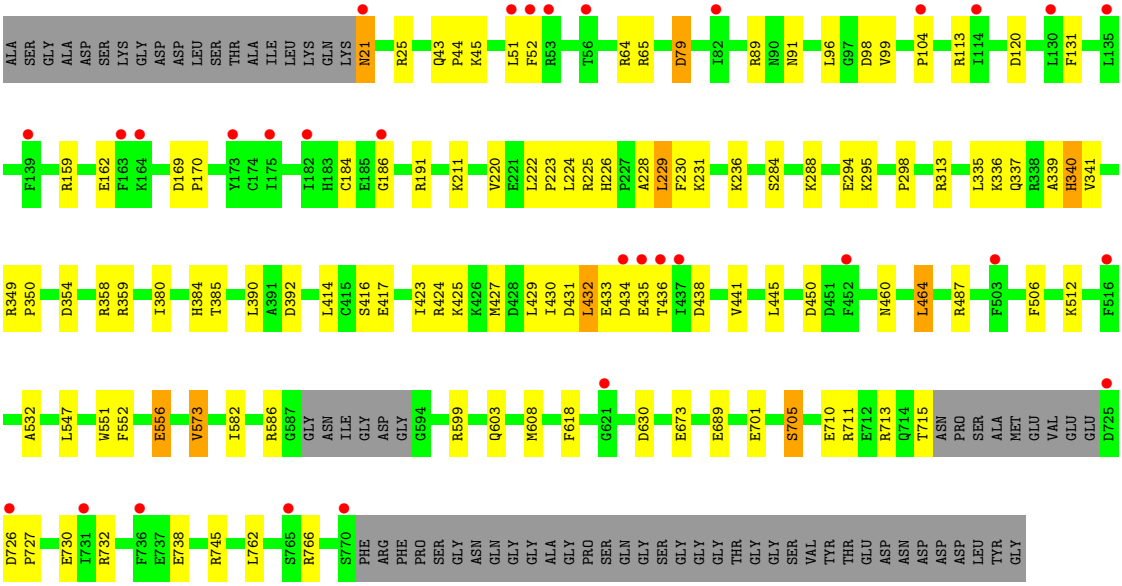
Chain I:





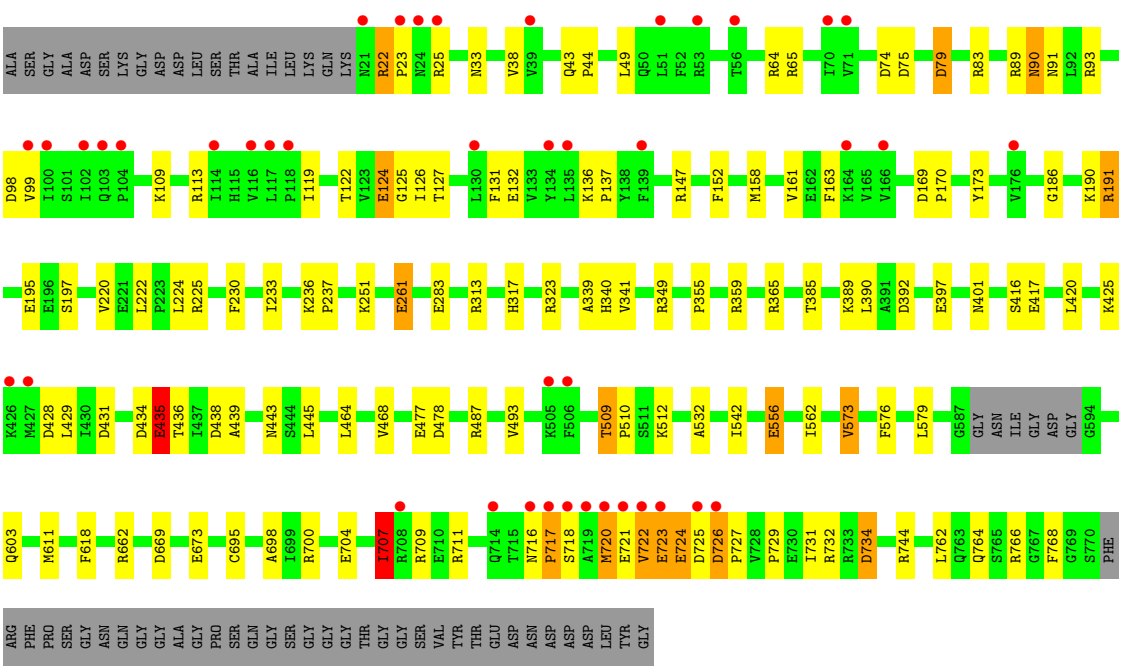
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain J:



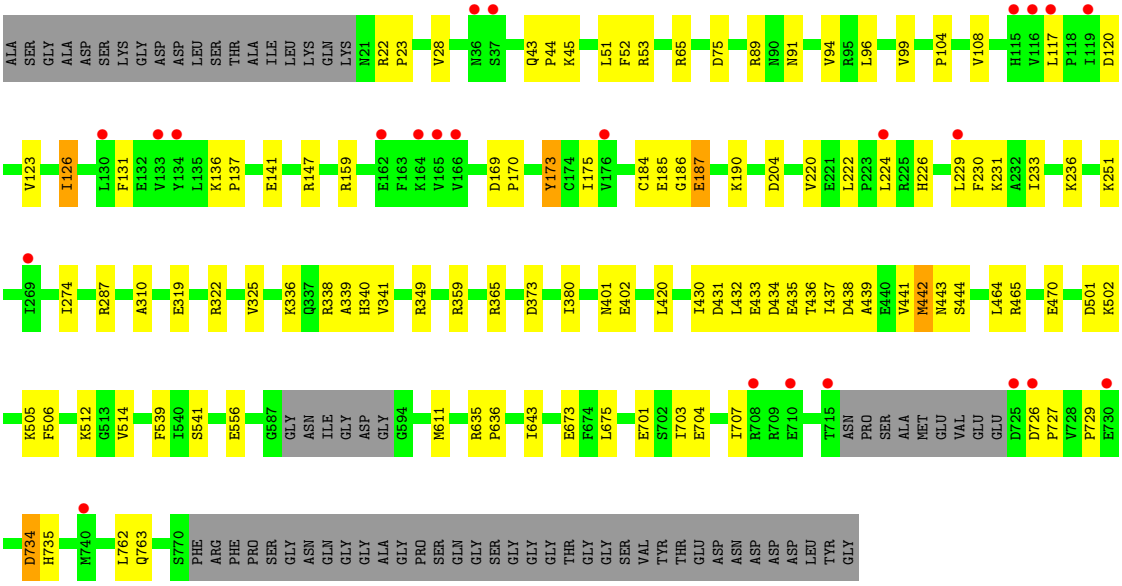
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain K:



• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain L:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.74 (at 3.77Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.190 , 0.254 0.193 , 0.256	Depositor DCC
R_{free} test set	6037 reflections (5.00%)	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)	0.36 , 125.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.059 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.29	0/5856	0.51	0/7906
1	B	0.30	0/5864	0.52	0/7917
1	C	0.29	0/5864	0.53	0/7917
1	D	0.27	0/5864	0.50	0/7917
1	E	0.30	0/5864	0.53	0/7917
1	F	0.30	0/5864	0.54	0/7917
1	G	0.29	0/5856	0.53	0/7906
1	H	0.29	0/5864	0.51	0/7917
1	I	0.28	0/5863	0.51	0/7913
1	J	0.29	0/5864	0.52	0/7917
1	K	0.30	0/5934	0.52	0/8014
1	L	0.29	0/5864	0.51	0/7917
All	All	0.29	0/70421	0.52	0/95075

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.

There are no bond angle outliers.

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5764	5814	5812	48	0
1	B	5771	5819	5819	57	0
1	C	5771	5818	5818	44	0
1	D	5771	5820	5820	46	0
1	E	5771	5818	5818	53	0
1	F	5771	5818	5819	54	0
1	G	5764	5812	5811	52	0
1	H	5771	5819	5819	63	0
1	I	5771	5818	5818	51	0
1	J	5771	5819	5819	47	0
1	K	5839	5880	5879	67	0
1	L	5771	5820	5819	53	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	595	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 (595) 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
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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:251:LYS:NZ	2:C:901:AGS:O2B	2.36	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
1:E:124:GLU:OE1	1:E:125:GLY:N	2.40	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: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:H:706:GLU:OE1	1:I:502:LYS:NZ	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:432:LEU:C	1:L:434:ASP:H	2.11	0.54
1:E:169:ASP:HB3	1:E:170:PRO:HD3	1.90	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: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:J:284:SER:OG	1:J:288:LYS:NZ	2.41	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:434:ASP:C	1:L:436:THR:H	2.14	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:432:LEU:C	1:F:434:ASP:H	2.16	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
1:L:51:LEU:HD21	1:L:104:PRO:HB3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:158:MET:HE1	1:I:445:LEU:HD13	1.97	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:F:434:ASP:C	1:F:436:THR:H	2.17	0.47
1:G:94:VAL:HG13	1:G:98:ASP:HB2	1.97	0.47
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:J:512:LYS:NZ	1:J:608:MET:O	2.42	0.46
1:L:75:ASP:OD1	1:L:75:ASP:N	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:I:75:ASP:OD1	1:I:75:ASP:N	2.49	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:K:716:ASN:C	1:K:718:SER:HA	2.35	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
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:D:136:LYS:HB3	1:D:137:PRO:HD3	1.98	0.45
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: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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:727:PRO:HB2	1:H:729:PRO:CD	2.48	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
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:H:512:LYS:NZ	1:H:608:MET:O	2.43	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:F:438:ASP:OD1	1:F:438:ASP:N	2.51	0.43
1:I:233:ILE:HG22	1:I:235:VAL:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:519:PRO:O	1:B:524:LYS:NZ	2.51	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:226:HIS:HB3	1:I:229:LEU:HG	2.02	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: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: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
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: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:H:427:MET:O	1:H:428:ASP:C	2.57	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:A:726:ASP:N	1:A:727:PRO:HD3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:120:ASP:OD1	1:H:120:ASP:N	2.53	0.42
1:J:298:PRO:HA	1:J:340:HIS:O	2.20	0.42
1:C:734:ASP:N	1:C:734:ASP:OD1	2.53	0.41
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
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: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:H:728:VAL:O	1:H:729:PRO:C	2.59	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:C:208:GLY:HA2	1:C:376:GLY:HA2	2.02	0.41
1:C:442:MET:HA	1:C:442:MET:HE2	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: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:C:727:PRO:C	1:C:729:PRO:HD3	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:204:ASP:OD1	1:L:204:ASP:N	2.54	0.41
1:D:158:MET:HE2	1:E:235:VAL:HG21	2.03	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: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
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: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:B:725:ASP:C	1:B:727:PRO:HD3	2.41	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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: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:G:335:LEU:C	1:G:337:GLN:N	2.74	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: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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	729/805 (91%)	705 (97%)	23 (3%)	1 (0%)	51	83
1	B	729/805 (91%)	703 (96%)	23 (3%)	3 (0%)	34	70
1	C	729/805 (91%)	704 (97%)	23 (3%)	2 (0%)	41	74
1	D	729/805 (91%)	707 (97%)	20 (3%)	2 (0%)	41	74
1	E	729/805 (91%)	704 (97%)	20 (3%)	5 (1%)	22	60
1	F	729/805 (91%)	703 (96%)	22 (3%)	4 (0%)	29	66
1	G	729/805 (91%)	706 (97%)	22 (3%)	1 (0%)	51	83
1	H	729/805 (91%)	702 (96%)	21 (3%)	6 (1%)	19	57
1	I	727/805 (90%)	705 (97%)	21 (3%)	1 (0%)	51	83
1	J	729/805 (91%)	707 (97%)	20 (3%)	2 (0%)	41	74
1	K	740/805 (92%)	700 (95%)	27 (4%)	13 (2%)	8	42
1	L	729/805 (91%)	706 (97%)	18 (2%)	5 (1%)	22	60
All	All	8757/9660 (91%)	8452 (96%)	260 (3%)	45 (0%)	29	66

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

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Mol	Chain	Res	Type
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
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	627/677 (93%)	584 (93%)	43 (7%)	15	46
1	B	628/677 (93%)	591 (94%)	37 (6%)	19	51
1	C	628/677 (93%)	589 (94%)	39 (6%)	18	49
1	D	628/677 (93%)	597 (95%)	31 (5%)	25	55
1	E	628/677 (93%)	590 (94%)	38 (6%)	18	50
1	F	628/677 (93%)	592 (94%)	36 (6%)	20	52
1	G	627/677 (93%)	588 (94%)	39 (6%)	18	49
1	H	628/677 (93%)	593 (94%)	35 (6%)	21	52
1	I	628/677 (93%)	583 (93%)	45 (7%)	14	45
1	J	628/677 (93%)	583 (93%)	45 (7%)	14	45
1	K	636/677 (94%)	594 (93%)	42 (7%)	16	48
1	L	628/677 (93%)	594 (95%)	34 (5%)	22	53
All	All	7542/8124 (93%)	7078 (94%)	464 (6%)	18	49

All (464) 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	184	CYS
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	313	ARG
1	A	317	HIS
1	A	336	LYS
1	A	349	ARG
1	A	351	ASN

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Mol	Chain	Res	Type
1	A	359	ARG
1	A	392	ASP
1	A	414	LEU
1	A	416	SER
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	464	LEU
1	A	487	ARG
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	124	GLU
1	B	131	PHE
1	B	155	ARG
1	B	184	CYS
1	B	235	VAL
1	B	236	LYS
1	B	268	LEU
1	B	278	LEU
1	B	295	LYS
1	B	313	ARG
1	B	317	HIS
1	B	349	ARG
1	B	375	THR

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Mol	Chain	Res	Type
1	B	392	ASP
1	B	416	SER
1	B	420	LEU
1	B	427	MET
1	B	429	LEU
1	B	433	GLU
1	B	464	LEU
1	B	465	ARG
1	B	487	ARG
1	B	556	GLU
1	B	706	GLU
1	B	707	ILE
1	B	714	GLN
1	B	731	ILE
1	B	737	GLU
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	130	LEU
1	C	131	PHE
1	C	173	TYR
1	C	179	ASP
1	C	184	CYS
1	C	187	GLU
1	C	230	PHE
1	C	233	ILE
1	C	235	VAL
1	C	236	LYS
1	C	288	LYS
1	C	313	ARG
1	C	317	HIS
1	C	336	LYS
1	C	349	ARG
1	C	359	ARG
1	C	420	LEU
1	C	427	MET
1	C	437	ILE
1	C	442	MET

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Mol	Chain	Res	Type
1	C	445	LEU
1	C	450	ASP
1	C	498	GLU
1	C	551	TRP
1	C	556	GLU
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	131	PHE
1	D	159	ARG
1	D	211	LYS
1	D	229	LEU
1	D	230	PHE
1	D	236	LYS
1	D	283	GLU
1	D	295	LYS
1	D	335	LEU
1	D	349	ARG
1	D	359	ARG
1	D	392	ASP
1	D	414	LEU
1	D	416	SER
1	D	425	LYS
1	D	430	ILE
1	D	435	GLU
1	D	436	THR
1	D	445	LEU
1	D	556	GLU
1	D	573	VAL
1	D	618	PHE
1	D	706	GLU

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Mol	Chain	Res	Type
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	159	ARG
1	E	184	CYS
1	E	190	LYS
1	E	229	LEU
1	E	230	PHE
1	E	231	LYS
1	E	236	LYS
1	E	292	GLU
1	E	295	LYS
1	E	313	ARG
1	E	317	HIS
1	E	336	LYS
1	E	349	ARG
1	E	351	ASN
1	E	392	ASP
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	487	ARG
1	E	508	MET
1	E	509	THR
1	E	556	GLU
1	E	573	VAL
1	E	669	ASP
1	E	713	ARG
1	E	734	ASP
1	E	762	LEU
1	F	45	LYS
1	F	52	PHE

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Mol	Chain	Res	Type
1	F	53	ARG
1	F	99	VAL
1	F	112	LYS
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	222	LEU
1	F	230	PHE
1	F	236	LYS
1	F	274	ILE
1	F	287	ARG
1	F	292	GLU
1	F	295	LYS
1	F	313	ARG
1	F	317	HIS
1	F	338	ARG
1	F	349	ARG
1	F	359	ARG
1	F	392	ASP
1	F	402	GLU
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	704	GLU
1	F	711	ARG
1	F	734	ASP
1	F	762	LEU
1	G	21	ASN
1	G	22	ARG
1	G	45	LYS
1	G	52	PHE
1	G	78	SER
1	G	99	VAL
1	G	107	ASP
1	G	113	ARG

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Mol	Chain	Res	Type
1	G	159	ARG
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	317	HIS
1	G	319	GLU
1	G	349	ARG
1	G	359	ARG
1	G	378	LEU
1	G	392	ASP
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	464	LEU
1	G	551	TRP
1	G	552	PHE
1	G	556	GLU
1	G	703	ILE
1	G	734	ASP
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	131	PHE
1	H	155	ARG
1	H	159	ARG
1	H	184	CYS

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Mol	Chain	Res	Type
1	H	211	LYS
1	H	229	LEU
1	H	236	LYS
1	H	256	ARG
1	H	261	GLU
1	H	268	LEU
1	H	313	ARG
1	H	317	HIS
1	H	349	ARG
1	H	359	ARG
1	H	392	ASP
1	H	420	LEU
1	H	425	LYS
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	668	LYS
1	H	700	ARG
1	H	711	ARG
1	H	731	ILE
1	H	762	LEU
1	I	22	ARG
1	I	45	LYS
1	I	52	PHE
1	I	53	ARG
1	I	80	GLU
1	I	99	VAL
1	I	107	ASP
1	I	109	LYS
1	I	112	LYS
1	I	113	ARG
1	I	130	LEU
1	I	131	PHE
1	I	173	TYR
1	I	184	CYS
1	I	229	LEU
1	I	230	PHE
1	I	233	ILE
1	I	236	LYS

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Mol	Chain	Res	Type
1	I	292	GLU
1	I	336	LYS
1	I	349	ARG
1	I	359	ARG
1	I	392	ASP
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	498	GLU
1	I	505	LYS
1	I	556	GLU
1	I	614	LYS
1	I	615	LYS
1	I	675	LEU
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	745	ARG
1	I	762	LEU
1	J	21	ASN
1	J	25	ARG
1	J	45	LYS
1	J	52	PHE
1	J	64	ARG
1	J	79	ASP
1	J	99	VAL
1	J	113	ARG
1	J	131	PHE
1	J	159	ARG
1	J	184	CYS
1	J	211	LYS
1	J	229	LEU
1	J	230	PHE
1	J	236	LYS

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Mol	Chain	Res	Type
1	J	295	LYS
1	J	335	LEU
1	J	336	LYS
1	J	349	ARG
1	J	359	ARG
1	J	392	ASP
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	556	GLU
1	J	573	VAL
1	J	618	PHE
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	762	LEU
1	K	22	ARG
1	K	49	LEU
1	K	64	ARG
1	K	79	ASP
1	K	90	ASN
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

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Mol	Chain	Res	Type
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	392	ASP
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	445	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	669	ASP
1	K	700	ARG
1	K	707	ILE
1	K	722	VAL
1	K	723	GLU
1	K	732	ARG
1	K	734	ASP
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

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Mol	Chain	Res	Type
1	L	222	LEU
1	L	230	PHE
1	L	236	LYS
1	L	274	ILE
1	L	287	ARG
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	420	LEU
1	L	431	ASP
1	L	442	MET
1	L	464	LEU
1	L	465	ARG
1	L	505	LYS
1	L	556	GLU
1	L	675	LEU
1	L	734	ASP
1	L	762	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	406	HIS
1	I	340	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	B	902	3	26,33,33	1.43	5 (19%)	26,52,52	1.71	5 (19%)
2	AGS	B	901	3	26,33,33	1.42	5 (19%)	26,52,52	1.62	3 (11%)
2	AGS	J	902	3	26,33,33	1.34	4 (15%)	26,52,52	1.52	2 (7%)
2	AGS	H	901	3	26,33,33	1.43	6 (23%)	26,52,52	1.73	5 (19%)
2	AGS	G	901	3	26,33,33	1.48	7 (26%)	26,52,52	1.70	5 (19%)
2	AGS	E	901	3	26,33,33	1.54	7 (26%)	26,52,52	1.79	4 (15%)
2	AGS	K	902	3	26,33,33	1.44	5 (19%)	26,52,52	1.65	5 (19%)
2	AGS	F	901	3	26,33,33	1.42	5 (19%)	26,52,52	1.78	4 (15%)
2	AGS	L	902	3	26,33,33	1.40	5 (19%)	26,52,52	1.59	3 (11%)
2	AGS	I	901	3	26,33,33	1.42	5 (19%)	26,52,52	1.71	4 (15%)
2	AGS	D	902	3	26,33,33	1.42	5 (19%)	26,52,52	1.54	5 (19%)
2	AGS	C	901	3	26,33,33	1.42	6 (23%)	26,52,52	1.76	4 (15%)
2	AGS	L	901	3	26,33,33	1.45	5 (19%)	26,52,52	1.76	4 (15%)
2	AGS	H	902	3	26,33,33	1.36	5 (19%)	26,52,52	1.69	5 (19%)
2	AGS	G	902	3	26,33,33	1.43	6 (23%)	26,52,52	1.62	4 (15%)
2	AGS	A	902	3	26,33,33	1.40	5 (19%)	26,52,52	1.63	5 (19%)
2	AGS	F	902	3	26,33,33	1.37	5 (19%)	26,52,52	1.70	4 (15%)
2	AGS	E	902	3	26,33,33	1.39	4 (15%)	26,52,52	1.53	4 (15%)
2	AGS	C	902	3	26,33,33	1.43	5 (19%)	26,52,52	1.65	4 (15%)
2	AGS	K	901	3	26,33,33	1.46	6 (23%)	26,52,52	1.62	5 (19%)
2	AGS	J	901	3	26,33,33	1.51	7 (26%)	26,52,52	1.68	5 (19%)
2	AGS	A	901	3	26,33,33	1.53	6 (23%)	26,52,52	1.63	4 (15%)
2	AGS	D	901	3	26,33,33	1.43	6 (23%)	26,52,52	1.57	4 (15%)
2	AGS	I	902	3	26,33,33	1.44	5 (19%)	26,52,52	1.71	4 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AGS	B	902	3	-	2/17/38/38	0/3/3/3
2	AGS	B	901	3	-	1/17/38/38	0/3/3/3
2	AGS	J	902	3	-	4/17/38/38	0/3/3/3
2	AGS	H	901	3	-	4/17/38/38	0/3/3/3
2	AGS	G	901	3	-	2/17/38/38	0/3/3/3
2	AGS	E	901	3	-	1/17/38/38	0/3/3/3
2	AGS	K	902	3	-	6/17/38/38	0/3/3/3
2	AGS	F	901	3	-	2/17/38/38	0/3/3/3
2	AGS	L	902	3	-	8/17/38/38	0/3/3/3
2	AGS	I	901	3	-	3/17/38/38	0/3/3/3
2	AGS	D	902	3	-	4/17/38/38	0/3/3/3
2	AGS	C	901	3	-	5/17/38/38	0/3/3/3
2	AGS	L	901	3	-	4/17/38/38	0/3/3/3
2	AGS	H	902	3	-	4/17/38/38	0/3/3/3
2	AGS	G	902	3	-	9/17/38/38	0/3/3/3
2	AGS	A	902	3	-	7/17/38/38	0/3/3/3
2	AGS	F	902	3	-	6/17/38/38	0/3/3/3
2	AGS	E	902	3	-	6/17/38/38	0/3/3/3
2	AGS	C	902	3	-	5/17/38/38	0/3/3/3
2	AGS	K	901	3	-	2/17/38/38	0/3/3/3
2	AGS	J	901	3	-	3/17/38/38	0/3/3/3
2	AGS	A	901	3	-	2/17/38/38	0/3/3/3
2	AGS	D	901	3	-	0/17/38/38	0/3/3/3
2	AGS	I	902	3	-	5/17/38/38	0/3/3/3

All (130) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	902	AGS	C2-N3	3.54	1.37	1.32
2	E	902	AGS	C2-N3	3.51	1.37	1.32
2	D	902	AGS	C2-N3	3.44	1.37	1.32
2	F	902	AGS	C2-N3	3.40	1.37	1.32
2	C	902	AGS	C2-N3	3.40	1.37	1.32
2	H	902	AGS	C2-N3	3.31	1.37	1.32
2	D	901	AGS	C2-N3	3.28	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	902	AGS	C2-N3	3.26	1.37	1.32
2	E	901	AGS	C2-N3	3.25	1.37	1.32
2	G	902	AGS	C2-N3	3.24	1.37	1.32
2	H	901	AGS	C2-N3	3.23	1.37	1.32
2	J	902	AGS	C2-N3	3.23	1.37	1.32
2	K	901	AGS	C2-N3	3.19	1.37	1.32
2	A	901	AGS	C2-N3	3.19	1.37	1.32
2	L	901	AGS	C2-N3	3.18	1.37	1.32
2	B	901	AGS	C2-N3	3.16	1.37	1.32
2	A	902	AGS	C2-N3	3.10	1.37	1.32
2	F	901	AGS	C2-N3	3.07	1.37	1.32
2	J	901	AGS	C2-N3	3.06	1.37	1.32
2	D	902	AGS	C6-N6	3.02	1.45	1.34
2	H	902	AGS	C6-N6	2.99	1.45	1.34
2	I	902	AGS	C6-N6	2.98	1.44	1.34
2	G	902	AGS	C6-N6	2.98	1.44	1.34
2	I	901	AGS	C2-N3	2.97	1.36	1.32
2	B	902	AGS	C6-N6	2.95	1.44	1.34
2	K	902	AGS	C2-N3	2.94	1.36	1.32
2	C	902	AGS	C6-N6	2.94	1.44	1.34
2	G	901	AGS	C2-N3	2.94	1.36	1.32
2	C	901	AGS	C2-N3	2.93	1.36	1.32
2	A	902	AGS	C6-N6	2.92	1.44	1.34
2	D	901	AGS	C6-N6	2.92	1.44	1.34
2	E	902	AGS	C6-N6	2.92	1.44	1.34
2	L	902	AGS	C6-N6	2.91	1.44	1.34
2	F	902	AGS	C6-N6	2.91	1.44	1.34
2	B	902	AGS	C2-N3	2.90	1.36	1.32
2	L	901	AGS	C6-N6	2.87	1.44	1.34
2	H	901	AGS	C6-N6	2.86	1.44	1.34
2	E	901	AGS	C6-N6	2.83	1.44	1.34
2	K	901	AGS	C6-N6	2.82	1.44	1.34
2	K	902	AGS	C6-N6	2.82	1.44	1.34
2	J	902	AGS	C6-N6	2.82	1.44	1.34
2	C	901	AGS	C6-N6	2.80	1.44	1.34
2	G	901	AGS	C6-N6	2.79	1.44	1.34
2	F	901	AGS	C6-N6	2.78	1.44	1.34
2	B	901	AGS	C6-N6	2.73	1.44	1.34
2	A	901	AGS	C6-N6	2.72	1.44	1.34
2	J	901	AGS	C6-N6	2.69	1.43	1.34
2	I	901	AGS	C6-N6	2.65	1.43	1.34
2	J	901	AGS	O2'-C2'	-2.65	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	901	AGS	O2'-C2'	-2.52	1.37	1.43
2	E	901	AGS	PG-S1G	2.50	1.96	1.90
2	A	901	AGS	O2'-C2'	-2.50	1.37	1.43
2	F	901	AGS	O2'-C2'	-2.47	1.37	1.43
2	I	902	AGS	O2'-C2'	-2.46	1.37	1.43
2	K	902	AGS	O2'-C2'	-2.45	1.37	1.43
2	E	902	AGS	PG-S1G	2.42	1.95	1.90
2	B	902	AGS	O2'-C2'	-2.40	1.37	1.43
2	L	902	AGS	O2'-C2'	-2.39	1.37	1.43
2	K	902	AGS	C2'-C3'	-2.39	1.46	1.53
2	I	901	AGS	PG-S1G	2.38	1.95	1.90
2	A	902	AGS	O2'-C2'	-2.37	1.37	1.43
2	B	902	AGS	C2'-C3'	-2.37	1.46	1.53
2	G	902	AGS	O2'-C2'	-2.36	1.37	1.43
2	C	901	AGS	O2'-C2'	-2.34	1.37	1.43
2	C	902	AGS	O2'-C2'	-2.33	1.37	1.43
2	D	901	AGS	O2'-C2'	-2.32	1.37	1.43
2	L	901	AGS	O2'-C2'	-2.32	1.37	1.43
2	G	901	AGS	O2'-C2'	-2.32	1.37	1.43
2	B	901	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	H	901	AGS	O2'-C2'	-2.31	1.37	1.43
2	I	901	AGS	O2'-C2'	-2.30	1.37	1.43
2	K	901	AGS	O2'-C2'	-2.29	1.37	1.43
2	A	901	AGS	O3'-C3'	-2.27	1.37	1.43
2	D	902	AGS	O2'-C2'	-2.25	1.37	1.43
2	A	901	AGS	C2'-C1'	-2.24	1.50	1.53
2	A	901	AGS	PG-S1G	2.24	1.95	1.90
2	H	901	AGS	O3'-C3'	-2.24	1.37	1.43
2	H	901	AGS	PG-S1G	2.23	1.95	1.90
2	G	901	AGS	C2'-C1'	-2.23	1.50	1.53
2	E	901	AGS	O3'-C3'	-2.22	1.37	1.43
2	D	901	AGS	PG-S1G	2.22	1.95	1.90
2	F	902	AGS	O2'-C2'	-2.21	1.37	1.43
2	H	902	AGS	O2'-C2'	-2.21	1.37	1.43
2	L	901	AGS	O3'-C3'	-2.21	1.37	1.43
2	F	902	AGS	PG-S1G	2.21	1.95	1.90
2	K	901	AGS	O3'-C3'	-2.20	1.37	1.43
2	K	902	AGS	O3'-C3'	-2.20	1.37	1.43
2	G	902	AGS	C2'-C3'	-2.20	1.47	1.53
2	E	901	AGS	C2'-C1'	-2.20	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	902	AGS	C2'-C3'	-2.20	1.47	1.53
2	E	901	AGS	C2'-C3'	-2.19	1.47	1.53
2	J	901	AGS	C2'-C3'	-2.19	1.47	1.53
2	G	901	AGS	O3'-C3'	-2.19	1.37	1.43
2	K	901	AGS	PG-S1G	2.19	1.95	1.90
2	J	901	AGS	PG-S1G	2.17	1.95	1.90
2	C	901	AGS	C2'-C3'	-2.17	1.47	1.53
2	B	901	AGS	PG-S1G	2.16	1.95	1.90
2	F	901	AGS	O3'-C3'	-2.15	1.37	1.43
2	B	902	AGS	O3'-C3'	-2.15	1.37	1.43
2	B	901	AGS	O3'-C3'	-2.14	1.37	1.43
2	G	902	AGS	PG-S1G	2.12	1.95	1.90
2	L	902	AGS	C2'-C3'	-2.12	1.47	1.53
2	J	901	AGS	O3'-C3'	-2.11	1.38	1.43
2	L	901	AGS	C2'-C3'	-2.09	1.47	1.53
2	G	901	AGS	C2'-C3'	-2.09	1.47	1.53
2	C	901	AGS	O3'-C3'	-2.09	1.38	1.43
2	F	902	AGS	C2'-C3'	-2.09	1.47	1.53
2	L	902	AGS	O3'-C3'	-2.09	1.38	1.43
2	H	901	AGS	C2'-C3'	-2.09	1.47	1.53
2	I	902	AGS	O3'-C3'	-2.08	1.38	1.43
2	J	901	AGS	C2'-C1'	-2.08	1.50	1.53
2	D	901	AGS	C2'-C3'	-2.08	1.47	1.53
2	H	902	AGS	C2'-C3'	-2.08	1.47	1.53
2	A	902	AGS	O3'-C3'	-2.07	1.38	1.43
2	E	902	AGS	O2'-C2'	-2.07	1.38	1.43
2	C	902	AGS	O3'-C3'	-2.07	1.38	1.43
2	D	902	AGS	PG-S1G	2.05	1.95	1.90
2	G	902	AGS	O3'-C3'	-2.05	1.38	1.43
2	I	902	AGS	PG-S1G	2.05	1.95	1.90
2	I	901	AGS	C2'-C3'	-2.05	1.47	1.53
2	D	902	AGS	O3'-C3'	-2.04	1.38	1.43
2	J	902	AGS	PG-S1G	2.04	1.95	1.90
2	F	901	AGS	C2'-C3'	-2.04	1.47	1.53
2	J	902	AGS	O2'-C2'	-2.03	1.38	1.43
2	H	902	AGS	O3'-C3'	-2.03	1.38	1.43
2	D	901	AGS	O3'-C3'	-2.02	1.38	1.43
2	K	901	AGS	C2'-C1'	-2.01	1.50	1.53
2	A	902	AGS	C3'-C4'	-2.00	1.47	1.53

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	902	AGS	N3-C2-N1	-5.74	119.70	128.68
2	J	902	AGS	N3-C2-N1	-5.69	119.79	128.68
2	L	901	AGS	N3-C2-N1	-5.63	119.88	128.68
2	B	902	AGS	N3-C2-N1	-5.58	119.96	128.68
2	G	901	AGS	N3-C2-N1	-5.56	119.98	128.68
2	L	902	AGS	N3-C2-N1	-5.52	120.06	128.68
2	H	902	AGS	N3-C2-N1	-5.51	120.07	128.68
2	C	902	AGS	N3-C2-N1	-5.47	120.13	128.68
2	G	902	AGS	N3-C2-N1	-5.46	120.14	128.68
2	A	902	AGS	N3-C2-N1	-5.46	120.14	128.68
2	I	902	AGS	N3-C2-N1	-5.46	120.15	128.68
2	K	902	AGS	N3-C2-N1	-5.44	120.18	128.68
2	A	901	AGS	N3-C2-N1	-5.42	120.20	128.68
2	E	901	AGS	N3-C2-N1	-5.41	120.22	128.68
2	D	901	AGS	N3-C2-N1	-5.41	120.22	128.68
2	K	901	AGS	N3-C2-N1	-5.36	120.31	128.68
2	D	902	AGS	N3-C2-N1	-5.35	120.32	128.68
2	J	901	AGS	N3-C2-N1	-5.33	120.35	128.68
2	F	901	AGS	N3-C2-N1	-5.29	120.41	128.68
2	C	901	AGS	N3-C2-N1	-5.25	120.47	128.68
2	I	901	AGS	N3-C2-N1	-5.22	120.53	128.68
2	E	902	AGS	N3-C2-N1	-5.16	120.62	128.68
2	H	901	AGS	N3-C2-N1	-5.11	120.68	128.68
2	B	901	AGS	N3-C2-N1	-5.00	120.86	128.68
2	E	901	AGS	PA-O3A-PB	-4.73	116.61	132.83
2	I	901	AGS	PA-O3A-PB	-4.04	118.96	132.83
2	F	901	AGS	PA-O3A-PB	-3.88	119.50	132.83
2	H	902	AGS	PA-O3A-PB	-3.81	119.76	132.83
2	C	901	AGS	PA-O3A-PB	-3.71	120.11	132.83
2	H	901	AGS	C3'-C2'-C1'	3.70	106.55	100.98
2	L	901	AGS	PA-O3A-PB	-3.70	120.14	132.83
2	H	901	AGS	PA-O3A-PB	-3.70	120.14	132.83
2	G	901	AGS	PA-O3A-PB	-3.62	120.41	132.83
2	A	901	AGS	PA-O3A-PB	-3.61	120.43	132.83
2	C	902	AGS	PA-O3A-PB	-3.60	120.49	132.83
2	J	901	AGS	PA-O3A-PB	-3.52	120.73	132.83
2	C	901	AGS	C3'-C2'-C1'	3.48	106.22	100.98
2	B	901	AGS	C3'-C2'-C1'	3.44	106.16	100.98
2	L	902	AGS	PA-O3A-PB	-3.44	121.03	132.83
2	I	902	AGS	PA-O3A-PB	-3.42	121.08	132.83
2	B	901	AGS	PA-O3A-PB	-3.31	121.48	132.83
2	B	902	AGS	PA-O3A-PB	-3.28	121.57	132.83
2	K	901	AGS	PA-O3A-PB	-3.22	121.77	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	902	AGS	C3'-C2'-C1'	3.18	105.77	100.98
2	L	901	AGS	C3'-C2'-C1'	3.17	105.75	100.98
2	E	901	AGS	C3'-C2'-C1'	3.14	105.71	100.98
2	G	902	AGS	PA-O3A-PB	-3.12	122.12	132.83
2	K	902	AGS	PA-O3A-PB	-3.10	122.20	132.83
2	J	901	AGS	C3'-C2'-C1'	3.08	105.62	100.98
2	F	901	AGS	C3'-C2'-C1'	3.08	105.61	100.98
2	D	901	AGS	PA-O3A-PB	-3.03	122.43	132.83
2	I	901	AGS	C3'-C2'-C1'	2.99	105.48	100.98
2	B	902	AGS	C3'-C2'-C1'	2.97	105.44	100.98
2	F	902	AGS	PA-O3A-PB	-2.91	122.83	132.83
2	K	901	AGS	C3'-C2'-C1'	2.82	105.22	100.98
2	A	901	AGS	C3'-C2'-C1'	2.81	105.20	100.98
2	A	902	AGS	C3'-C2'-C1'	2.78	105.16	100.98
2	F	902	AGS	C3'-C2'-C1'	2.77	105.15	100.98
2	G	901	AGS	C3'-C2'-C1'	2.76	105.14	100.98
2	E	901	AGS	O4'-C4'-C3'	2.75	110.56	105.11
2	E	902	AGS	PA-O3A-PB	-2.73	123.46	132.83
2	G	902	AGS	C3'-C2'-C1'	2.71	105.06	100.98
2	D	902	AGS	PA-O3A-PB	-2.67	123.67	132.83
2	I	901	AGS	O4'-C4'-C3'	2.65	110.37	105.11
2	J	901	AGS	O4'-C4'-C3'	2.64	110.34	105.11
2	K	902	AGS	C3'-C2'-C1'	2.62	104.92	100.98
2	J	902	AGS	PA-O3A-PB	-2.57	124.00	132.83
2	A	902	AGS	PA-O3A-PB	-2.57	124.02	132.83
2	G	901	AGS	O4'-C4'-C3'	2.49	110.05	105.11
2	F	901	AGS	O4'-C4'-C3'	2.47	110.00	105.11
2	L	901	AGS	O4'-C4'-C3'	2.43	109.93	105.11
2	A	901	AGS	O4'-C4'-C3'	2.41	109.87	105.11
2	C	902	AGS	C3'-C2'-C1'	2.38	104.57	100.98
2	H	901	AGS	O4'-C4'-C3'	2.38	109.81	105.11
2	K	902	AGS	O4'-C4'-C3'	2.36	109.78	105.11
2	C	901	AGS	O4'-C4'-C3'	2.36	109.78	105.11
2	H	901	AGS	C4-C5-N7	-2.35	106.94	109.40
2	E	902	AGS	C3'-C2'-C1'	2.32	104.48	100.98
2	L	902	AGS	C4-C5-N7	-2.32	106.98	109.40
2	H	902	AGS	C3'-C2'-C1'	2.32	104.46	100.98
2	D	902	AGS	C3'-C2'-C1'	2.29	104.43	100.98
2	E	902	AGS	C4-C5-N7	-2.28	107.02	109.40
2	F	902	AGS	O4'-C4'-C3'	2.24	109.55	105.11
2	C	902	AGS	O3G-PG-O3B	2.22	112.07	104.64
2	A	902	AGS	C4-C5-N7	-2.22	107.08	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	902	AGS	C4-C5-N7	-2.21	107.10	109.40
2	I	902	AGS	O4'-C4'-C3'	2.20	109.46	105.11
2	D	901	AGS	C3'-C2'-C1'	2.19	104.27	100.98
2	G	902	AGS	O4'-C4'-C3'	2.19	109.44	105.11
2	B	902	AGS	O4'-C4'-C3'	2.18	109.42	105.11
2	D	901	AGS	C4-C5-N7	-2.14	107.16	109.40
2	A	902	AGS	O4'-C4'-C3'	2.14	109.35	105.11
2	K	901	AGS	O4'-C4'-C3'	2.14	109.35	105.11
2	H	902	AGS	O4'-C4'-C3'	2.11	109.30	105.11
2	H	902	AGS	C4-C5-N7	-2.09	107.22	109.40
2	B	902	AGS	C4-C5-N7	-2.08	107.23	109.40
2	D	902	AGS	O3G-PG-O3B	2.05	111.47	104.64
2	D	902	AGS	C4-C5-N7	-2.04	107.28	109.40
2	K	901	AGS	C4-C5-N7	-2.03	107.28	109.40
2	J	901	AGS	C4-C5-N7	-2.02	107.30	109.40
2	G	901	AGS	O4'-C1'-C2'	2.01	109.86	106.93

There are no chirality outliers.

All (95) 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	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	902	AGS	C5'-O5'-PA-O1A
2	C	902	AGS	C5'-O5'-PA-O2A
2	D	902	AGS	C5'-O5'-PA-O1A
2	D	902	AGS	C5'-O5'-PA-O2A
2	E	902	AGS	PB-O3B-PG-O2G
2	E	902	AGS	PB-O3B-PG-O3G
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

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Mol	Chain	Res	Type	Atoms
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	K	902	AGS	PB-O3B-PG-O2G
2	K	902	AGS	PB-O3B-PG-O3G
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	I	902	AGS	C3'-C4'-C5'-O5'
2	I	902	AGS	O4'-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	C5'-O5'-PA-O3A
2	D	902	AGS	C5'-O5'-PA-O3A
2	J	902	AGS	C5'-O5'-PA-O3A
2	L	902	AGS	C5'-O5'-PA-O3A
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
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	L	901	AGS	C5'-O5'-PA-O1A
2	G	901	AGS	O4'-C4'-C5'-O5'

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

There are no ring outliers.

19 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	902	AGS	1	0
2	B	901	AGS	3	0
2	J	902	AGS	2	0
2	H	901	AGS	1	0
2	G	901	AGS	1	0

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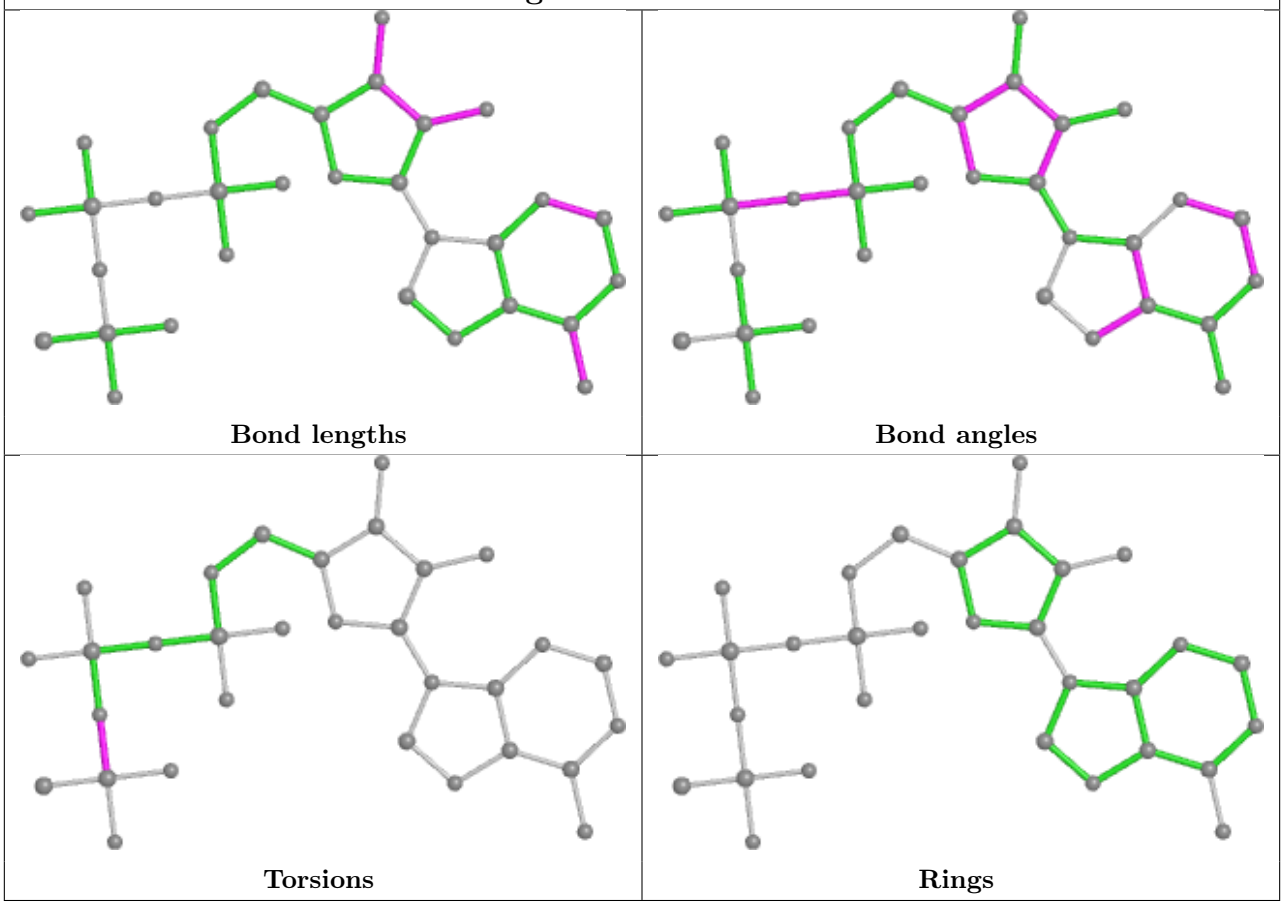
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	901	AGS	2	0
2	K	902	AGS	1	0
2	F	901	AGS	5	0
2	L	902	AGS	2	0
2	I	901	AGS	2	0
2	C	901	AGS	2	0
2	L	901	AGS	2	0
2	G	902	AGS	1	0
2	F	902	AGS	1	0
2	E	902	AGS	1	0
2	C	902	AGS	1	0
2	K	901	AGS	1	0
2	J	901	AGS	2	0
2	I	902	AGS	2	0

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

Ligand AGS B 902



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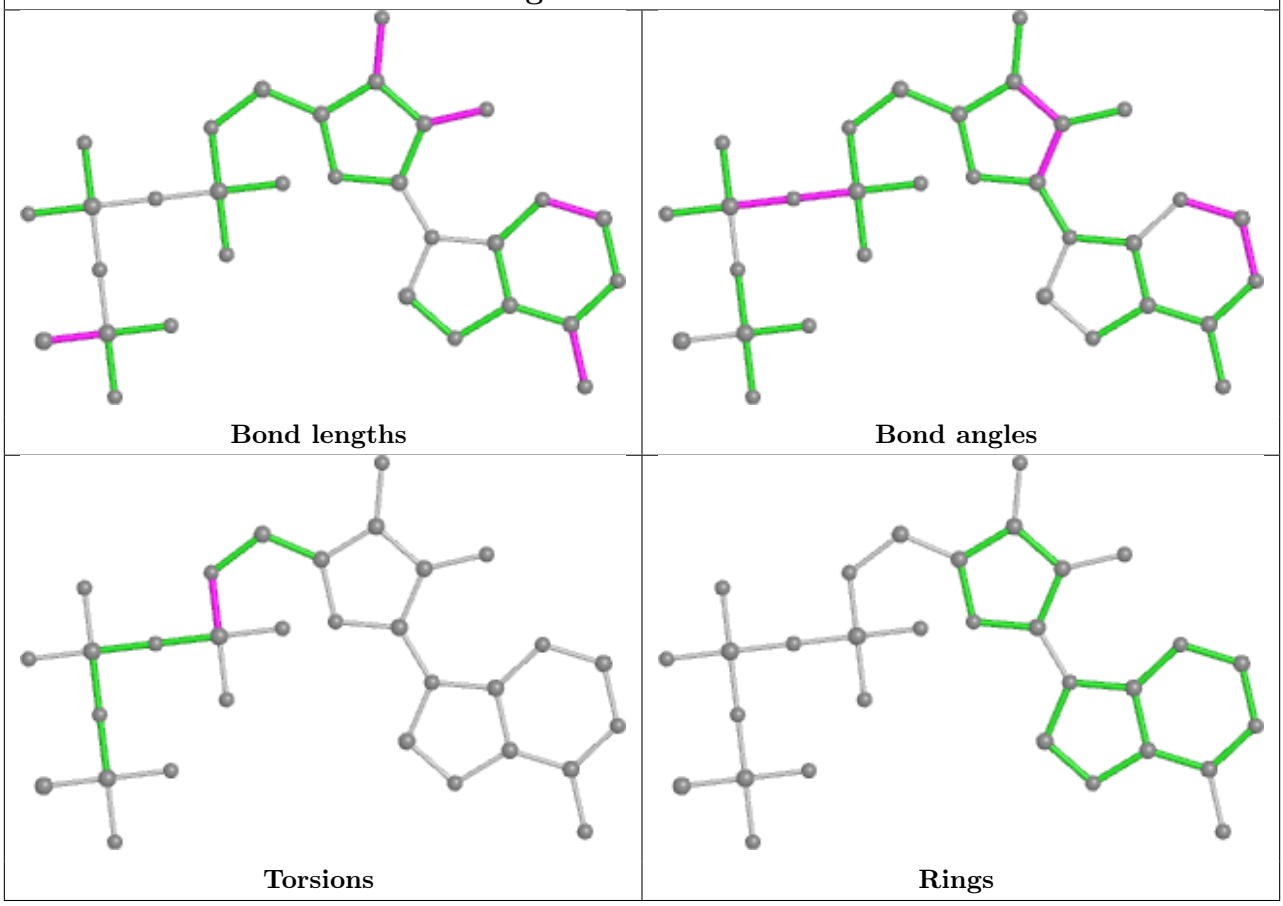

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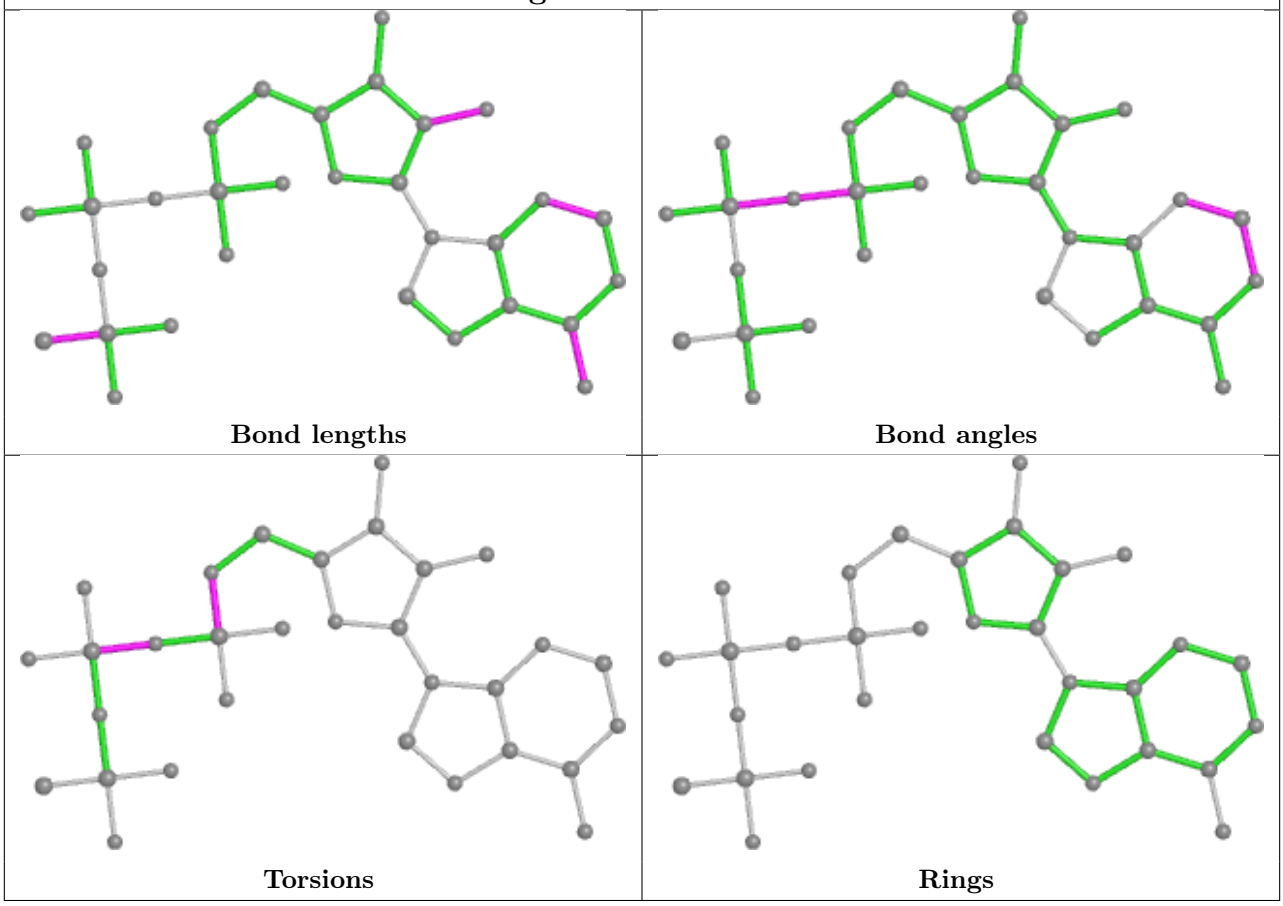

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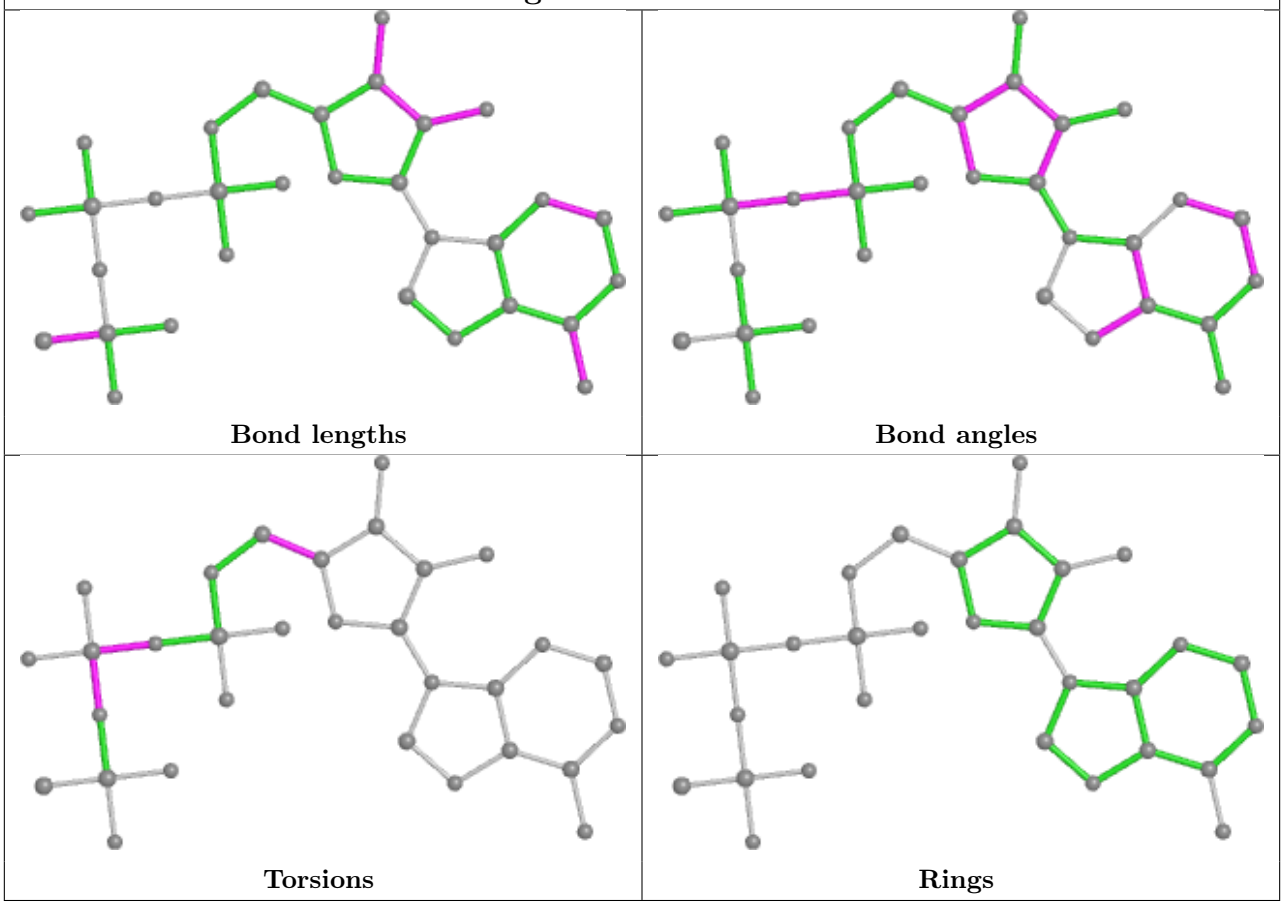

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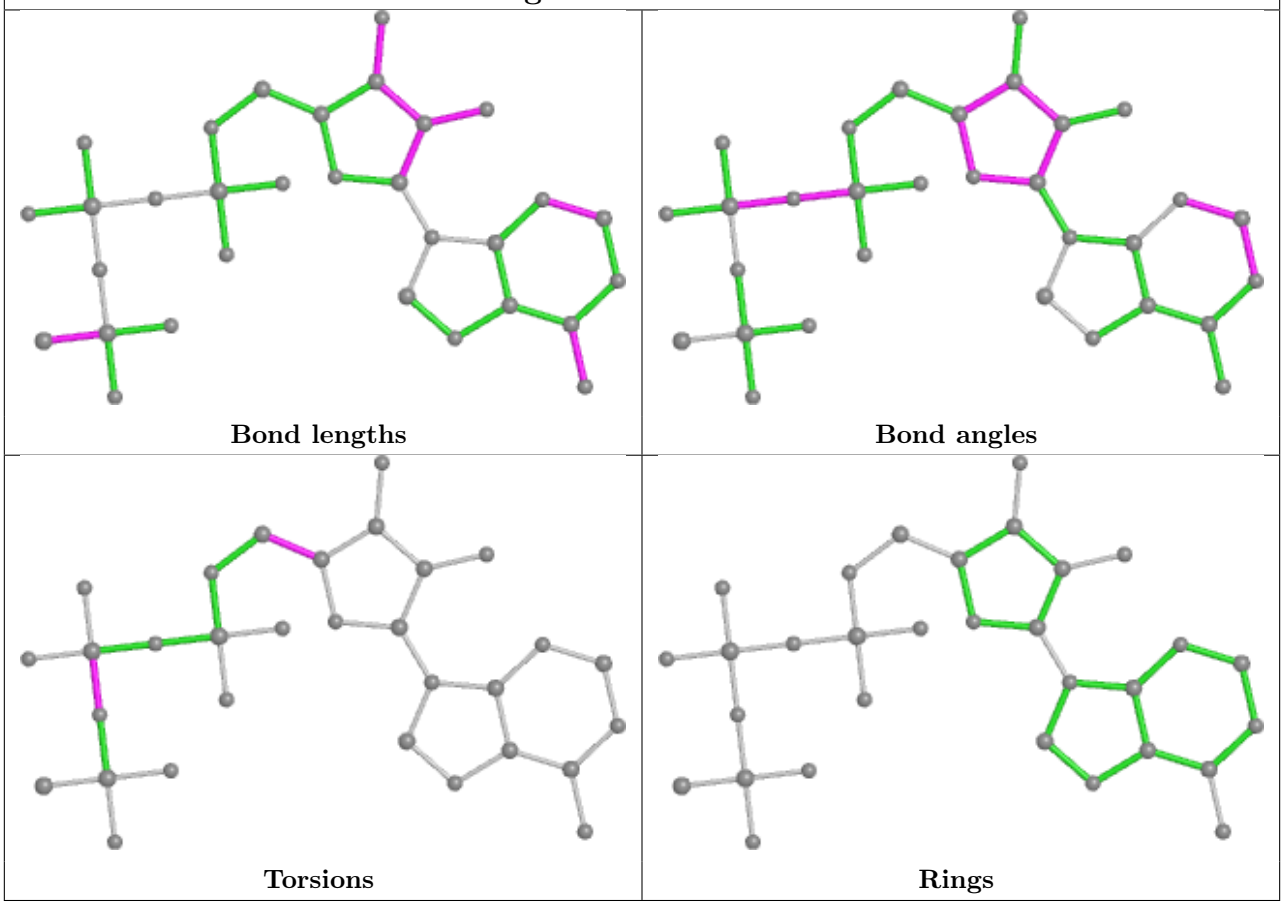

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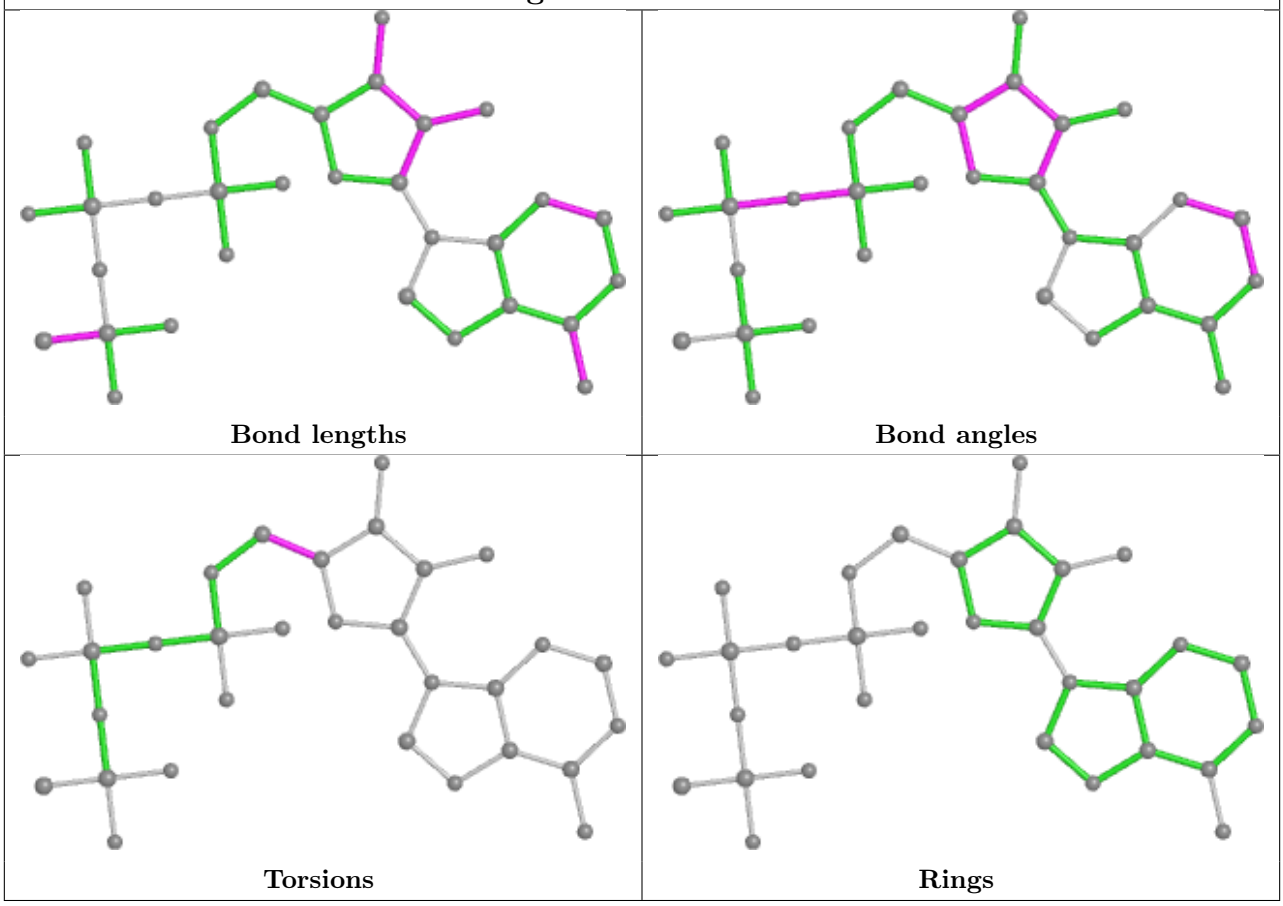

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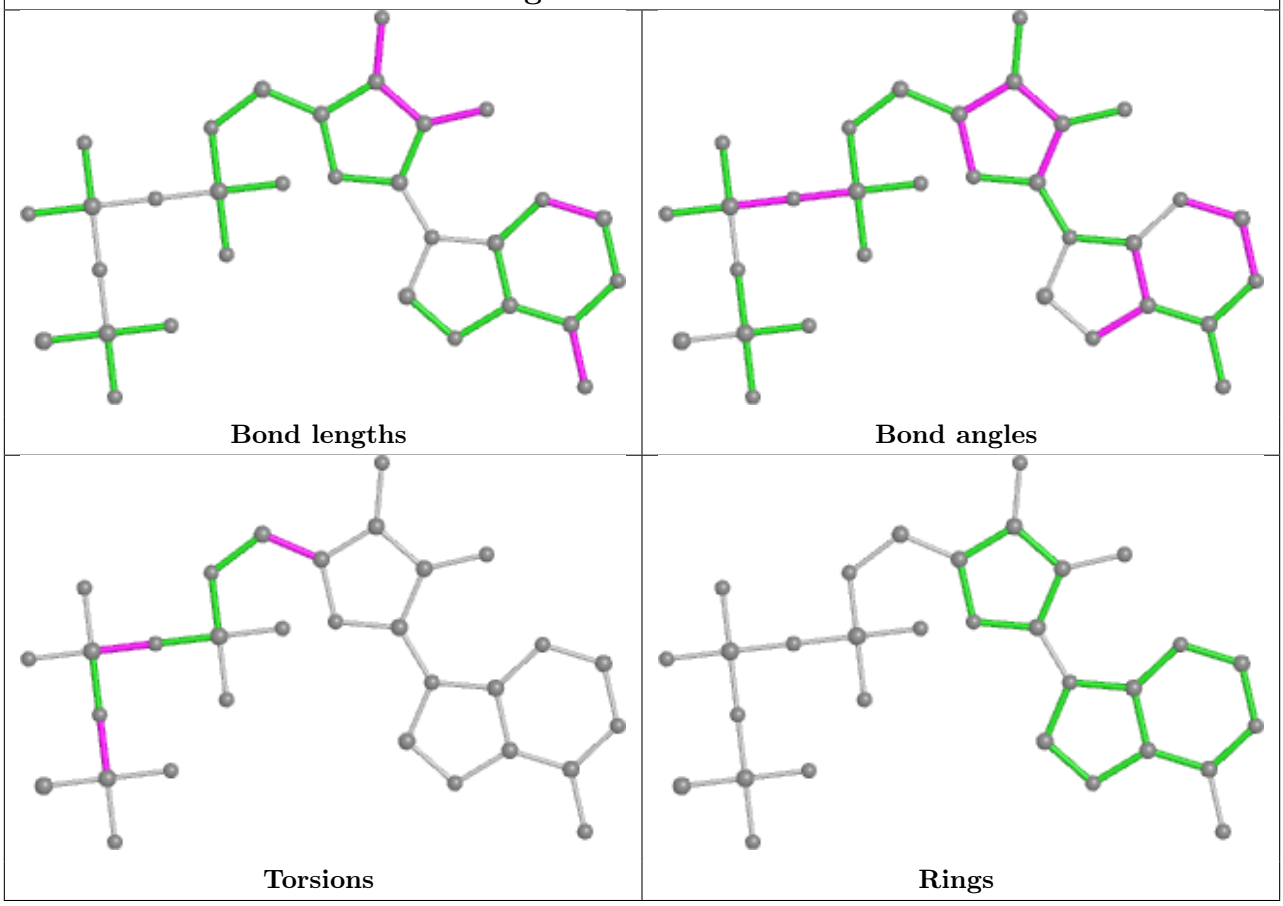

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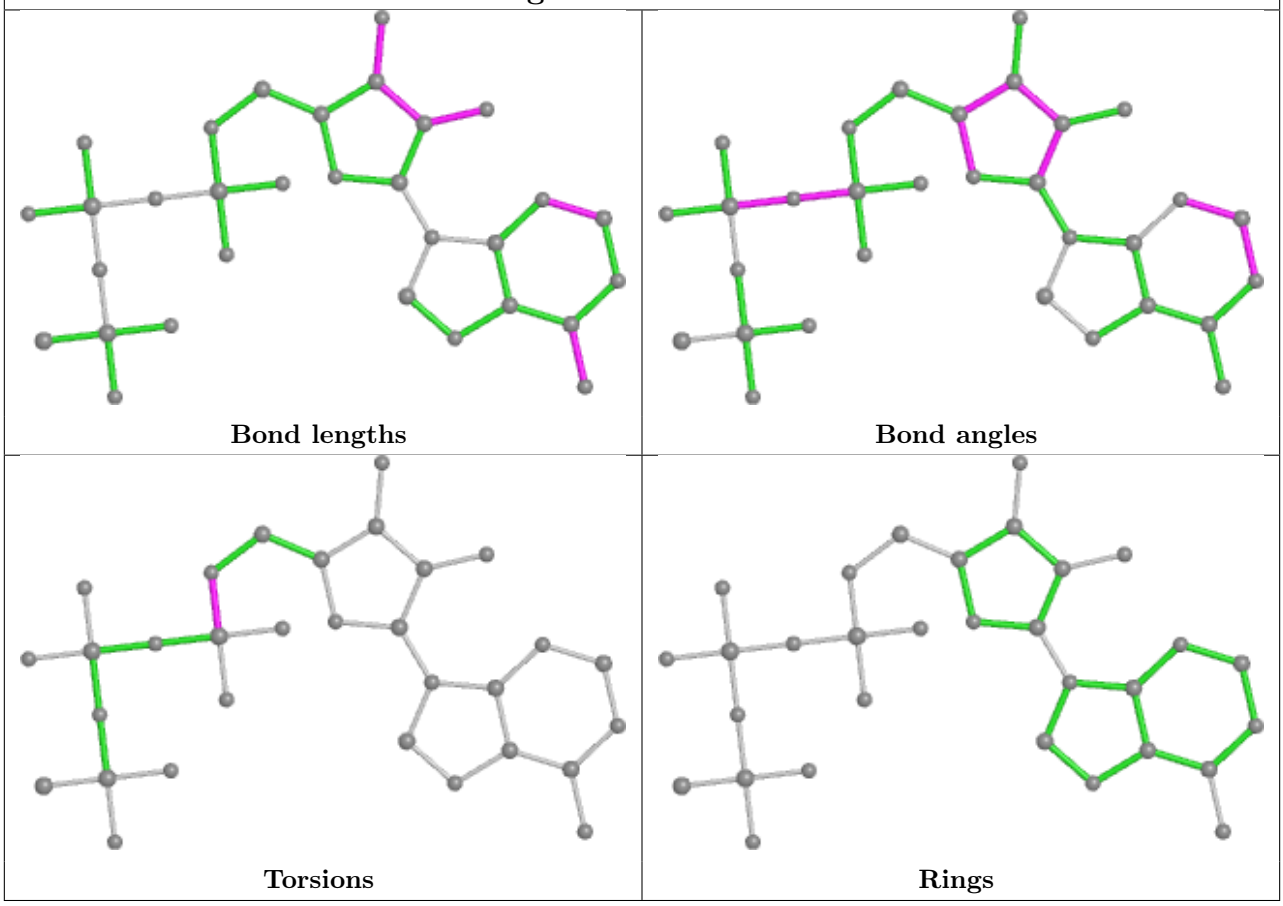

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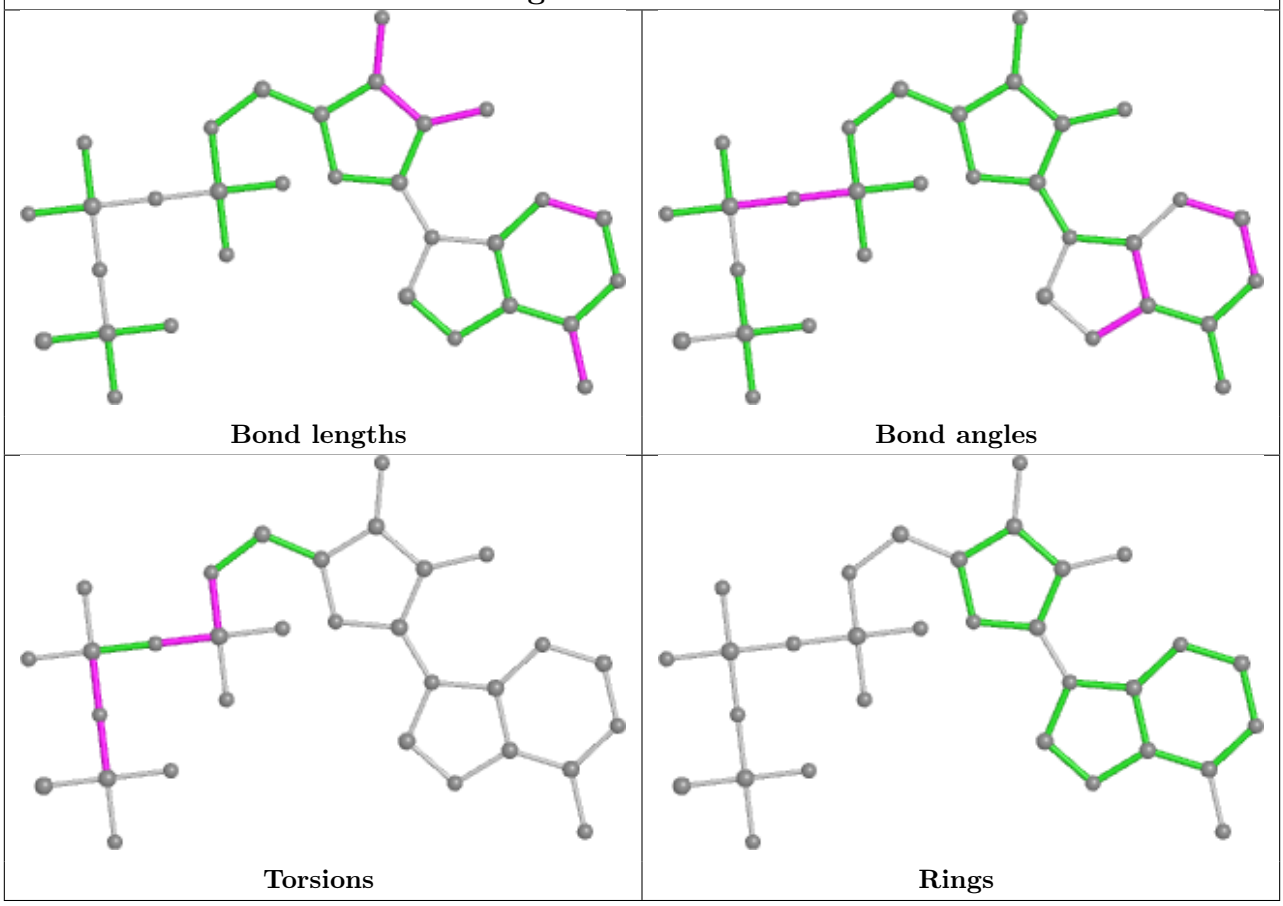

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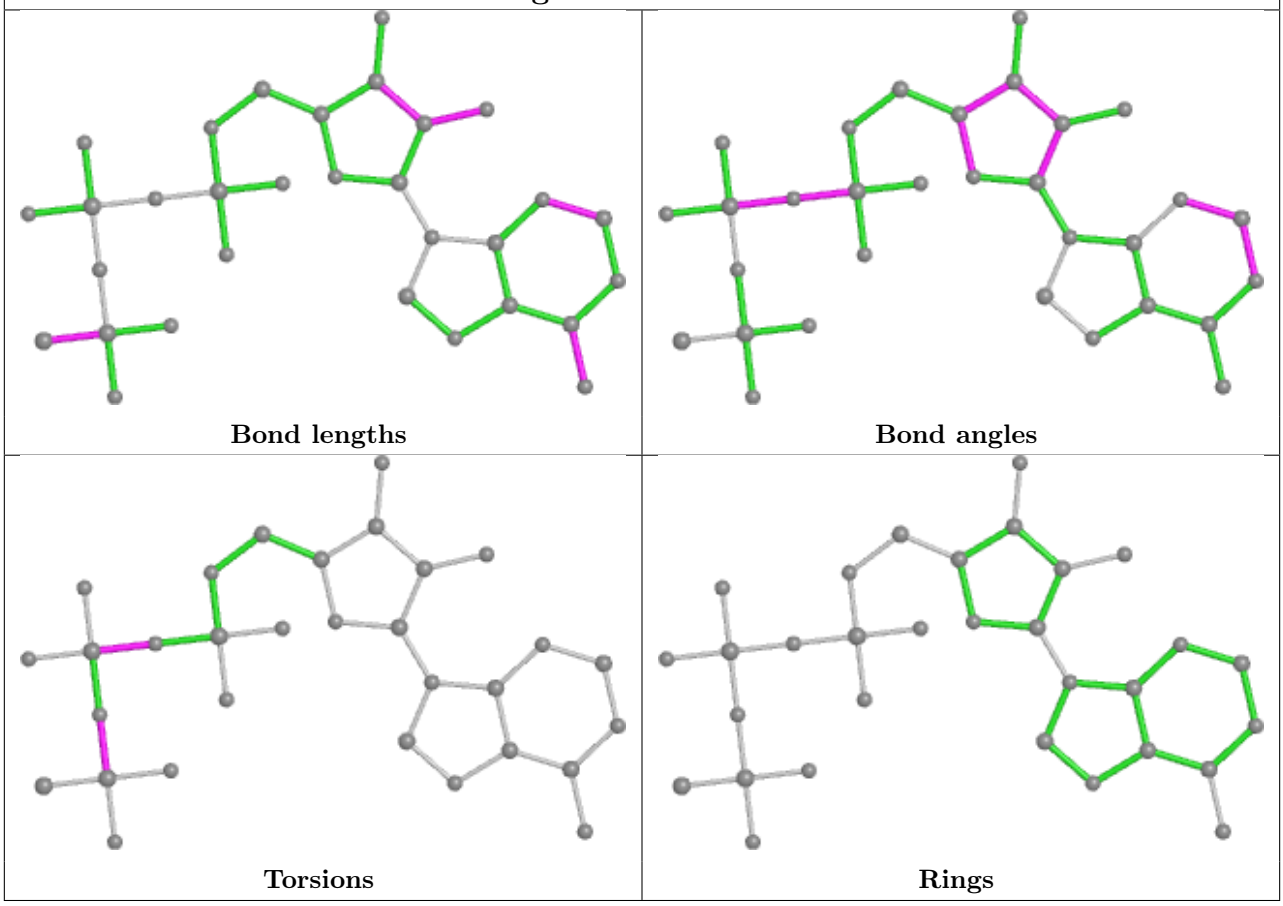

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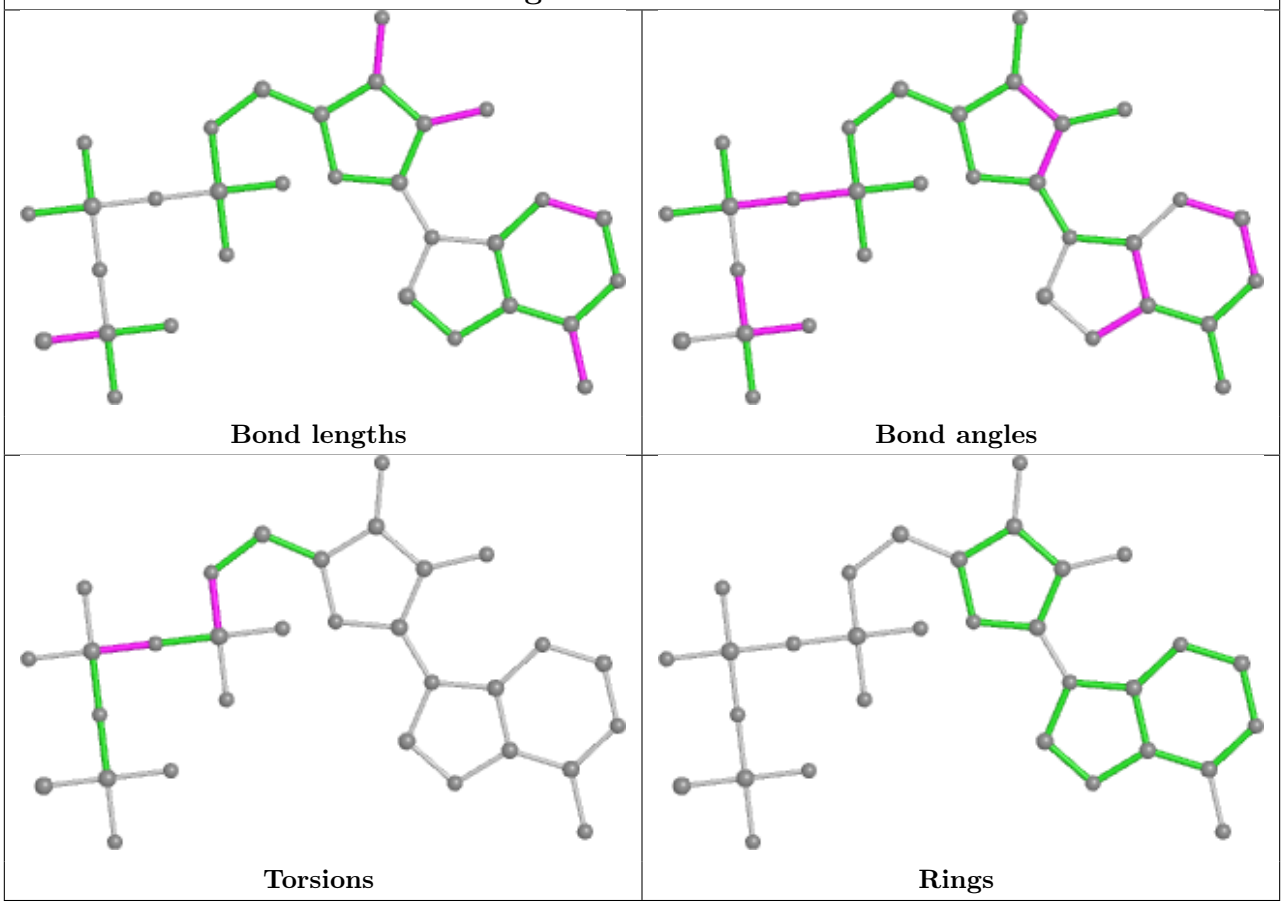

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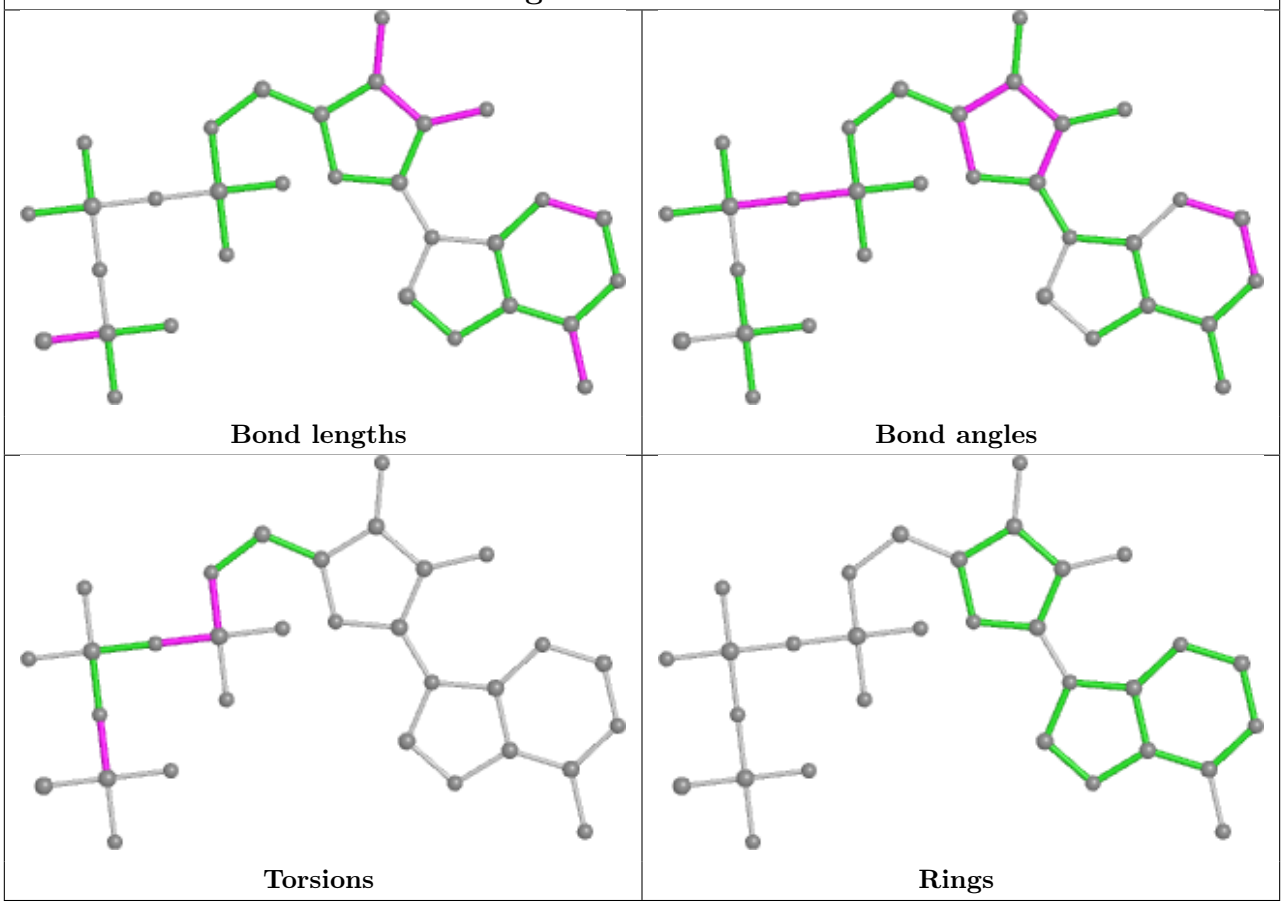

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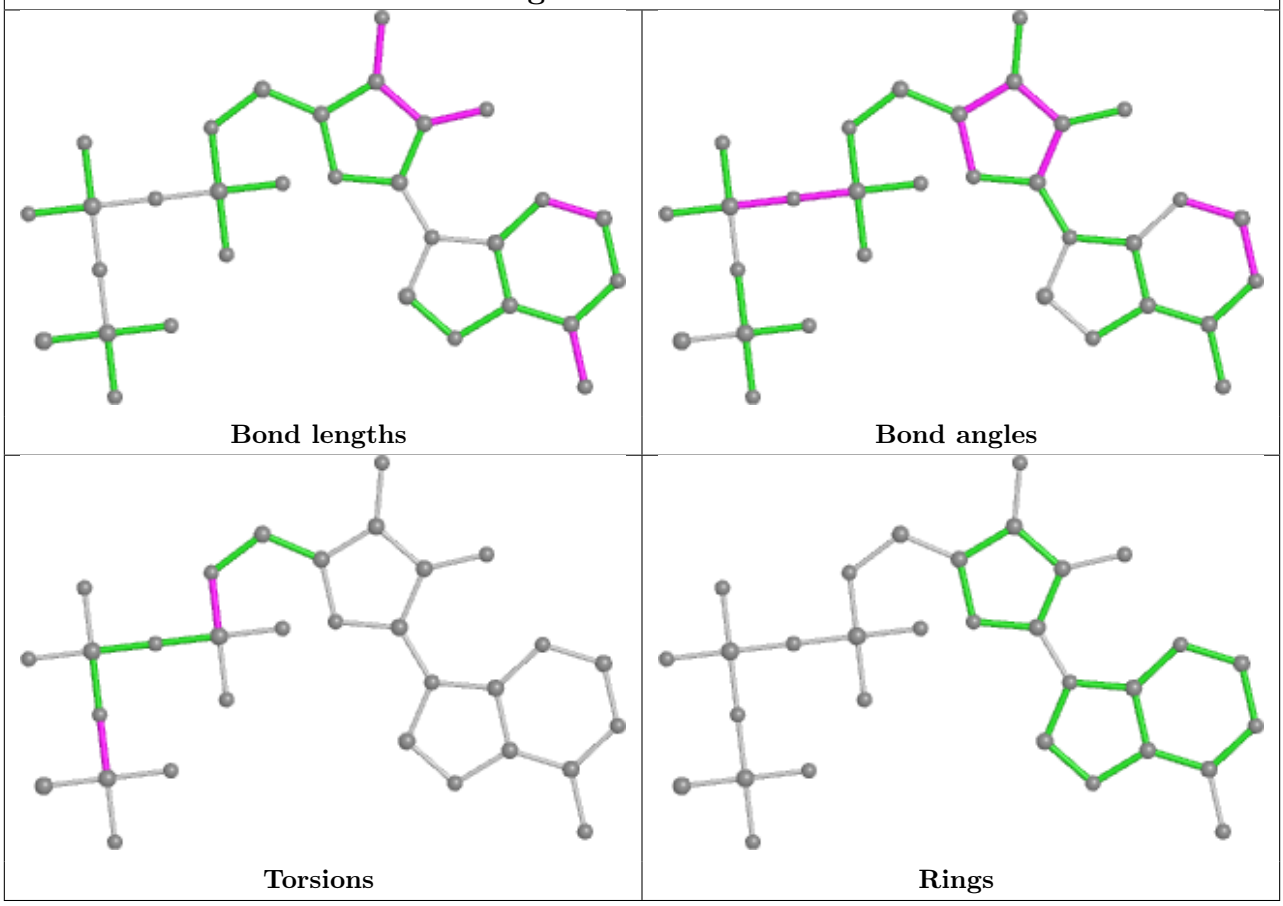

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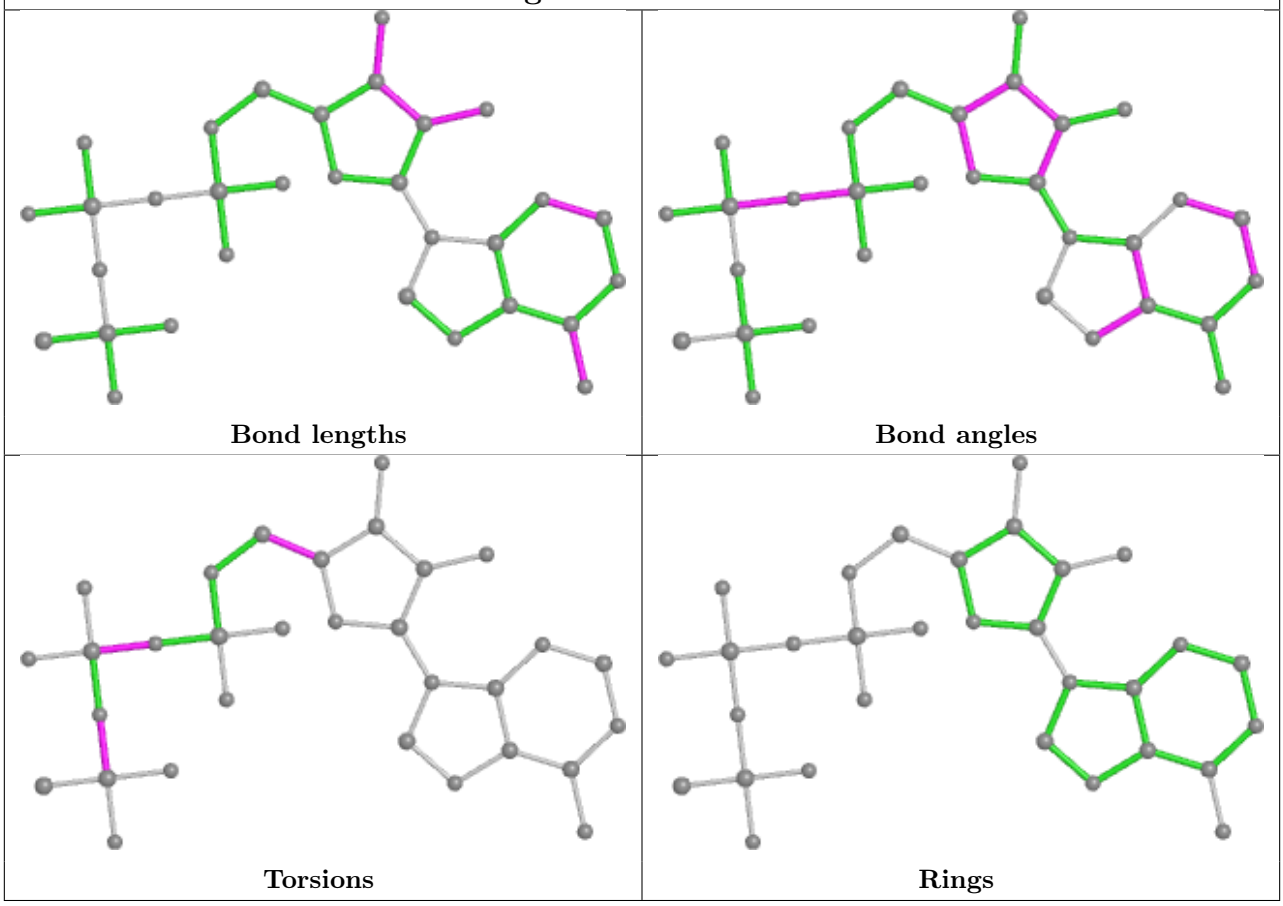
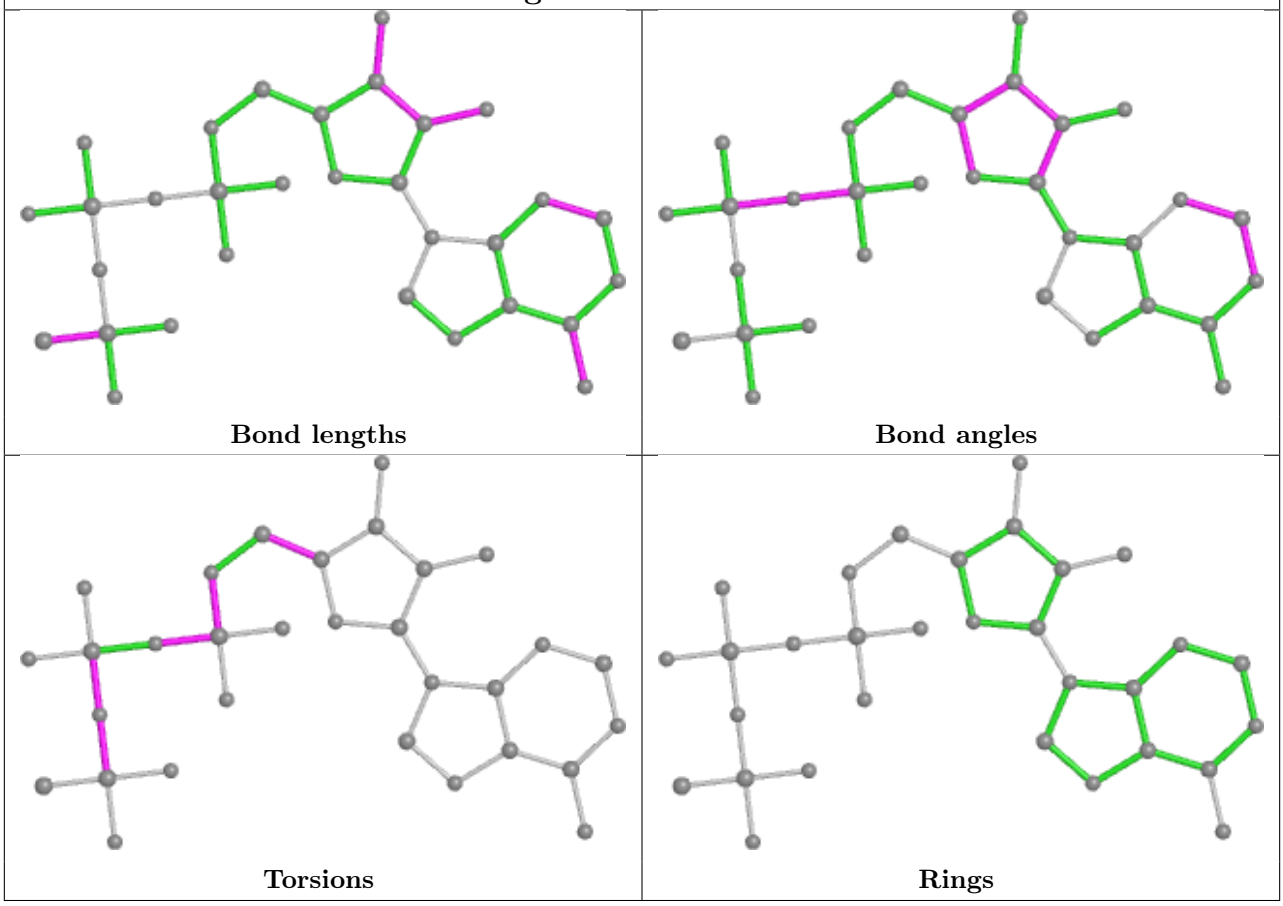
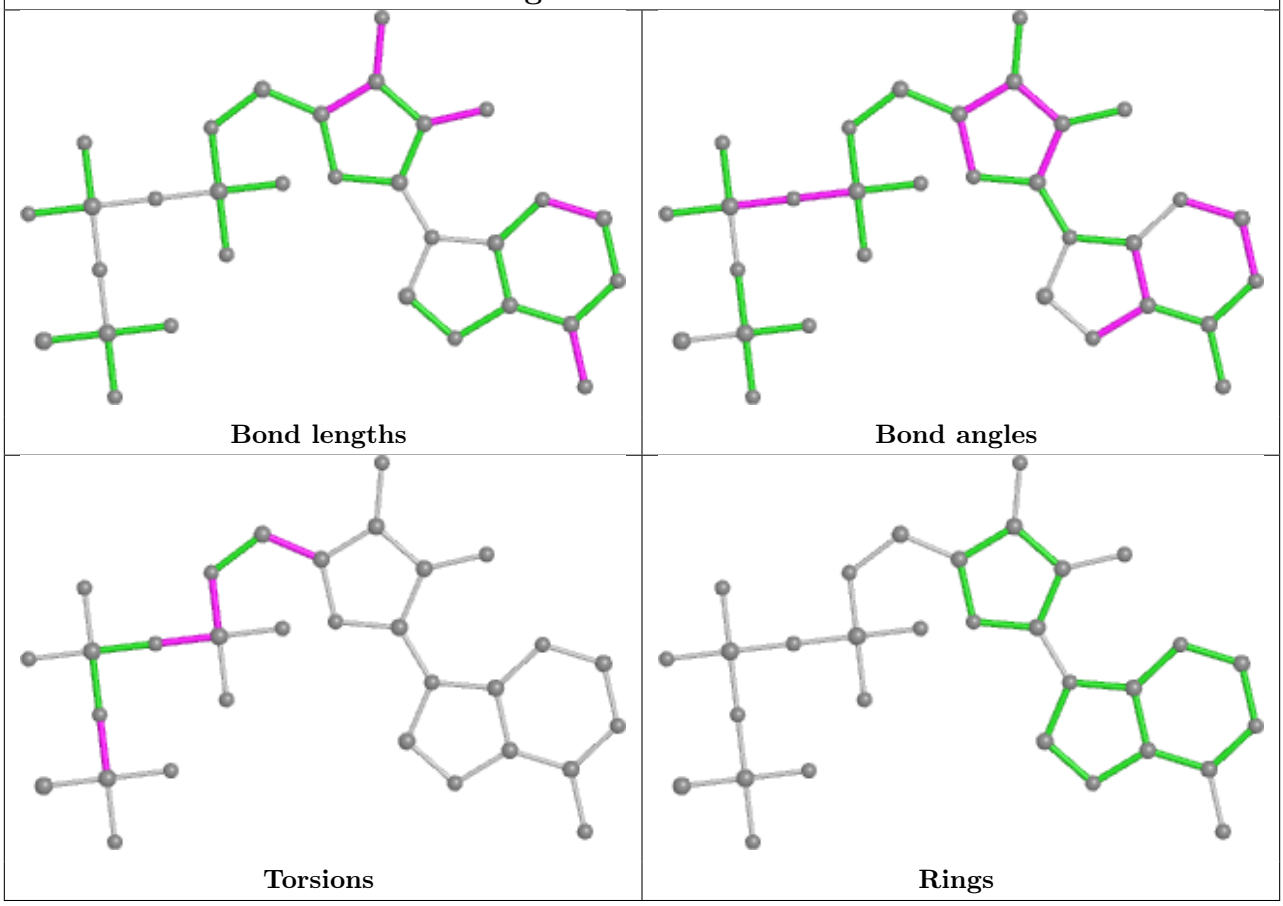


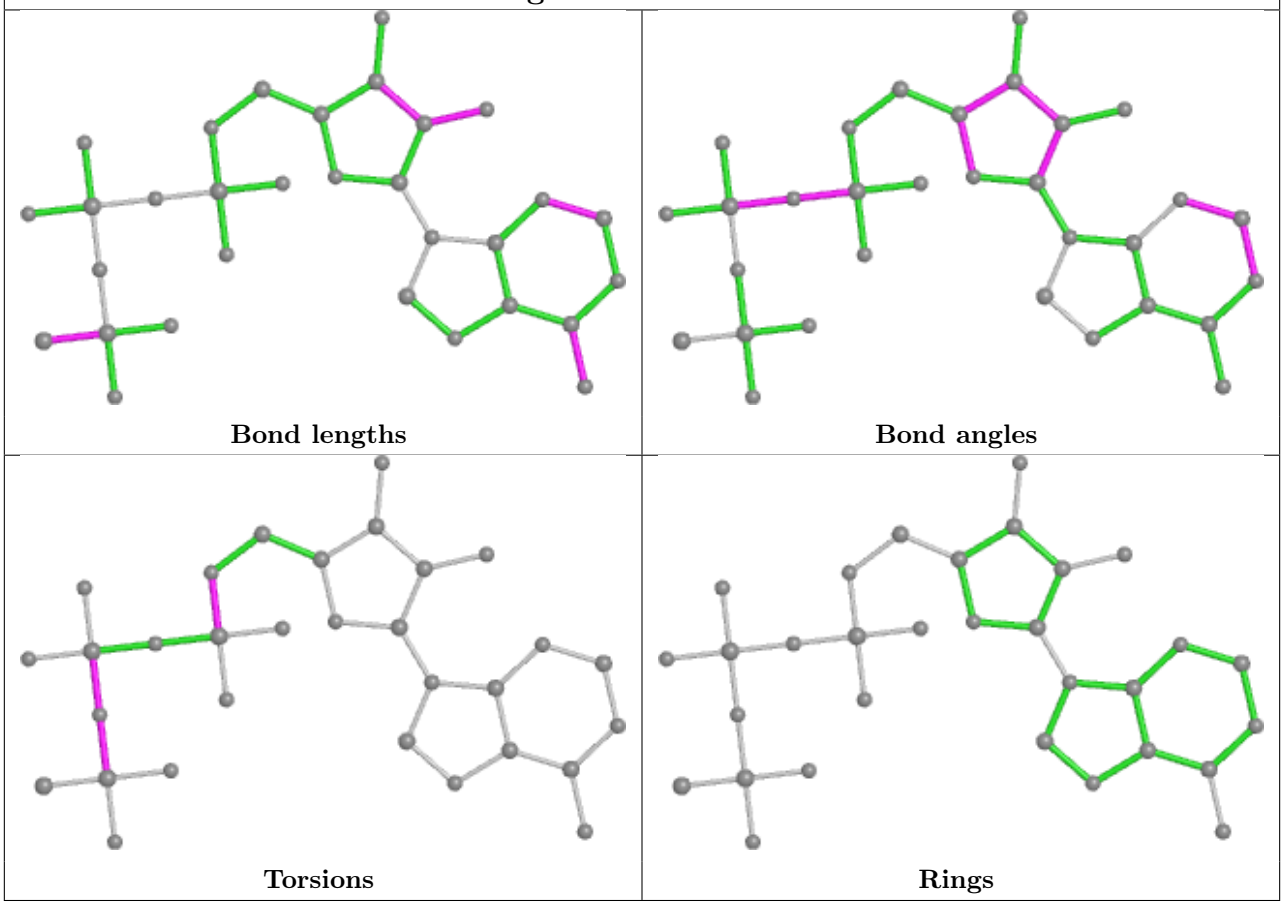
Ligand AGS G 902



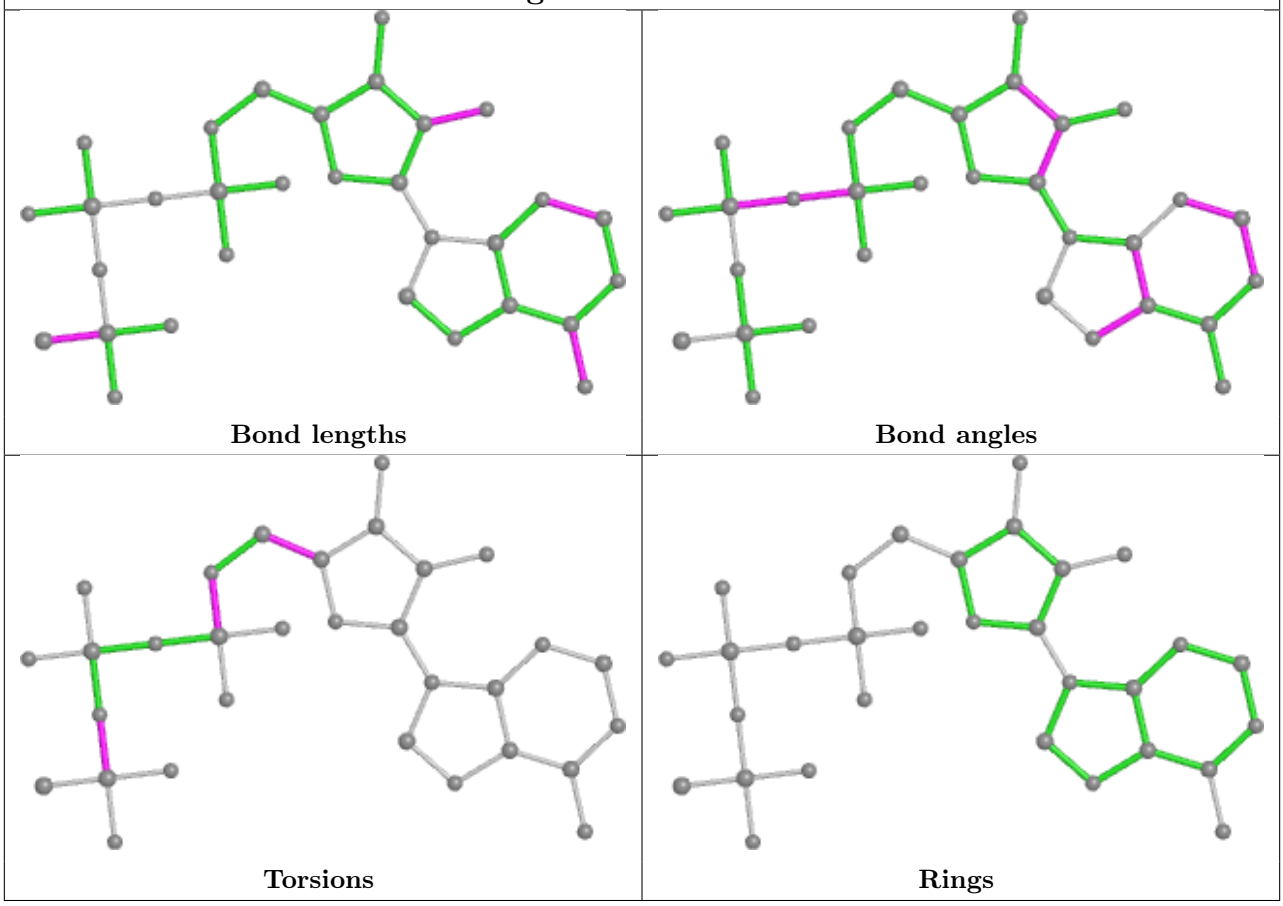
Ligand AGS A 902



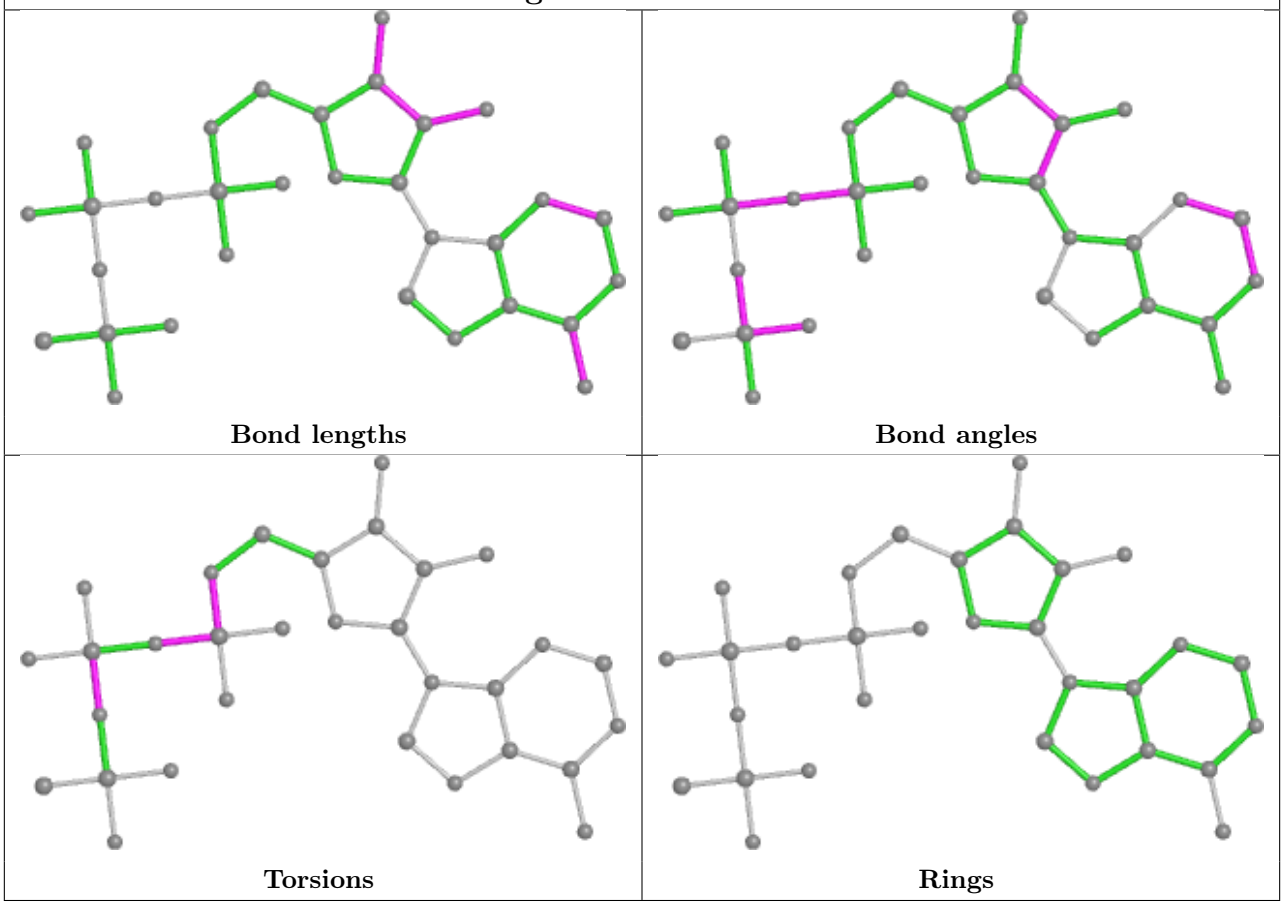
Ligand AGS F 902



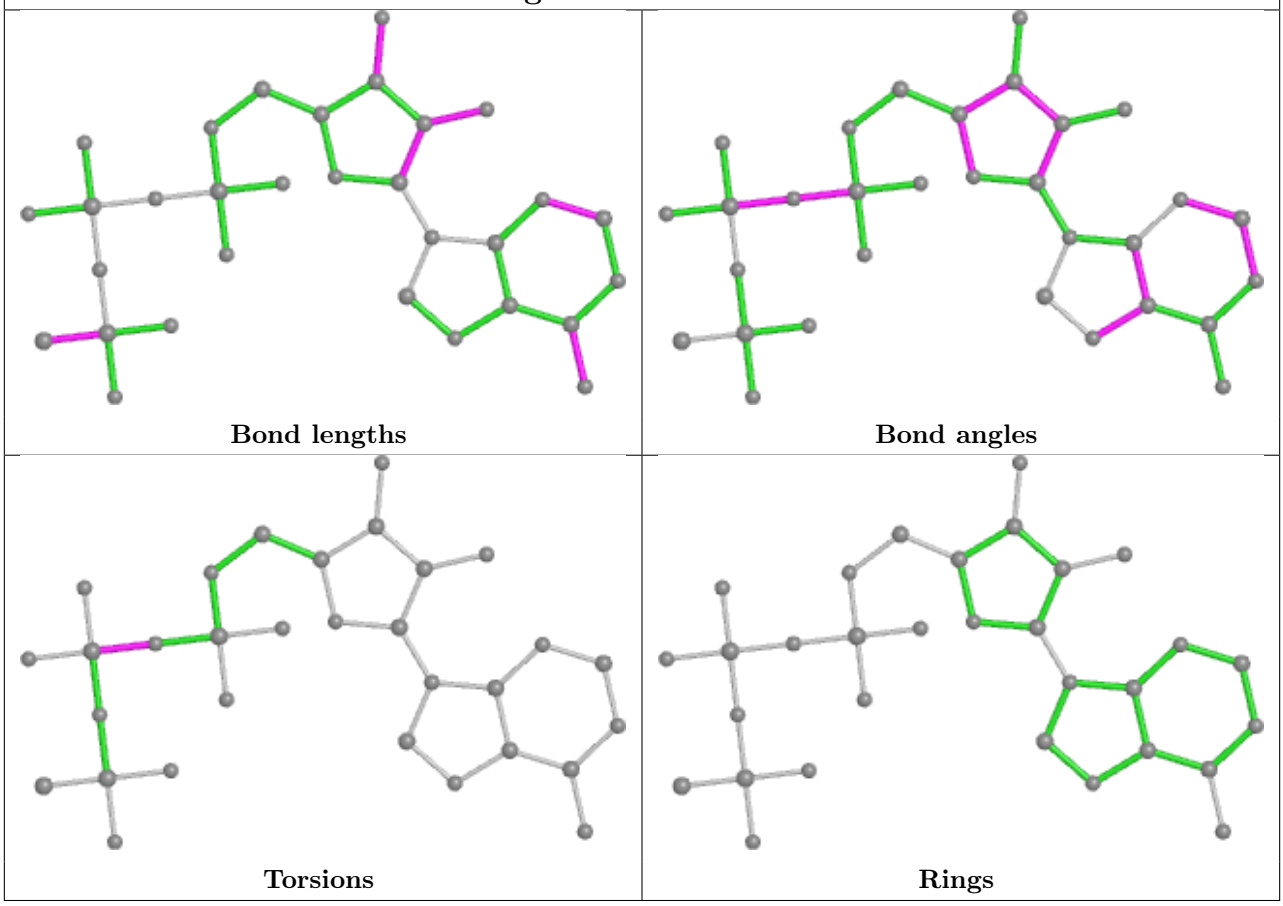
Ligand AGS E 902



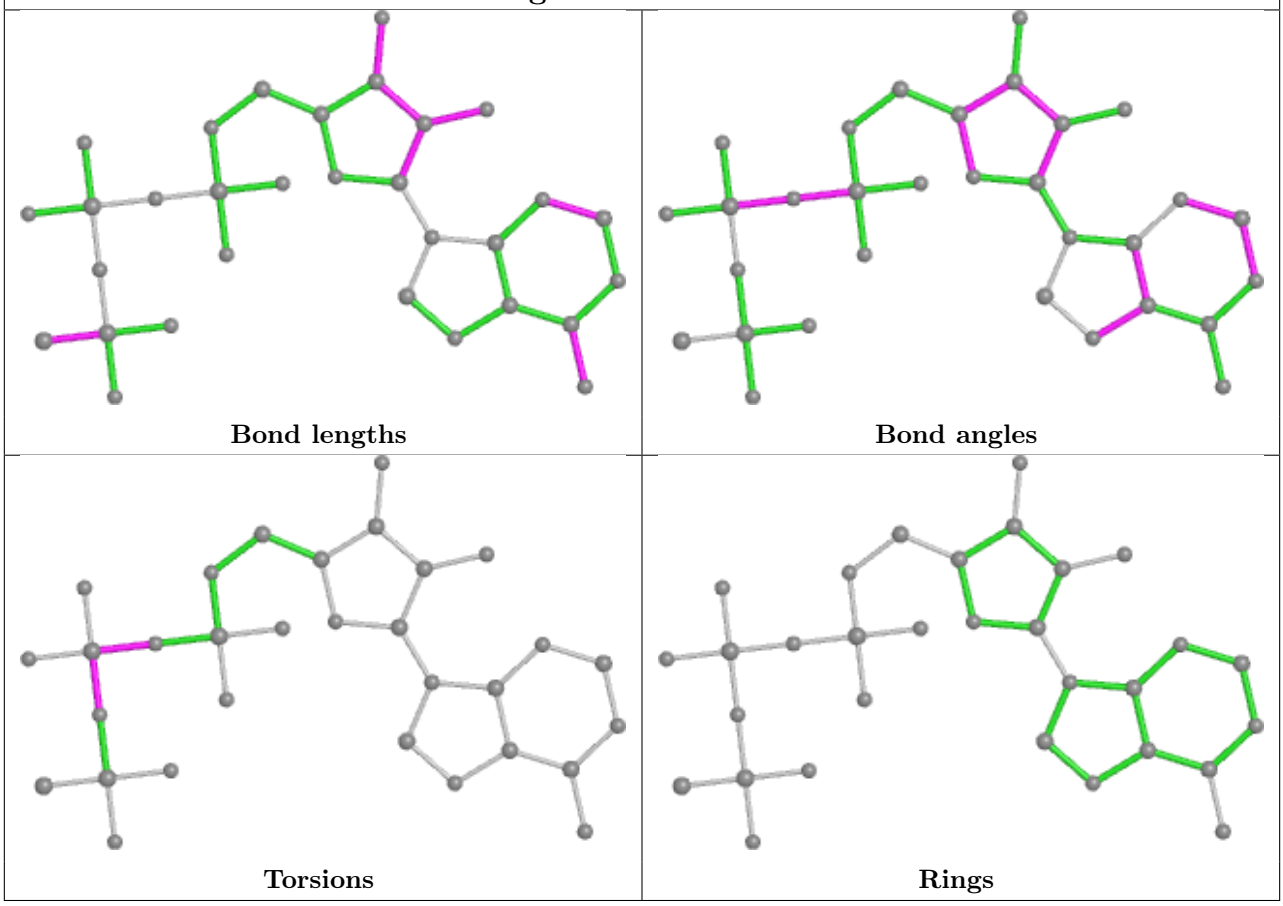
Ligand AGS C 902



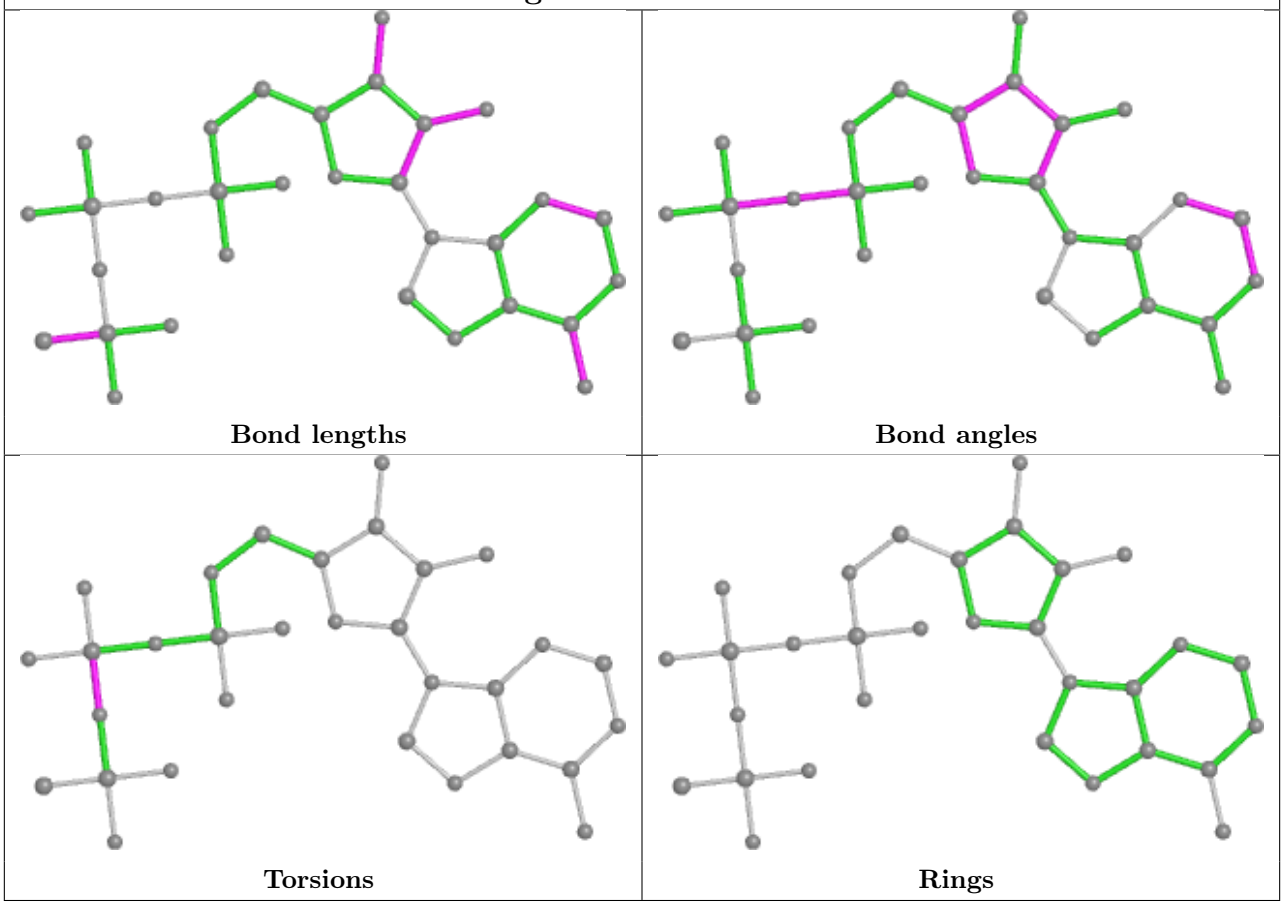
Ligand AGS K 901



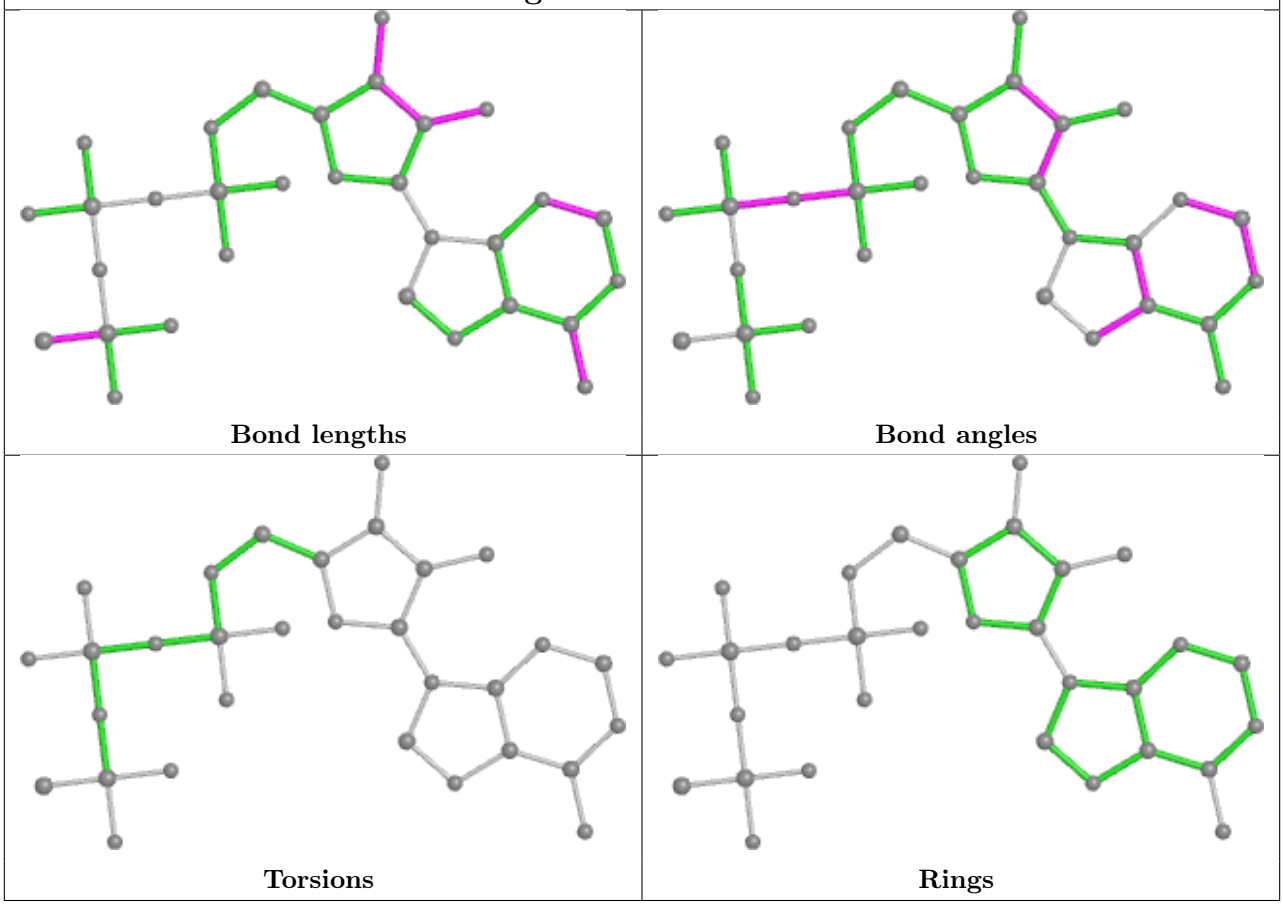
Ligand AGS J 901



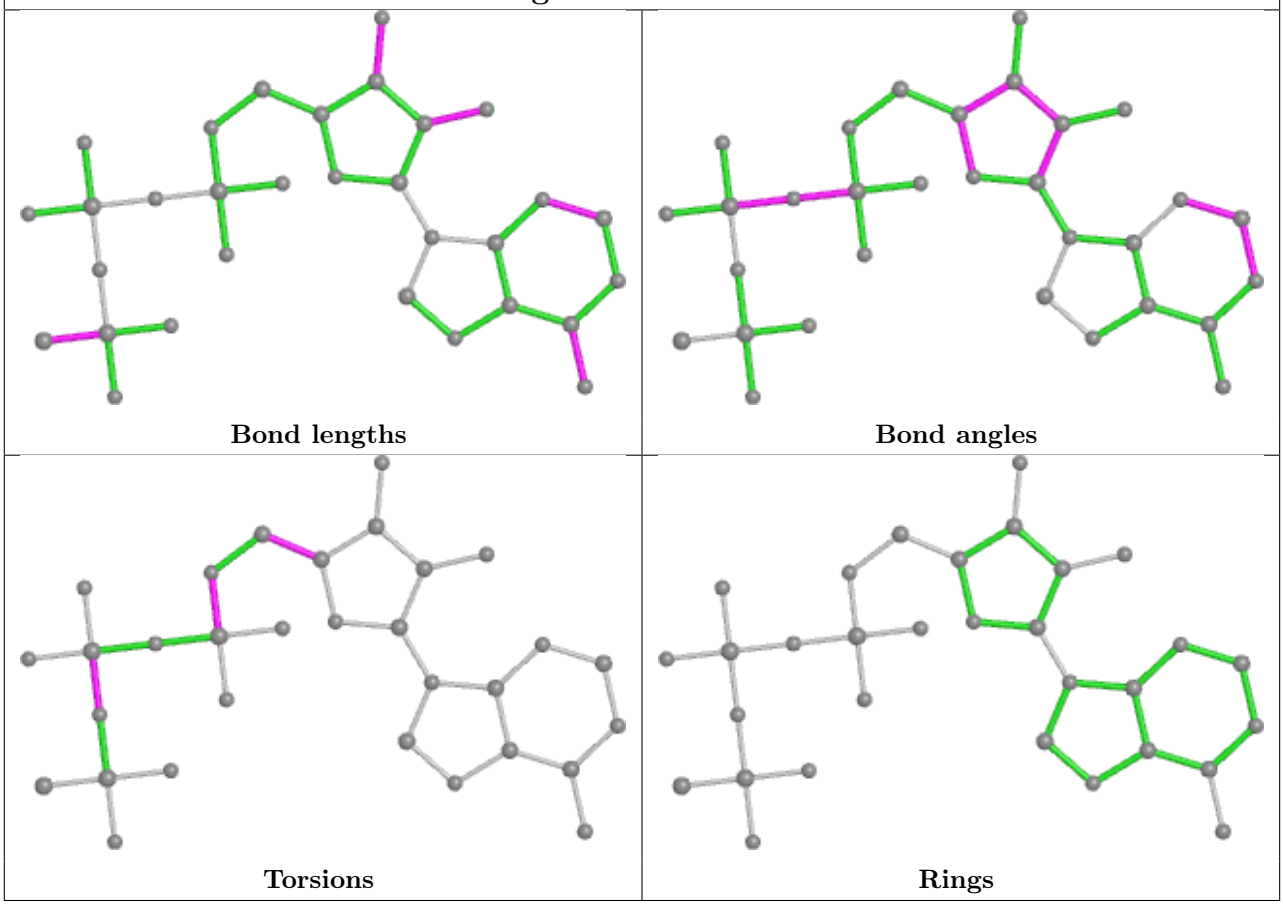
Ligand AGS A 901



Ligand AGS D 901



Ligand AGS I 902



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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	735/805 (91%)	0.26	23 (3%)	49	40	104, 177, 239, 332	0
1	B	735/805 (91%)	0.25	19 (2%)	56	47	101, 170, 246, 376	0
1	C	735/805 (91%)	0.30	30 (4%)	37	31	112, 181, 249, 329	0
1	D	735/805 (91%)	0.46	60 (8%)	11	9	118, 195, 263, 337	0
1	E	735/805 (91%)	0.23	20 (2%)	54	45	105, 173, 252, 352	0
1	F	735/805 (91%)	0.21	19 (2%)	56	47	98, 170, 249, 333	0
1	G	735/805 (91%)	0.25	16 (2%)	62	54	104, 173, 246, 315	0
1	H	735/805 (91%)	0.28	21 (2%)	51	42	104, 178, 245, 307	0
1	I	735/805 (91%)	0.34	32 (4%)	34	29	115, 185, 262, 351	0
1	J	735/805 (91%)	0.29	31 (4%)	36	30	109, 179, 240, 435	0
1	K	744/805 (92%)	0.35	42 (5%)	24	20	98, 173, 255, 362	0
1	L	735/805 (91%)	0.25	24 (3%)	46	38	100, 170, 243, 341	0
All	All	8829/9660 (91%)	0.29	337 (3%)	40	33	98, 177, 250, 435	0

All (337) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	770	SER	8.3
1	J	435	GLU	7.8
1	K	21	ASN	6.3
1	A	434	ASP	6.0
1	C	435	GLU	5.4
1	B	436	THR	5.0
1	J	434	ASP	4.8
1	J	436	THR	4.8
1	C	436	THR	4.7
1	K	427	MET	4.6
1	B	432	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	146	ILE	4.4
1	L	134	TYR	4.4
1	J	437	ILE	4.4
1	J	725	ASP	4.3
1	D	736	PHE	4.2
1	C	99	VAL	4.2
1	D	108	VAL	4.2
1	C	100	ILE	4.1
1	C	62	LYS	4.1
1	F	667	ALA	4.1
1	D	26	LEU	4.1
1	A	770	SER	4.1
1	H	435	GLU	4.0
1	G	108	VAL	4.0
1	K	24	ASN	4.0
1	H	116	VAL	4.0
1	L	726	ASP	4.0
1	I	745	ARG	3.9
1	L	162	GLU	3.9
1	D	69	CYS	3.9
1	F	433	GLU	3.9
1	J	726	ASP	3.9
1	I	116	VAL	3.8
1	C	552	PHE	3.8
1	B	117	LEU	3.8
1	F	23	PRO	3.8
1	G	736	PHE	3.8
1	B	21	ASN	3.8
1	D	49	LEU	3.7
1	D	434	ASP	3.7
1	K	23	PRO	3.7
1	E	770	SER	3.7
1	I	63	LYS	3.7
1	L	176	VAL	3.6
1	L	116	VAL	3.6
1	I	679	THR	3.6
1	C	460	ASN	3.6
1	D	92	LEU	3.6
1	A	340	HIS	3.6
1	K	134	TYR	3.6
1	D	235	VAL	3.5
1	D	105	CYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	736	PHE	3.5
1	K	116	VAL	3.5
1	A	621	GLY	3.5
1	B	428	ASP	3.5
1	C	26	LEU	3.4
1	K	102	ILE	3.4
1	F	435	GLU	3.4
1	D	731	ILE	3.4
1	I	731	ILE	3.4
1	I	186	GLY	3.4
1	D	56	THR	3.4
1	L	119	ILE	3.3
1	J	52	PHE	3.3
1	E	40	SER	3.3
1	I	770	SER	3.3
1	K	722	VAL	3.3
1	D	164	LYS	3.2
1	D	51	LEU	3.2
1	J	135	LEU	3.2
1	E	768	PHE	3.2
1	D	71	VAL	3.2
1	D	681	GLY	3.2
1	F	666	VAL	3.2
1	L	164	LYS	3.2
1	D	672	LEU	3.1
1	K	53	ARG	3.1
1	D	100	ILE	3.1
1	D	37	SER	3.1
1	D	67	ALA	3.1
1	B	731	ILE	3.1
1	K	176	VAL	3.1
1	A	67	ALA	3.1
1	H	51	LEU	3.0
1	K	51	LEU	3.0
1	J	186	GLY	3.0
1	D	712	GLU	3.0
1	K	117	LEU	3.0
1	I	508	MET	3.0
1	D	437	ILE	2.9
1	A	41	LEU	2.9
1	E	437	ILE	2.9
1	D	682	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	731	ILE	2.9
1	A	435	GLU	2.9
1	C	102	ILE	2.9
1	D	59	LEU	2.9
1	J	164	LYS	2.9
1	I	127	THR	2.9
1	K	426	LYS	2.9
1	I	26	LEU	2.9
1	H	102	ILE	2.9
1	K	118	PRO	2.9
1	I	552	PHE	2.9
1	B	666	VAL	2.9
1	C	731	ILE	2.9
1	E	432	LEU	2.8
1	A	82	ILE	2.8
1	B	152	PHE	2.8
1	E	436	THR	2.8
1	D	70	ILE	2.8
1	C	429	LEU	2.8
1	C	164	LYS	2.8
1	E	427	MET	2.8
1	K	164	LYS	2.8
1	K	166	VAL	2.8
1	C	45	LYS	2.8
1	L	730	GLU	2.8
1	D	679	THR	2.8
1	L	133	VAL	2.8
1	B	126	ILE	2.8
1	K	718	SER	2.7
1	A	682	PHE	2.7
1	D	103	GLN	2.7
1	K	135	LEU	2.7
1	B	116	VAL	2.7
1	D	104	PRO	2.7
1	E	494	GLN	2.7
1	K	25	ARG	2.7
1	K	726	ASP	2.7
1	F	731	ILE	2.7
1	J	56	THR	2.7
1	A	437	ILE	2.7
1	E	116	VAL	2.7
1	K	70	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	L	37	SER	2.7
1	D	139	PHE	2.7
1	L	725	ASP	2.7
1	B	712	GLU	2.7
1	K	708	ARG	2.7
1	K	100	ILE	2.7
1	K	39	VAL	2.6
1	J	182	ILE	2.6
1	D	730	GLU	2.6
1	I	678	MET	2.6
1	H	768	PHE	2.6
1	K	71	VAL	2.6
1	A	46	MET	2.6
1	G	41	LEU	2.6
1	H	694	ALA	2.6
1	D	758	PHE	2.6
1	G	682	PHE	2.6
1	K	99	VAL	2.6
1	H	100	ILE	2.6
1	K	139	PHE	2.6
1	B	99	VAL	2.6
1	D	154	VAL	2.6
1	I	739	ALA	2.6
1	F	736	PHE	2.6
1	A	51	LEU	2.6
1	E	39	VAL	2.6
1	E	675	LEU	2.6
1	D	645	ILE	2.5
1	F	670	VAL	2.5
1	K	719	ALA	2.5
1	F	53	ARG	2.5
1	B	233	ILE	2.5
1	F	768	PHE	2.5
1	I	71	VAL	2.5
1	I	428	ASP	2.5
1	L	165	VAL	2.5
1	L	115	HIS	2.5
1	D	38	VAL	2.5
1	L	36	ASN	2.5
1	E	498	GLU	2.5
1	G	164	LYS	2.5
1	K	506	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	708	ARG	2.5
1	B	460	ASN	2.5
1	J	21	ASN	2.5
1	K	725	ASP	2.5
1	E	762	LEU	2.5
1	J	139	PHE	2.5
1	C	594	GLY	2.5
1	D	57	VAL	2.5
1	C	622	ALA	2.5
1	D	66	GLU	2.5
1	D	72	LEU	2.5
1	D	68	VAL	2.5
1	C	134	TYR	2.4
1	E	731	ILE	2.4
1	H	666	VAL	2.4
1	J	53	ARG	2.4
1	G	172	PRO	2.4
1	L	269	ILE	2.4
1	I	114	ILE	2.4
1	F	52	PHE	2.4
1	K	56	THR	2.4
1	C	428	ASP	2.4
1	K	716	ASN	2.4
1	B	552	PHE	2.4
1	H	729	PRO	2.4
1	A	765	SER	2.4
1	H	503	PHE	2.4
1	I	452	PHE	2.4
1	I	108	VAL	2.4
1	I	165	VAL	2.4
1	K	720	MET	2.4
1	K	103	GLN	2.4
1	I	682	PHE	2.4
1	C	130	LEU	2.4
1	I	185	GLU	2.4
1	I	41	LEU	2.4
1	L	715	THR	2.4
1	D	36	ASN	2.4
1	L	166	VAL	2.4
1	J	516	PHE	2.4
1	I	725	ASP	2.4
1	J	51	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	480	GLY	2.4
1	L	710	GLU	2.3
1	H	239	ARG	2.3
1	G	672	LEU	2.3
1	G	388	MET	2.3
1	C	56	THR	2.3
1	I	115	HIS	2.3
1	K	717	PRO	2.3
1	A	681	GLY	2.3
1	D	102	ILE	2.3
1	E	765	SER	2.3
1	F	21	ASN	2.3
1	A	747	VAL	2.3
1	D	140	LEU	2.3
1	D	675	LEU	2.3
1	D	747	VAL	2.3
1	F	735	HIS	2.3
1	H	506	PHE	2.3
1	D	687	LEU	2.3
1	F	443	ASN	2.3
1	G	445	LEU	2.3
1	A	726	ASP	2.3
1	H	41	LEU	2.3
1	D	715	THR	2.3
1	I	102	ILE	2.3
1	K	505	LYS	2.3
1	D	173	TYR	2.3
1	C	648	PRO	2.3
1	B	49	LEU	2.2
1	A	436	THR	2.2
1	I	460	ASN	2.2
1	J	452	PHE	2.2
1	C	50	GLN	2.2
1	A	25	ARG	2.2
1	H	767	GLY	2.2
1	K	723	GLU	2.2
1	D	150	ASP	2.2
1	J	104	PRO	2.2
1	D	755	TYR	2.2
1	A	108	VAL	2.2
1	I	187	GLU	2.2
1	H	53	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	551	TRP	2.2
1	D	145	PRO	2.2
1	C	59	LEU	2.2
1	C	666	VAL	2.2
1	G	100	ILE	2.2
1	L	229	LEU	2.2
1	I	506	PHE	2.2
1	K	130	LEU	2.2
1	A	99	VAL	2.2
1	G	71	VAL	2.2
1	J	82	ILE	2.2
1	H	736	PHE	2.2
1	L	130	LEU	2.2
1	D	162	GLU	2.2
1	K	104	PRO	2.2
1	F	517	TYR	2.2
1	J	765	SER	2.2
1	J	736	PHE	2.2
1	D	711	ARG	2.1
1	B	768	PHE	2.1
1	C	690	ILE	2.1
1	E	452	PHE	2.1
1	L	224	LEU	2.1
1	C	679	THR	2.1
1	E	100	ILE	2.1
1	J	114	ILE	2.1
1	A	736	PHE	2.1
1	I	715	THR	2.1
1	J	163	PHE	2.1
1	J	130	LEU	2.1
1	D	24	ASN	2.1
1	C	461	PRO	2.1
1	L	708	ARG	2.1
1	K	114	ILE	2.1
1	H	50	GLN	2.1
1	D	699	ILE	2.1
1	I	49	LEU	2.1
1	F	682	PHE	2.1
1	G	50	GLN	2.1
1	C	551	TRP	2.1
1	E	41	LEU	2.1
1	A	59	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	147	ARG	2.1
1	D	172	PRO	2.1
1	D	436	THR	2.1
1	G	230	PHE	2.1
1	C	94	VAL	2.1
1	L	117	LEU	2.1
1	H	502	LYS	2.1
1	D	176	VAL	2.1
1	K	714	GLN	2.1
1	J	621	GLY	2.1
1	E	495	TYR	2.1
1	I	128	GLY	2.1
1	J	503	PHE	2.1
1	H	508	MET	2.0
1	J	731	ILE	2.0
1	A	230	PHE	2.0
1	L	740	MET	2.0
1	D	431	ASP	2.0
1	F	715	THR	2.0
1	G	506	PHE	2.0
1	G	84	MET	2.0
1	J	175	ILE	2.0
1	C	117	LEU	2.0
1	F	117	LEU	2.0
1	H	52	PHE	2.0
1	I	117	LEU	2.0
1	J	173	TYR	2.0
1	K	721	GLU	2.0
1	C	57	VAL	2.0
1	D	727	PRO	2.0
1	F	687	LEU	2.0
1	G	116	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	AGS	E	902	31/31	0.82	0.30	102,148,179,184	0
3	MG	J	903	1/1	0.84	0.72	105,105,105,105	0
2	AGS	I	902	31/31	0.85	0.31	125,150,180,187	0
2	AGS	F	902	31/31	0.85	0.30	122,150,185,190	0
2	AGS	G	902	31/31	0.88	0.32	112,139,179,187	0
2	AGS	D	902	31/31	0.89	0.25	111,144,182,204	0
2	AGS	C	902	31/31	0.90	0.28	105,140,172,196	0
3	MG	C	903	1/1	0.90	0.38	94,94,94,94	0
3	MG	F	904	1/1	0.90	0.58	149,149,149,149	0
3	MG	H	904	1/1	0.90	0.49	134,134,134,134	0
2	AGS	H	902	31/31	0.90	0.25	110,139,165,169	0
2	AGS	J	901	31/31	0.91	0.29	111,139,167,210	0
2	AGS	J	902	31/31	0.91	0.27	99,140,168,181	0
2	AGS	K	902	31/31	0.91	0.30	96,121,149,154	0
2	AGS	L	902	31/31	0.91	0.27	112,136,166,169	0
3	MG	D	903	1/1	0.92	0.49	122,122,122,122	0
2	AGS	B	901	31/31	0.92	0.32	102,131,160,170	0
2	AGS	A	902	31/31	0.92	0.24	120,142,172,177	0
2	AGS	F	901	31/31	0.92	0.31	94,131,160,160	0
2	AGS	E	901	31/31	0.93	0.26	105,131,164,179	0
2	AGS	G	901	31/31	0.93	0.27	104,134,164,210	0
2	AGS	D	901	31/31	0.93	0.27	103,137,166,208	0
2	AGS	B	902	31/31	0.93	0.27	101,128,152,156	0
2	AGS	I	901	31/31	0.93	0.26	105,131,158,186	0
3	MG	G	903	1/1	0.94	0.64	113,113,113,113	0
2	AGS	C	901	31/31	0.94	0.27	105,138,166,177	0
2	AGS	H	901	31/31	0.94	0.30	105,133,162,165	0
3	MG	L	903	1/1	0.94	0.31	117,117,117,117	0
3	MG	A	904	1/1	0.95	0.24	128,128,128,128	0
2	AGS	L	901	31/31	0.95	0.29	102,132,160,173	0
2	AGS	A	901	31/31	0.95	0.29	102,125,153,197	0
3	MG	A	903	1/1	0.95	0.51	110,110,110,110	0
3	MG	L	904	1/1	0.95	0.51	115,115,115,115	0
3	MG	E	904	1/1	0.96	0.34	151,151,151,151	0
2	AGS	K	901	31/31	0.96	0.27	100,132,164,172	0
3	MG	I	903	1/1	0.96	0.32	138,138,138,138	0
3	MG	E	903	1/1	0.97	0.26	113,113,113,113	0

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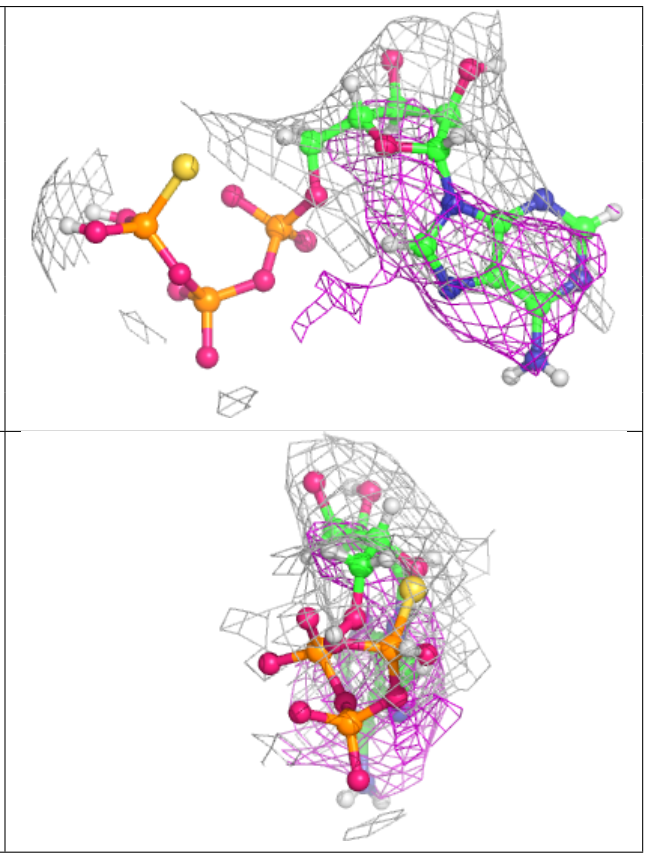
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	I	904	1/1	0.97	0.41	145,145,145,145	0
3	MG	D	904	1/1	0.97	0.34	127,127,127,127	0
3	MG	G	904	1/1	0.97	0.58	119,119,119,119	0
3	MG	F	903	1/1	0.97	0.40	94,94,94,94	0
3	MG	B	904	1/1	0.98	0.53	114,114,114,114	0
3	MG	J	904	1/1	0.98	0.37	112,112,112,112	0
3	MG	B	903	1/1	0.98	0.38	113,113,113,113	0
3	MG	H	903	1/1	0.98	0.33	132,132,132,132	0
3	MG	K	904	1/1	0.99	0.38	99,99,99,99	0
3	MG	C	904	1/1	0.99	0.38	137,137,137,137	0
3	MG	K	903	1/1	0.99	0.33	112,112,112,112	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.

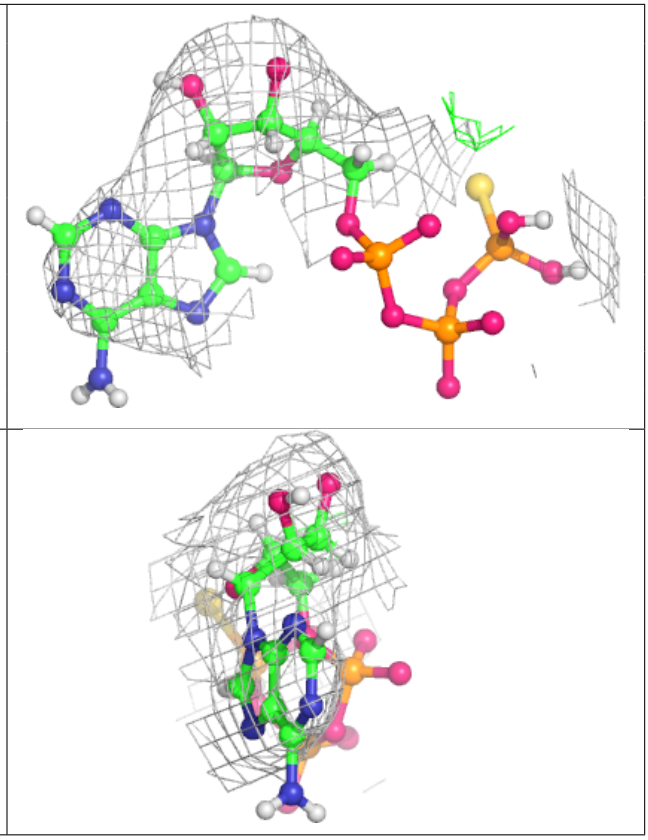
Electron density around AGS E 902:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



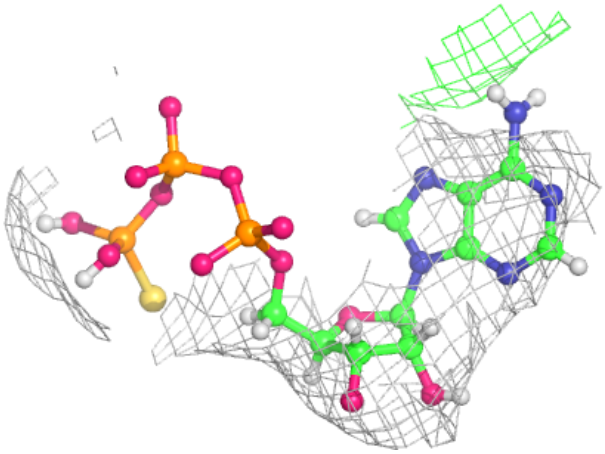
Electron density around AGS I 902:

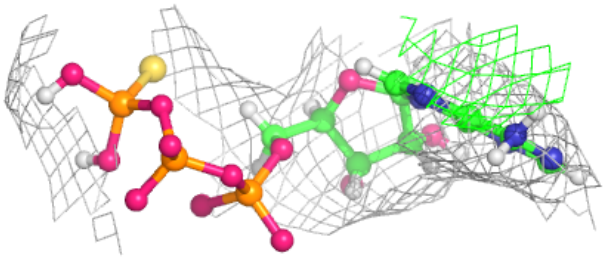
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

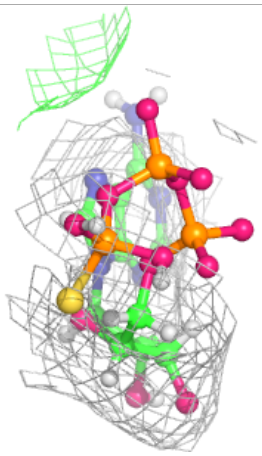


Electron density around AGS F 902:

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

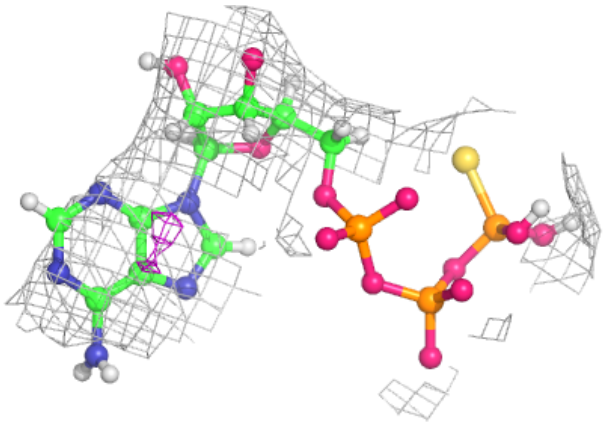


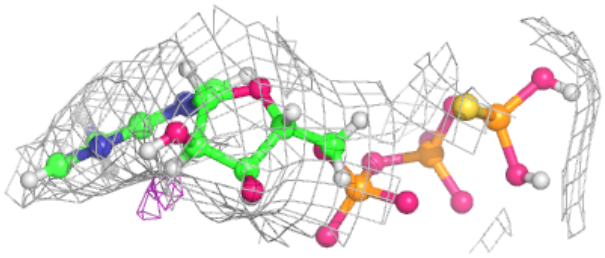


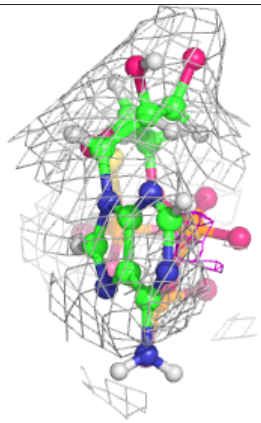


Electron density around AGS G 902:

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

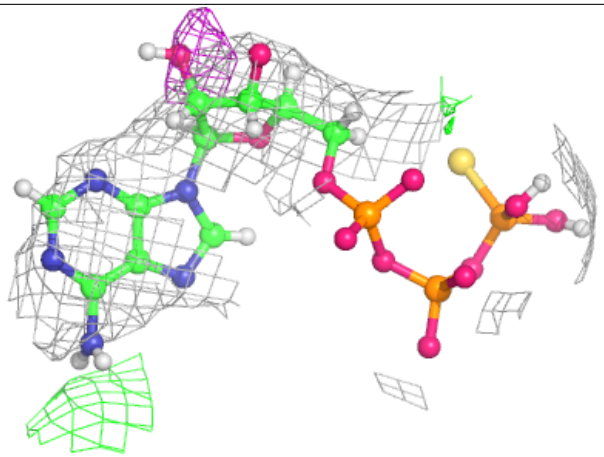


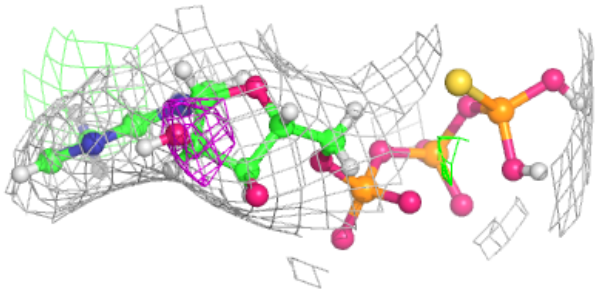


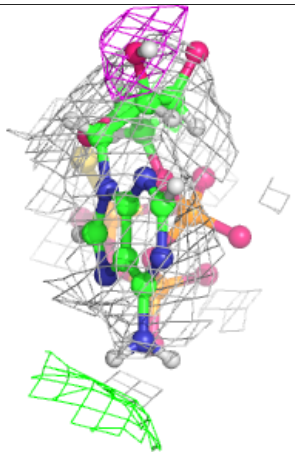


Electron density around AGS D 902:

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

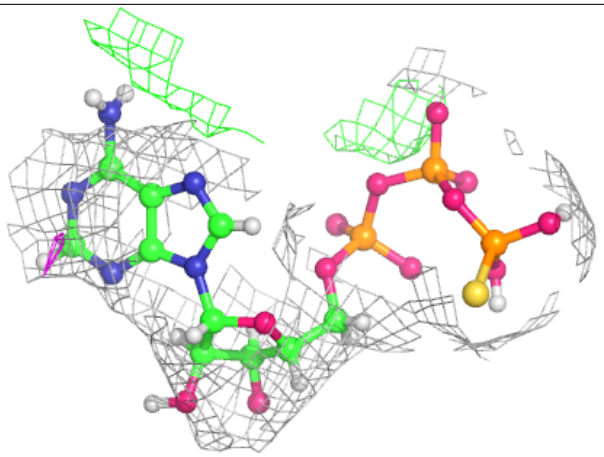


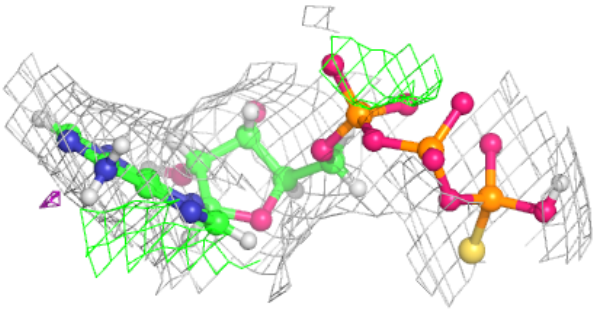


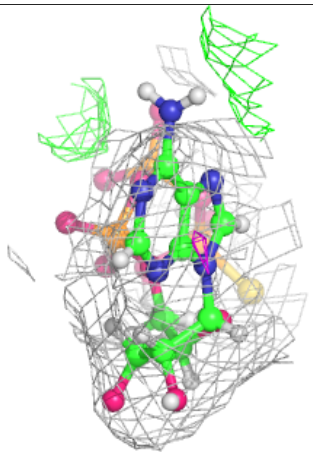


Electron density around AGS C 902:

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

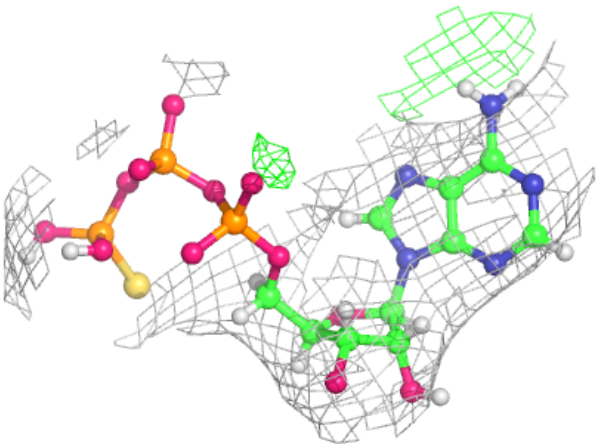


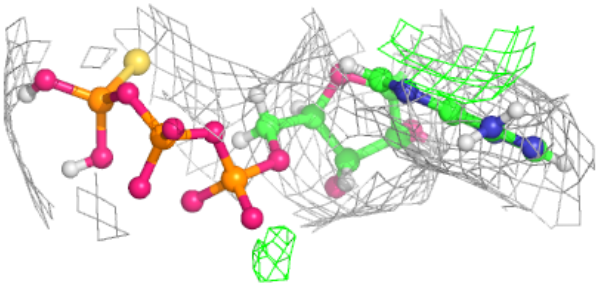


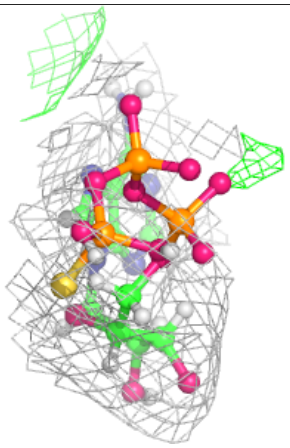


Electron density around AGS H 902:

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

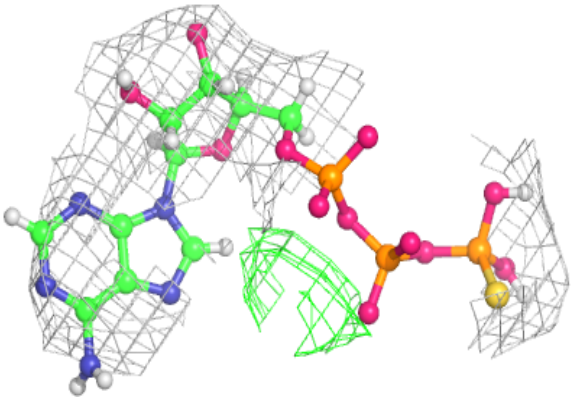


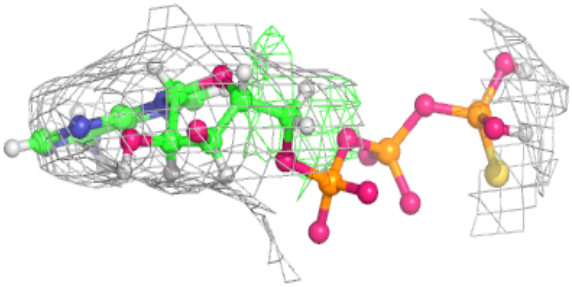


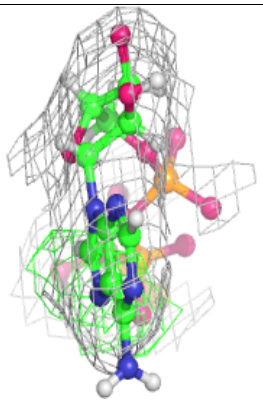


Electron density around AGS J 901:

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

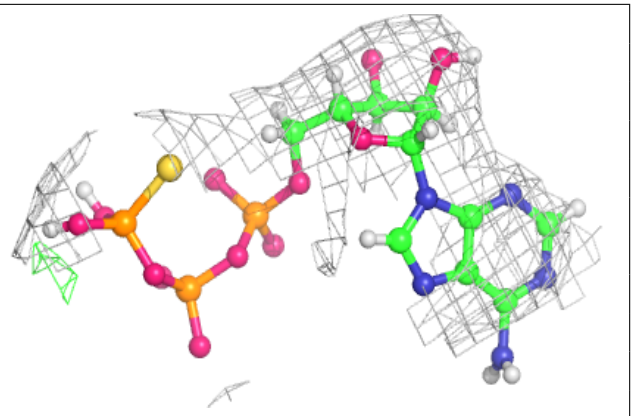


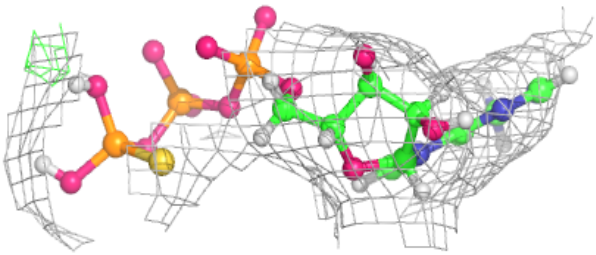


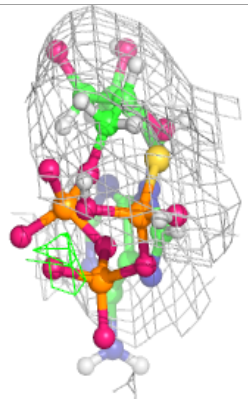


Electron density around AGS J 902:

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

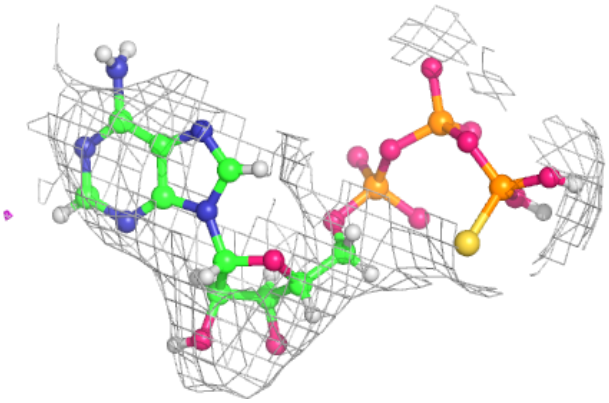


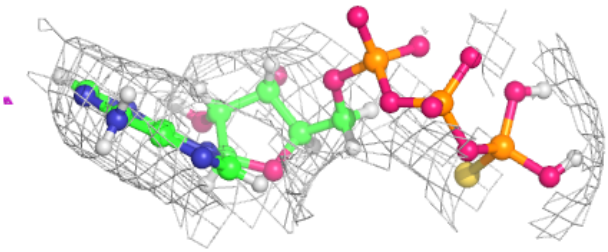


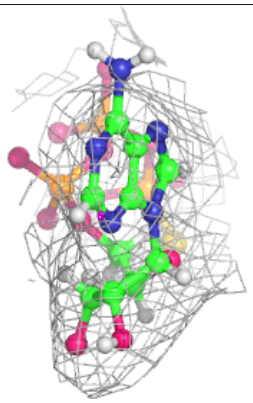


Electron density around AGS K 902:

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

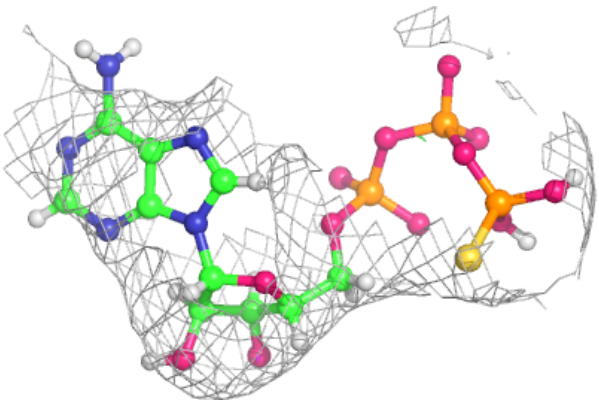


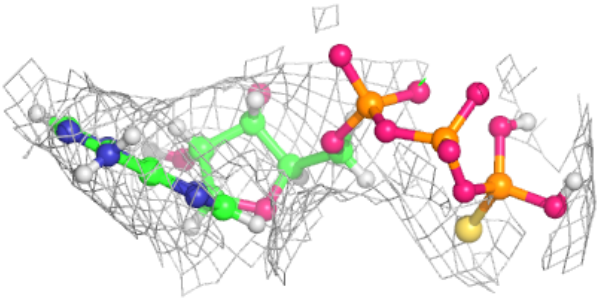


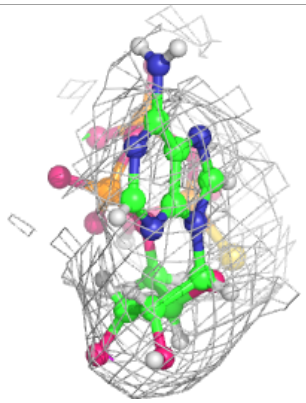


Electron density around AGS L 902:

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

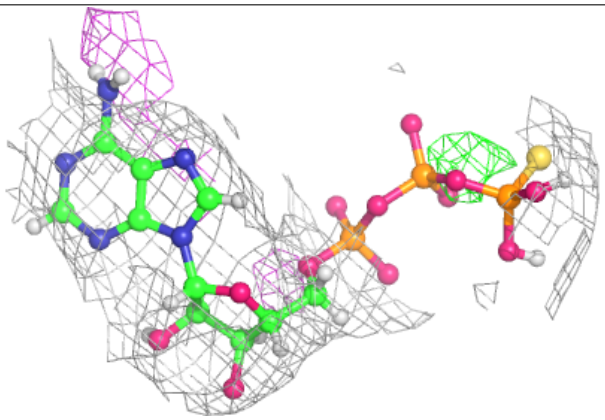


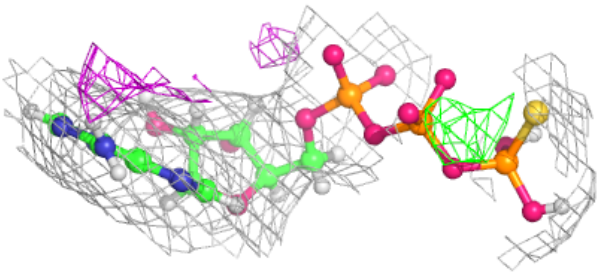


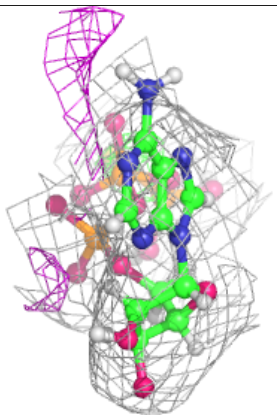


Electron density around AGS B 901:

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

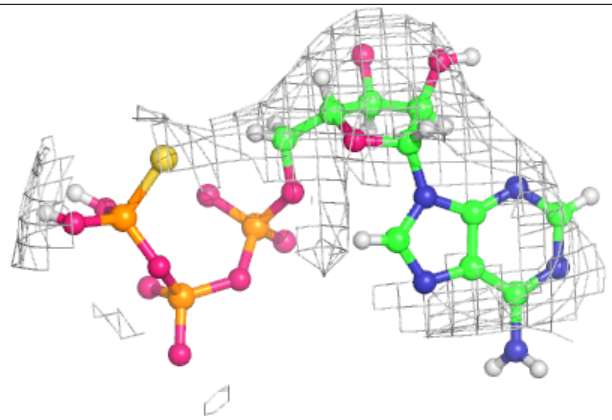


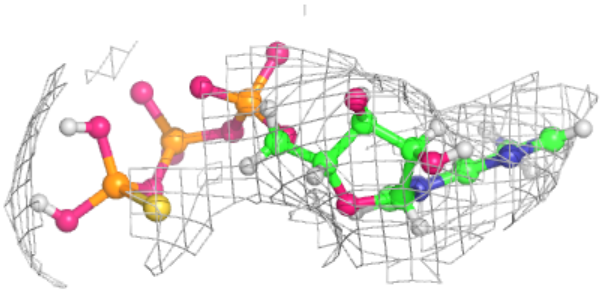


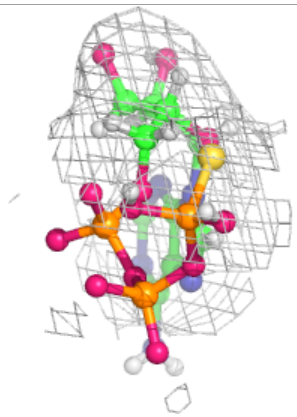


Electron density around AGS A 902:

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

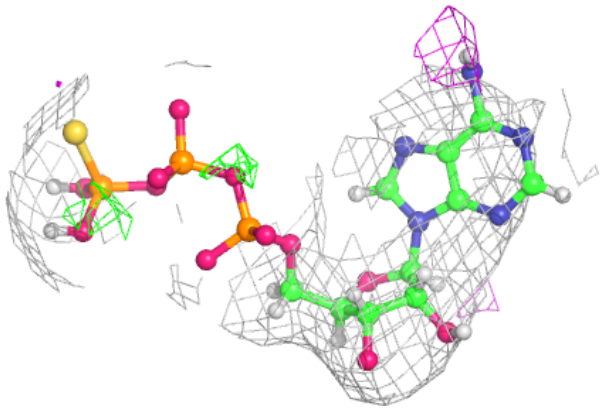


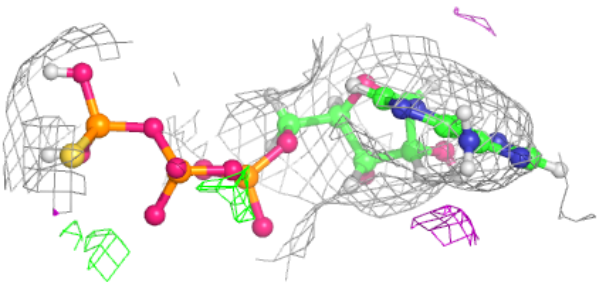


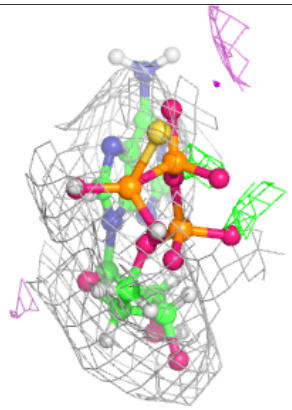


Electron density around AGS F 901:

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

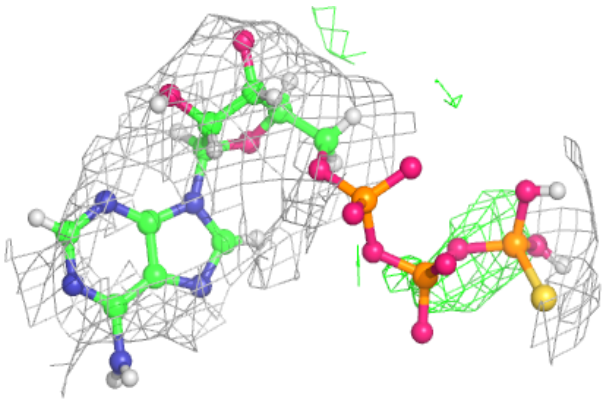


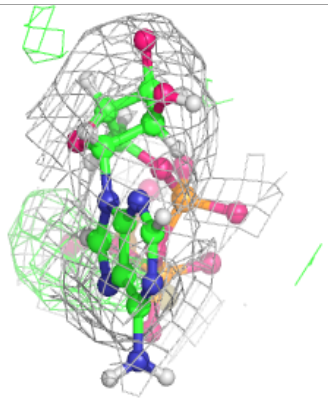




Electron density around AGS E 901:

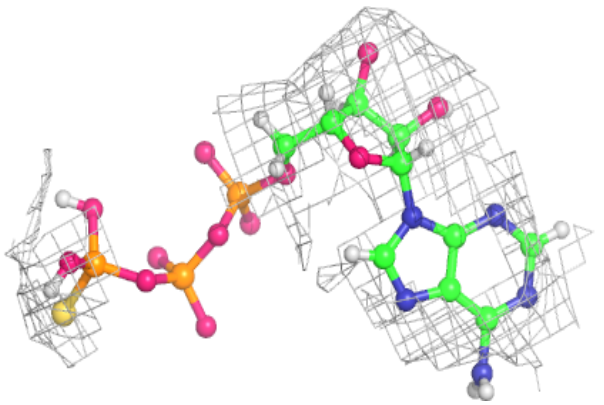
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

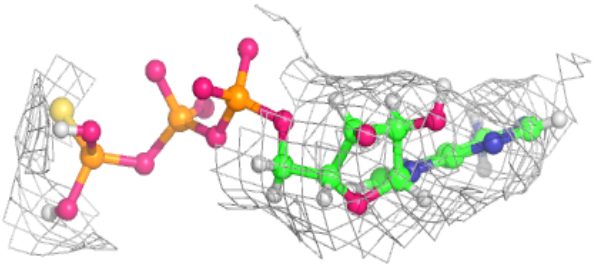


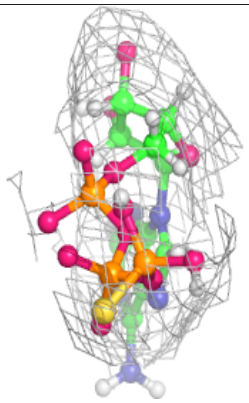


Electron density around AGS G 901:

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

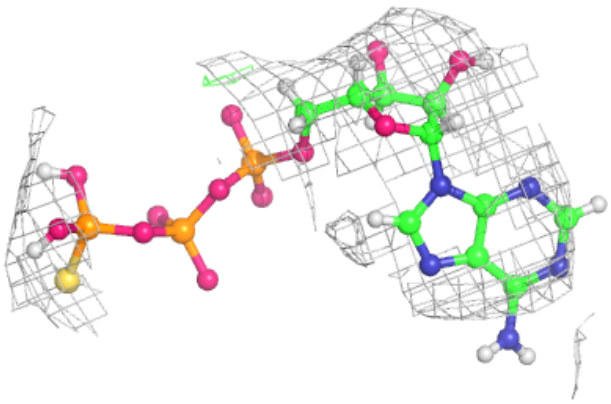


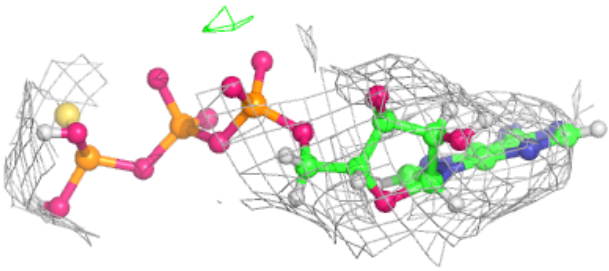


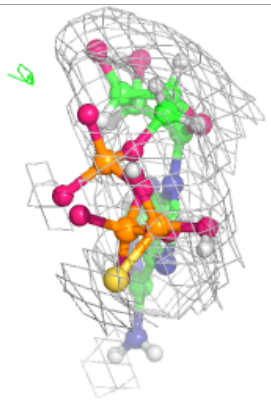


Electron density around AGS D 901:

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

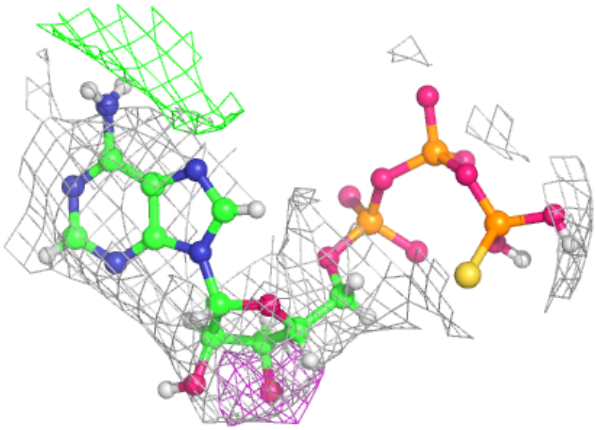


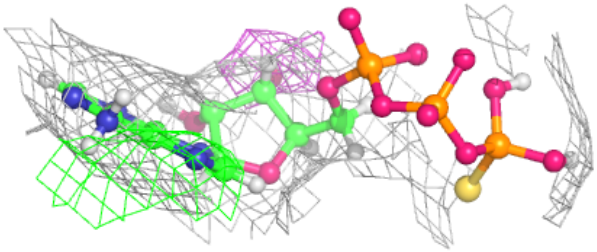


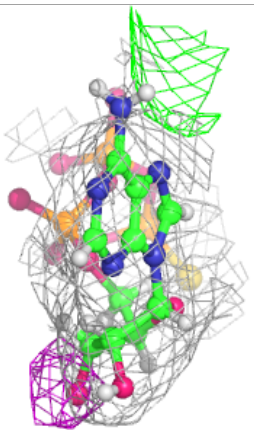


Electron density around AGS B 902:

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

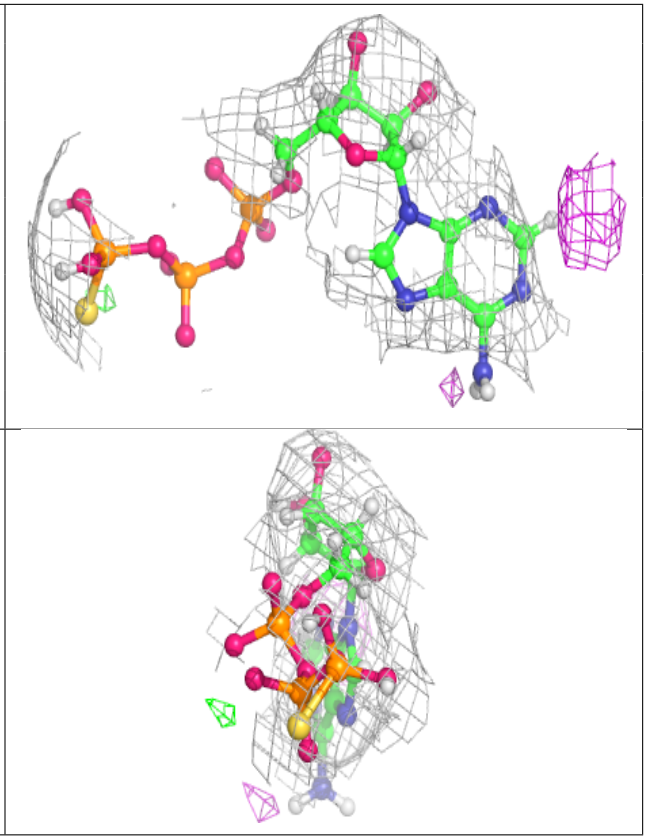


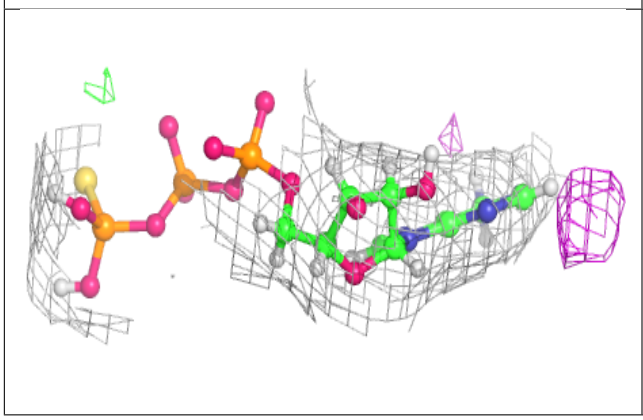




Electron density around AGS I 901:

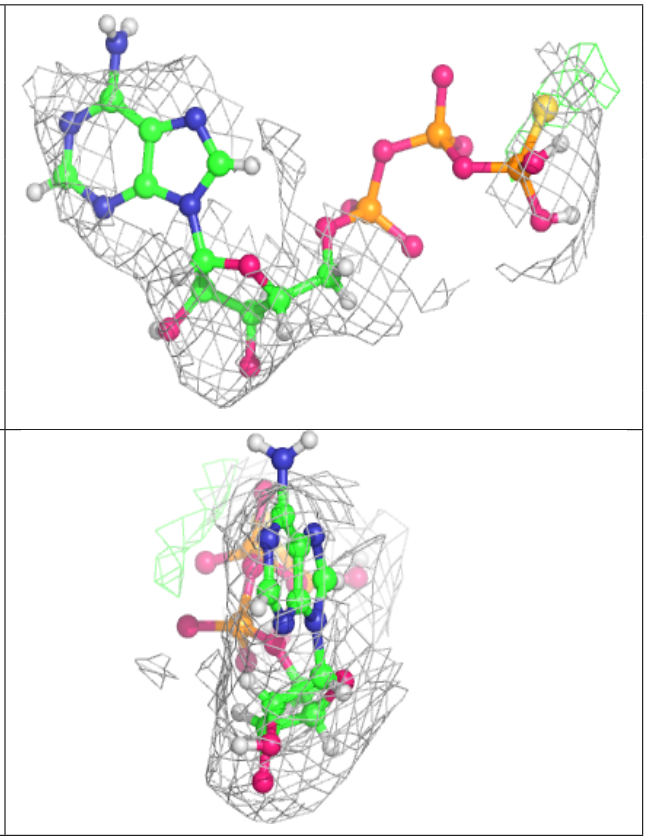
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

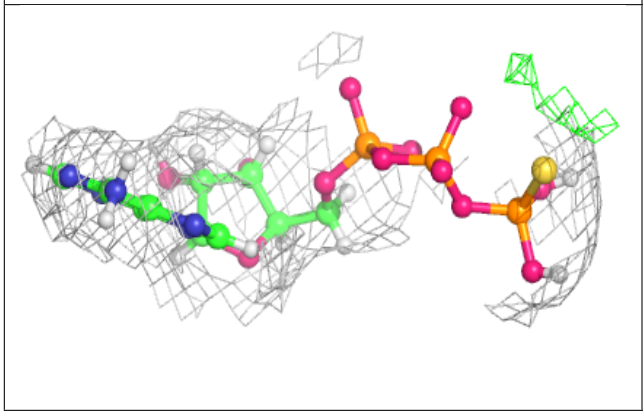




Electron density around AGS C 901:

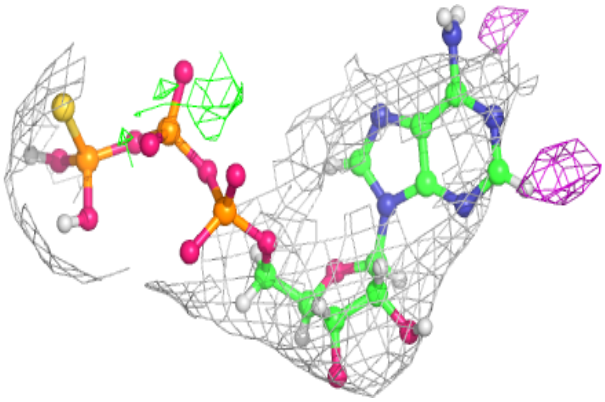
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

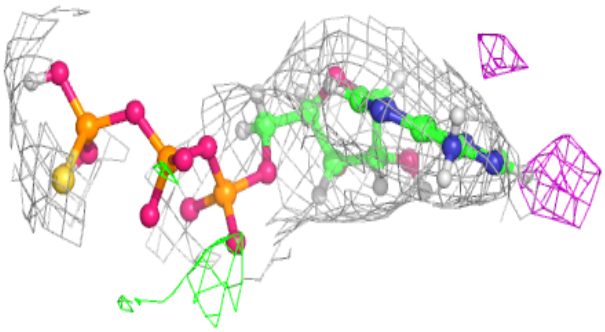


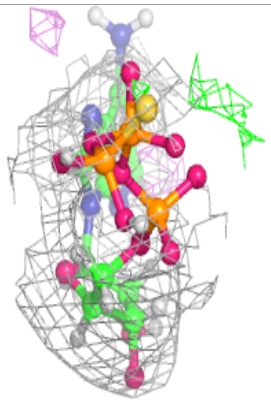


Electron density around AGS H 901:

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

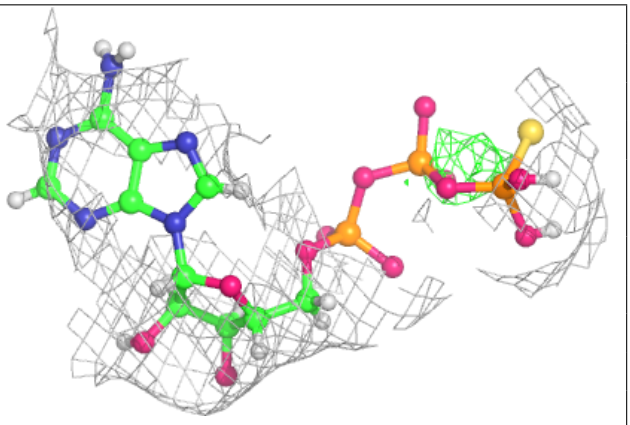


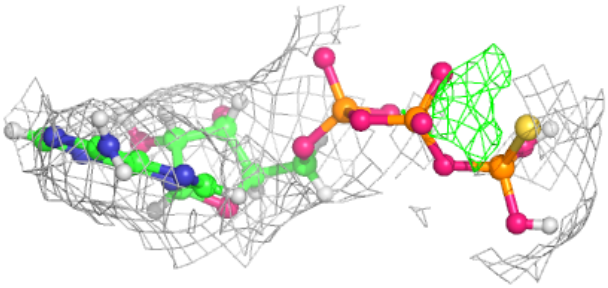


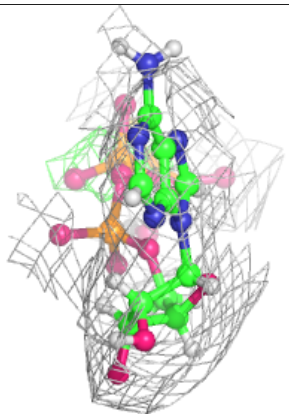


Electron density around AGS L 901:

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

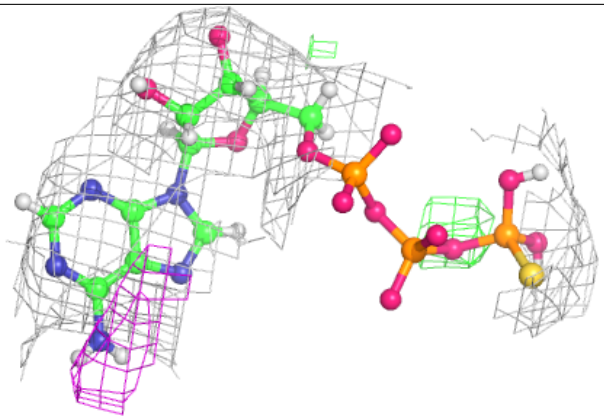


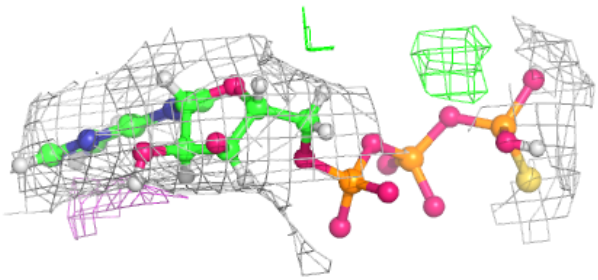


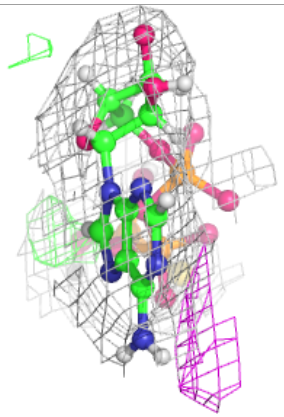


Electron density around AGS A 901:

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

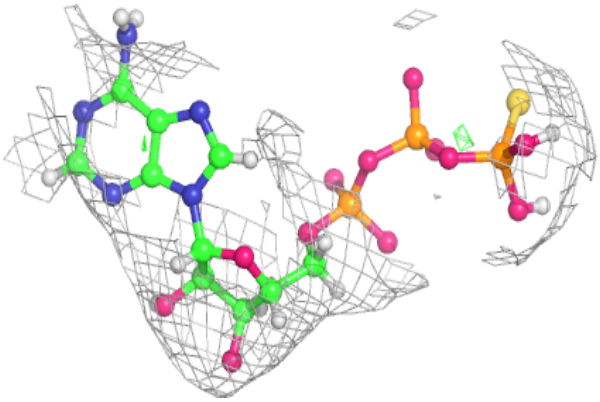


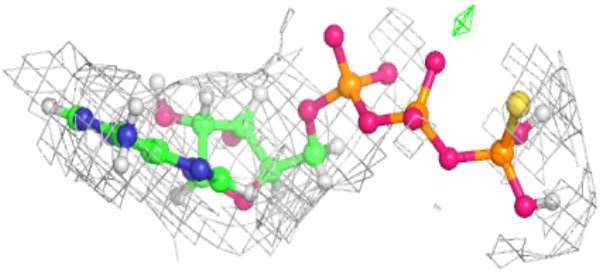


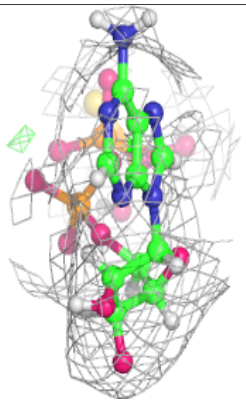


Electron density around AGS K 901:

$2mF_o$-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.