



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 02:04 AM UTC

PDB ID : 1KP8 / pdb_00001kp8
Title : Structural Basis for GroEL-assisted Protein Folding from the Crystal Structure of (GroEL-KMgATP)₁₄ at 2.0 Å Resolution
Authors : Wang, J.
Deposited on : 2001-12-30
Resolution : 2.00 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

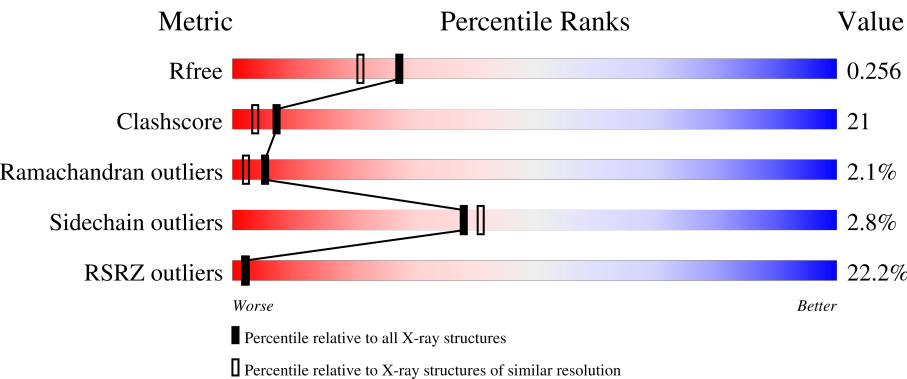
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	547	19% 61% 31% . .
1	B	547	25% 61% 31% . .
1	C	547	27% 63% 29% . .
1	D	547	11% 64% 29% . .
1	E	547	22% 62% 31% . .

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Mol	Chain	Length	Quality of chain
1	F	547	25% 64% 28%
1	G	547	17% 64% 29%
1	H	547	16% 63% 29%
1	I	547	20% 63% 29%
1	J	547	21% 63% 29%
1	K	547	27% 62% 30%
1	L	547	22% 63% 30%
1	M	547	29% 61% 31%
1	N	547	18% 65% 27%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 57085 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called groEL protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	B	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	C	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	D	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	E	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	F	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	G	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	H	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	I	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	J	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	K	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	L	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	M	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	N	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
A	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
B	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
B	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
B	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
C	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
C	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
C	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
D	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
D	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
D	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
E	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
E	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
E	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
F	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
F	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
F	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
G	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
G	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
G	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
H	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
H	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
H	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
I	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
I	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
I	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
J	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
J	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
J	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
K	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
K	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
K	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
L	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
L	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
L	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
M	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
M	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
M	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
N	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
N	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
N	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	J	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	M	1	Total	O	S	0	0
			5	4	1		
2	M	1	Total	O	S	0	0
			5	4	1		
2	N	1	Total	O	S	0	0
			5	4	1		
2	N	1	Total	O	S	0	0
			5	4	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		
3	G	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		
3	I	1	Total	Mg	0	0
			1	1		
3	J	1	Total	Mg	0	0
			1	1		
3	K	1	Total	Mg	0	0
			1	1		

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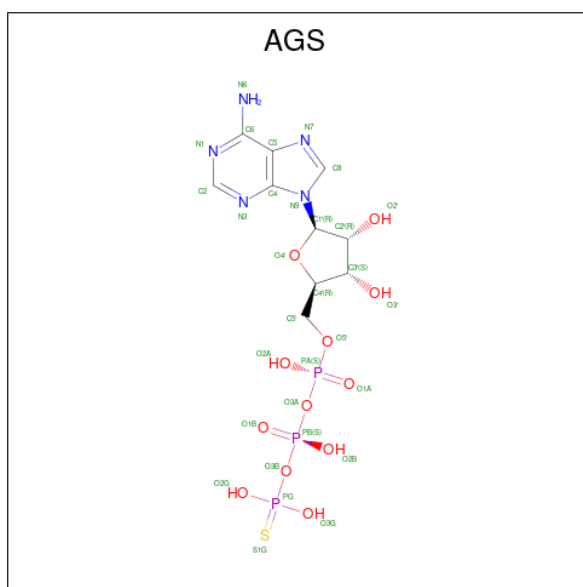
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	1	Total 1	Mg 1	0	0
3	M	1	Total 1	Mg 1	0	0
3	N	1	Total 1	Mg 1	0	0

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

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

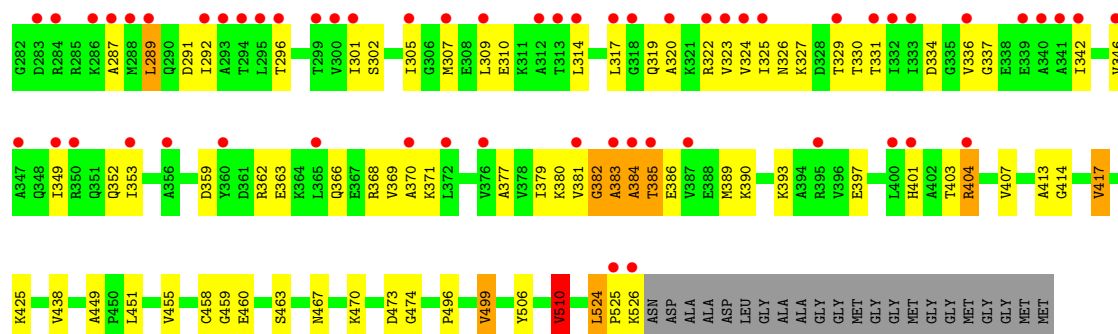
- Molecule 5 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



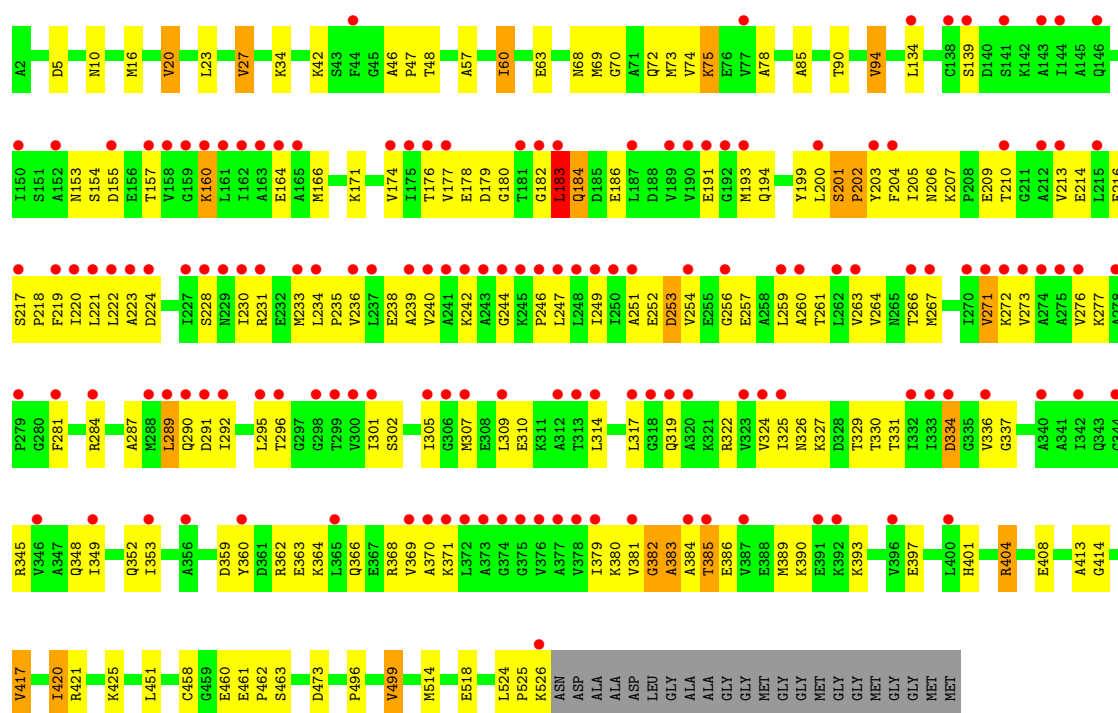
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
5	B	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
5	C	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
5	D	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
5	E	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
5	F	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
5	G	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
5	H	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
5	I	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
5	J	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
5	K	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
5	L	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
5	M	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
5	N	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0

- Molecule 6 is water.

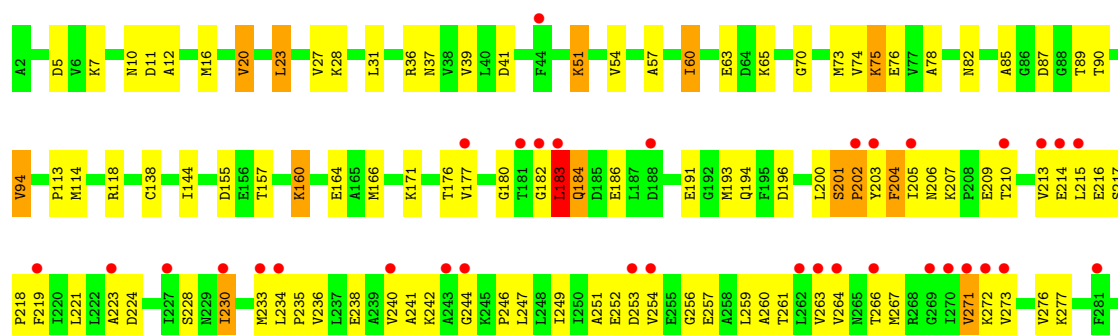
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	156	Total 156	O 156	0	0
6	B	214	Total 214	O 214	0	0
6	C	149	Total 149	O 149	0	0
6	D	261	Total 261	O 261	0	0
6	E	217	Total 217	O 217	0	0
6	F	200	Total 200	O 200	0	0
6	G	269	Total 269	O 269	0	0
6	H	204	Total 204	O 204	0	0
6	I	145	Total 145	O 145	0	0
6	J	139	Total 139	O 139	0	0
6	K	133	Total 133	O 133	0	0
6	L	163	Total 163	O 163	0	0
6	M	138	Total 138	O 138	0	0
6	N	153	Total 153	O 153	0	0

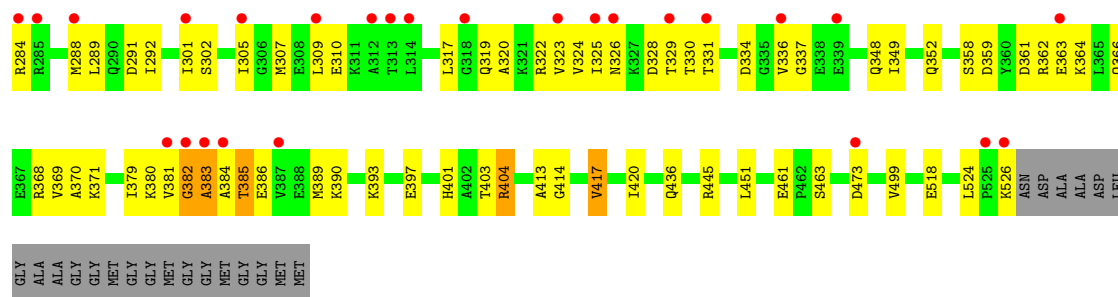


• Molecule 1: groEL protein

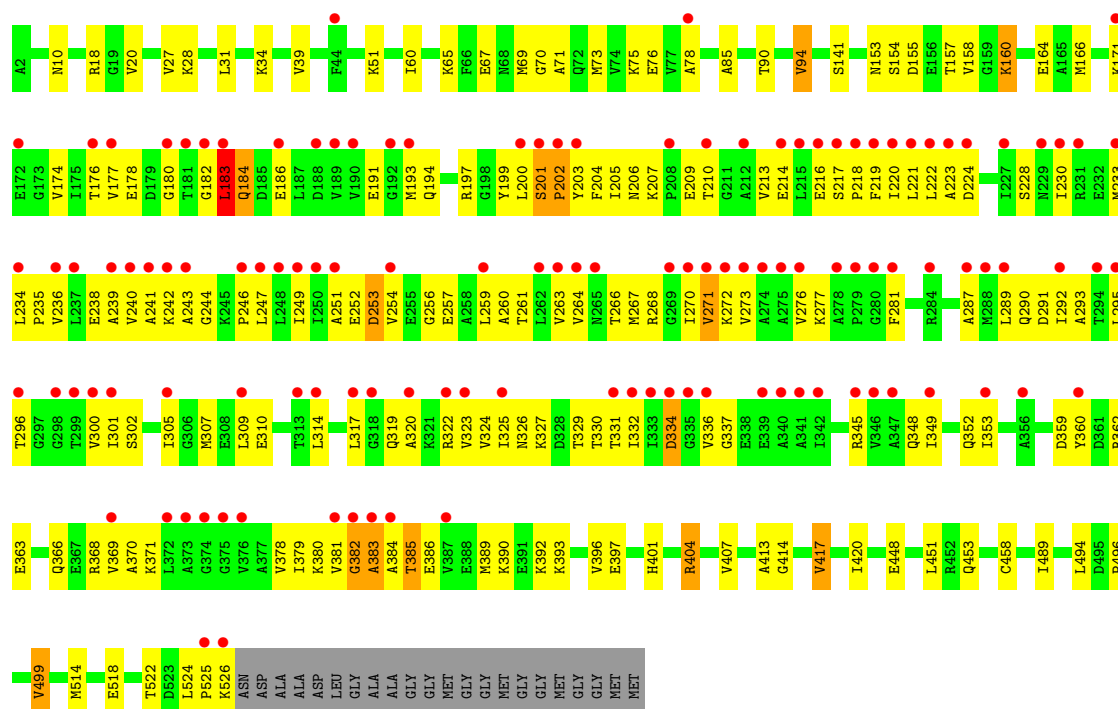


• Molecule 1: groEL protein

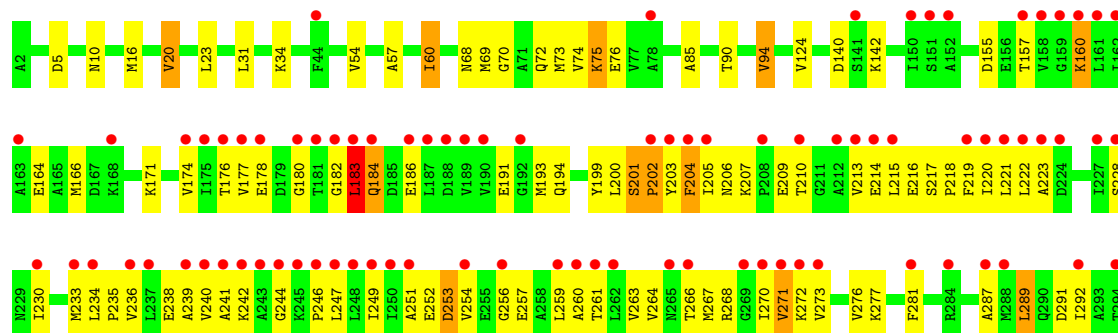


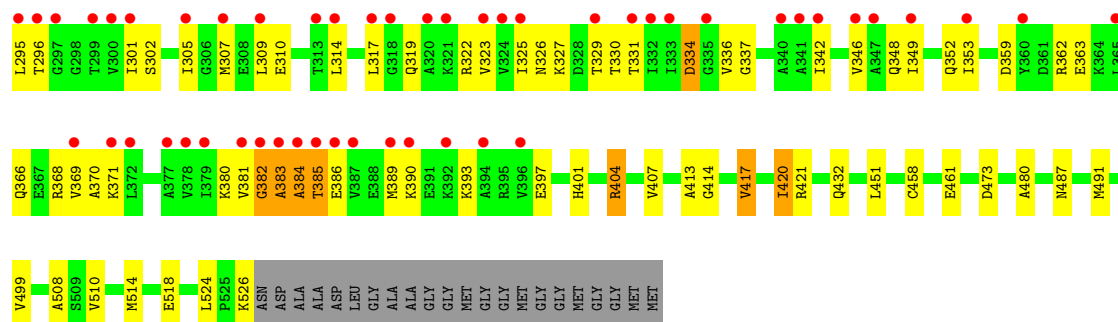


• Molecule 1: groEL protein

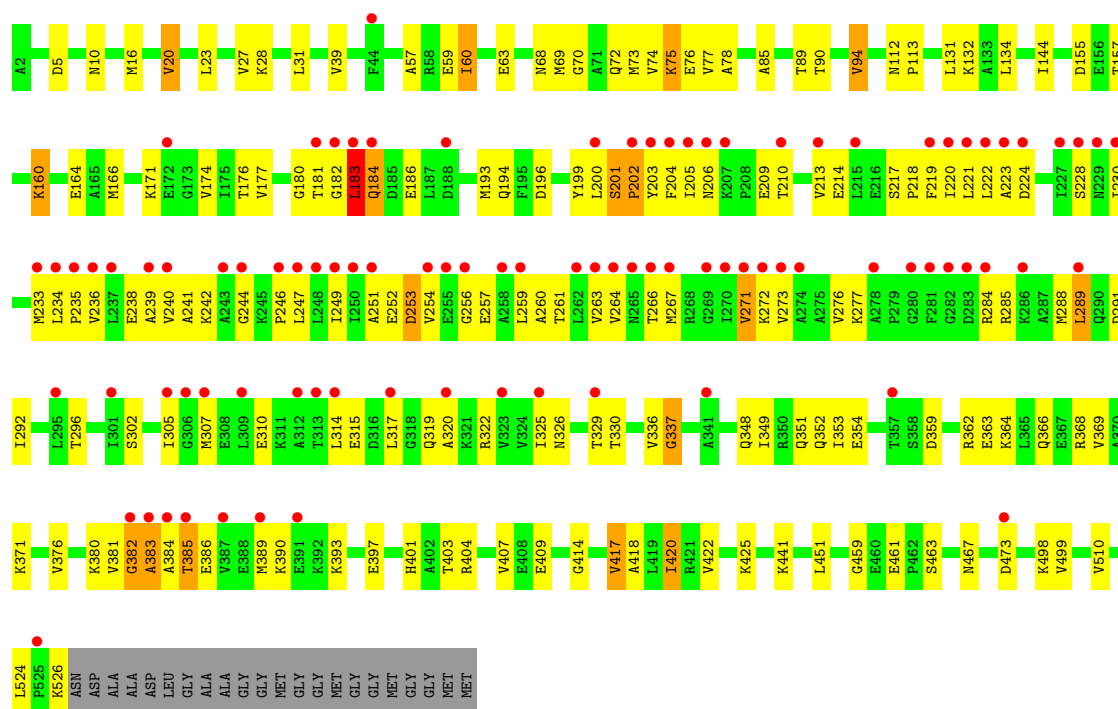


• Molecule 1: groEL protein

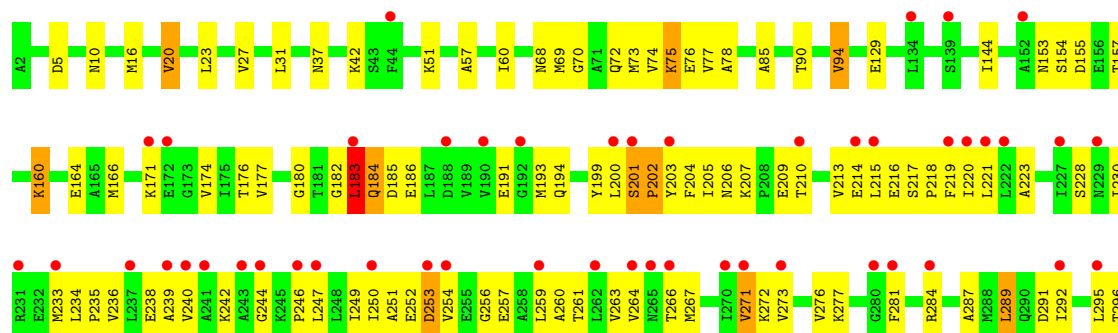


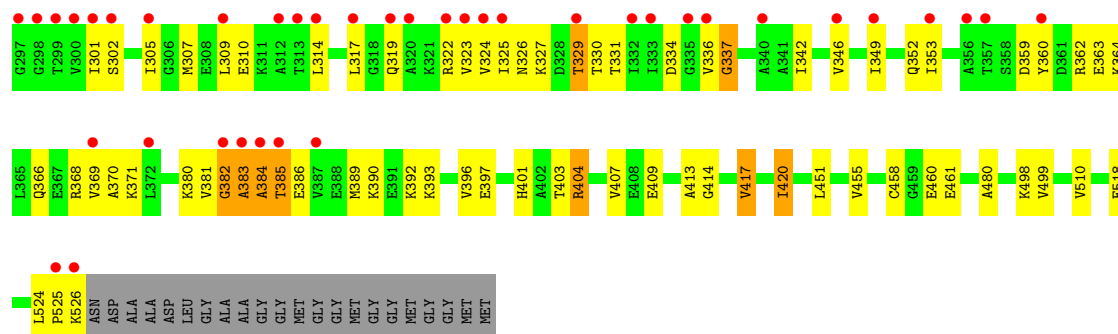


• Molecule 1: groEL protein

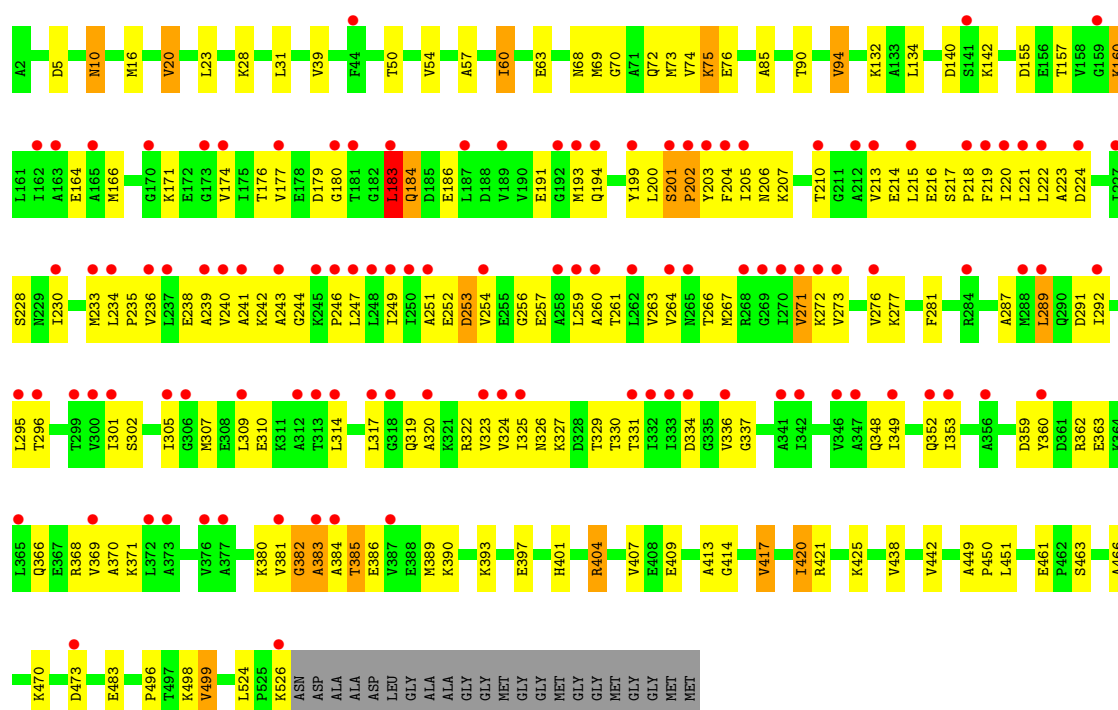


• Molecule 1: groEL protein

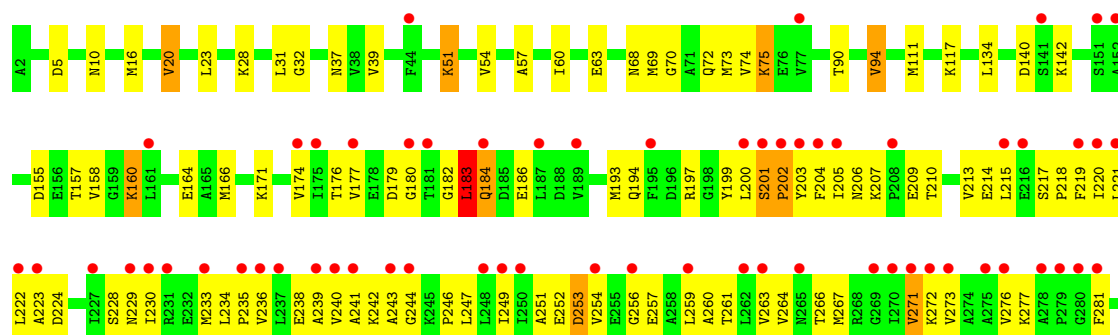


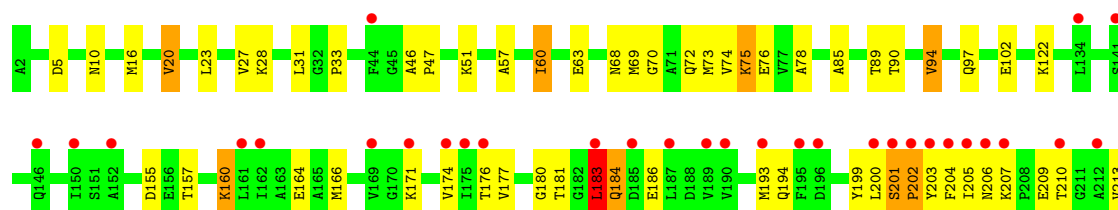


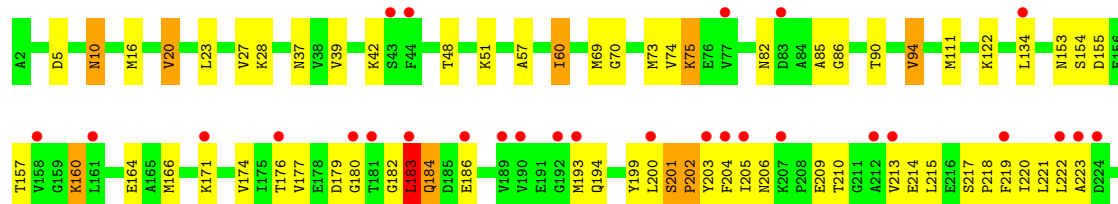
• Molecule 1: groEL protein

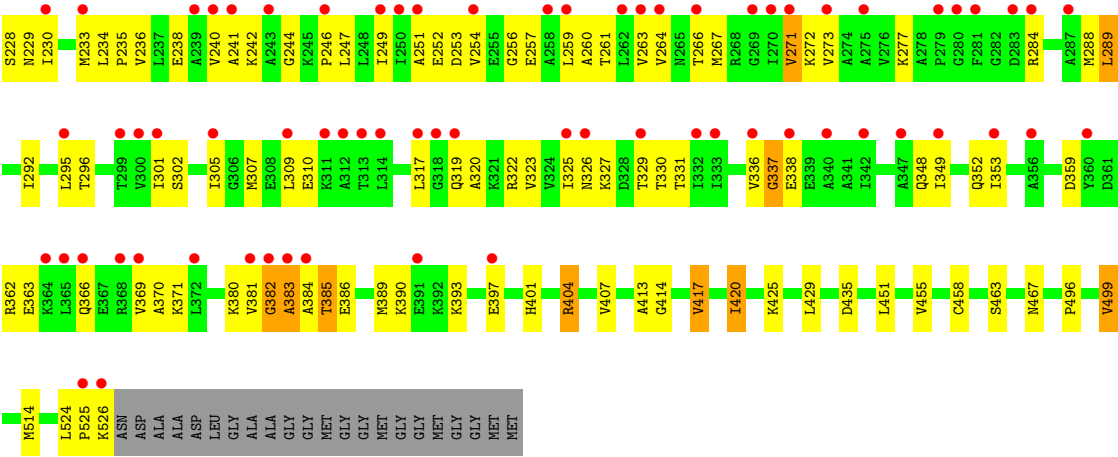


• Molecule 1: groEL protein









4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.57Å 260.11Å 150.20Å 90.00° 101.14° 90.00°	Depositor
Resolution (Å)	39.89 – 2.00 39.89 – 2.00	Depositor EDS
% Data completeness (in resolution range)	78.9 (39.89-2.00) 79.0 (39.89-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.57 (at 2.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.243 , 0.258 0.241 , 0.256	Depositor DCC
R_{free} test set	12780 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.362	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	57085	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AGS, MG, SO4, K

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	0.41	0/3883	0.87	9/5243 (0.2%)
1	B	0.44	0/3883	0.87	7/5243 (0.1%)
1	C	0.41	0/3883	0.87	6/5243 (0.1%)
1	D	0.47	0/3883	0.89	11/5243 (0.2%)
1	E	0.46	0/3883	0.88	3/5243 (0.1%)
1	F	0.42	0/3883	0.85	6/5243 (0.1%)
1	G	0.46	0/3883	0.88	9/5243 (0.2%)
1	H	0.42	0/3883	0.85	6/5243 (0.1%)
1	I	0.39	0/3883	0.86	7/5243 (0.1%)
1	J	0.40	0/3883	0.86	9/5243 (0.2%)
1	K	0.39	0/3883	0.85	7/5243 (0.1%)
1	L	0.42	0/3883	0.85	7/5243 (0.1%)
1	M	0.39	0/3883	0.85	5/5243 (0.1%)
1	N	0.40	0/3883	0.85	4/5243 (0.1%)
All	All	0.42	0/54362	0.86	96/73402 (0.1%)

There are no bond length outliers.

The worst 5 of 96 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	510	VAL	CB-CA-C	-8.18	100.94	112.22
1	E	60	ILE	N-CA-C	7.25	118.41	108.84
1	J	461	GLU	CA-C-N	7.17	126.70	119.24
1	J	461	GLU	C-N-CA	7.17	126.70	119.24
1	C	5	ASP	N-CA-C	-7.10	98.15	109.59

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3855	0	3982	173	0
1	B	3855	0	3982	183	0
1	C	3855	0	3982	164	0
1	D	3855	0	3982	160	0
1	E	3855	0	3982	165	0
1	F	3855	0	3982	151	0
1	G	3855	0	3982	164	1
1	H	3855	0	3982	158	0
1	I	3855	0	3982	165	0
1	J	3855	0	3982	163	0
1	K	3855	0	3982	167	0
1	L	3855	0	3982	162	0
1	M	3855	0	3982	169	0
1	N	3855	0	3982	156	1
2	A	15	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	E	10	0	0	1	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	10	0	0	0	0
2	J	10	0	0	0	0
2	K	10	0	0	0	0
2	L	5	0	0	0	0
2	M	10	0	0	0	0
2	N	10	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
5	A	31	0	12	3	0
5	B	31	0	12	4	0
5	C	31	0	12	3	0
5	D	31	0	12	4	0
5	E	31	0	12	4	0
5	F	31	0	12	3	0
5	G	31	0	12	5	0
5	H	31	0	12	4	0
5	I	31	0	12	4	0
5	J	31	0	12	4	0
5	K	31	0	12	5	0
5	L	31	0	12	5	0
5	M	31	0	12	5	0
5	N	31	0	12	4	0
6	A	156	0	0	7	0
6	B	214	0	0	8	0
6	C	149	0	0	9	0
6	D	261	0	0	19	0
6	E	217	0	0	12	0
6	F	200	0	0	6	0
6	G	269	0	0	12	0
6	H	204	0	0	7	0
6	I	145	0	0	5	0
6	J	139	0	0	2	0
6	K	133	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	L	163	0	0	9	0
6	M	138	0	0	6	0
6	N	153	0	0	7	0
All	All	57085	0	55916	2271	1

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 21.

The worst 5 of 2271 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)
5:B:1:AGS:PG	5:B:1:AGS:S1G	1.50	1.50
5:A:1:AGS:PG	5:A:1:AGS:S1G	1.50	1.49
5:H:1:AGS:S1G	5:H:1:AGS:PG	1.49	1.49
5:M:1:AGS:PG	5:M:1:AGS:S1G	1.49	1.48
5:D:551:AGS:PG	5:D:551:AGS:S1G	1.48	1.48

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:315:GLU:OE2	1:N:338:GLU:OE1[1_554]	2.17	0.03

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	523/547 (96%)	487 (93%)	27 (5%)	9 (2%)	7 3
1	B	523/547 (96%)	487 (93%)	24 (5%)	12 (2%)	5 2
1	C	523/547 (96%)	488 (93%)	24 (5%)	11 (2%)	5 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	523/547 (96%)	492 (94%)	22 (4%)	9 (2%)	7	3
1	E	523/547 (96%)	485 (93%)	27 (5%)	11 (2%)	5	2
1	F	523/547 (96%)	487 (93%)	24 (5%)	12 (2%)	5	2
1	G	523/547 (96%)	489 (94%)	23 (4%)	11 (2%)	5	2
1	H	523/547 (96%)	487 (93%)	24 (5%)	12 (2%)	5	2
1	I	523/547 (96%)	486 (93%)	27 (5%)	10 (2%)	6	3
1	J	523/547 (96%)	486 (93%)	25 (5%)	12 (2%)	5	2
1	K	523/547 (96%)	484 (92%)	29 (6%)	10 (2%)	6	3
1	L	523/547 (96%)	488 (93%)	23 (4%)	12 (2%)	5	2
1	M	523/547 (96%)	487 (93%)	25 (5%)	11 (2%)	5	2
1	N	523/547 (96%)	487 (93%)	26 (5%)	10 (2%)	6	3
All	All	7322/7658 (96%)	6820 (93%)	350 (5%)	152 (2%)	5	2

5 of 152 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	183	LEU
1	E	183	LEU
1	A	183	LEU
1	A	256	GLY
1	A	271	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	404/413 (98%)	392 (97%)	12 (3%)	36	38
1	B	404/413 (98%)	394 (98%)	10 (2%)	42	45
1	C	404/413 (98%)	393 (97%)	11 (3%)	39	42
1	D	404/413 (98%)	391 (97%)	13 (3%)	34	35
1	E	404/413 (98%)	395 (98%)	9 (2%)	45	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	404/413 (98%)	392 (97%)	12 (3%)	36	38
1	G	404/413 (98%)	393 (97%)	11 (3%)	39	42
1	H	404/413 (98%)	392 (97%)	12 (3%)	36	38
1	I	404/413 (98%)	392 (97%)	12 (3%)	36	38
1	J	404/413 (98%)	392 (97%)	12 (3%)	36	38
1	K	404/413 (98%)	393 (97%)	11 (3%)	39	42
1	L	404/413 (98%)	393 (97%)	11 (3%)	39	42
1	M	404/413 (98%)	392 (97%)	12 (3%)	36	38
1	N	404/413 (98%)	393 (97%)	11 (3%)	39	42
All	All	5656/5782 (98%)	5497 (97%)	159 (3%)	38	41

5 of 159 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	20	VAL
1	M	289	LEU
1	K	183	LEU
1	L	183	LEU
1	N	75	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 120 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	351	GLN
1	M	401	HIS
1	I	326	ASN
1	M	351	GLN
1	N	401	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 66 ligands modelled in this entry, 30 are monoatomic - leaving 36 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	SO4	L	4003	-	4,4,4	1.51	1 (25%)	6,6,6	1.13	0
2	SO4	A	4001	-	4,4,4	1.51	1 (25%)	6,6,6	1.14	0
5	AGS	N	1	3,4	32,33,33	3.59	4 (12%)	45,52,52	1.00	2 (4%)
5	AGS	J	1	3,4	32,33,33	3.49	2 (6%)	45,52,52	0.96	1 (2%)
2	SO4	F	4004	-	4,4,4	1.45	1 (25%)	6,6,6	1.15	0
2	SO4	C	4012	-	4,4,4	1.54	1 (25%)	6,6,6	1.13	0
2	SO4	K	4022	-	4,4,4	1.50	1 (25%)	6,6,6	1.12	0
5	AGS	B	1	3,4	32,33,33	3.58	4 (12%)	45,52,52	1.05	1 (2%)
2	SO4	M	4014	-	4,4,4	1.53	1 (25%)	6,6,6	1.11	0
2	SO4	K	4021	-	4,4,4	1.54	1 (25%)	6,6,6	1.12	0
2	SO4	A	4007	-	4,4,4	1.49	1 (25%)	6,6,6	1.13	0
5	AGS	I	1	3,4	32,33,33	3.56	3 (9%)	45,52,52	1.02	2 (4%)
2	SO4	B	4010	-	4,4,4	1.53	1 (25%)	6,6,6	1.11	0
2	SO4	A	4008	-	4,4,4	1.51	1 (25%)	6,6,6	1.11	0
2	SO4	H	4017	-	4,4,4	1.52	1 (25%)	6,6,6	1.12	0
5	AGS	L	1	3,4	32,33,33	3.54	3 (9%)	45,52,52	1.02	1 (2%)
5	AGS	H	1	3,4	32,33,33	3.57	3 (9%)	45,52,52	1.09	2 (4%)
5	AGS	F	1	3,4	32,33,33	3.48	2 (6%)	45,52,52	0.97	1 (2%)
5	AGS	M	1	3,4	32,33,33	3.57	4 (12%)	45,52,52	1.05	3 (6%)
2	SO4	E	4006	-	4,4,4	1.52	1 (25%)	6,6,6	1.10	0
2	SO4	E	4005	-	4,4,4	1.43	1 (25%)	6,6,6	1.14	0
2	SO4	H	4018	-	4,4,4	1.51	1 (25%)	6,6,6	1.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	N	4016	-	4,4,4	1.51	1 (25%)	6,6,6	1.12	0
2	SO4	C	4011	-	4,4,4	1.51	1 (25%)	6,6,6	1.11	0
2	SO4	N	4015	-	4,4,4	1.52	1 (25%)	6,6,6	1.13	0
5	AGS	K	1	3,4	32,33,33	3.56	4 (12%)	45,52,52	1.01	2 (4%)
5	AGS	E	1	3,4	32,33,33	3.63	5 (15%)	45,52,52	1.10	1 (2%)
5	AGS	A	1	3,4	32,33,33	3.54	4 (12%)	45,52,52	1.06	2 (4%)
5	AGS	C	1	3,4	32,33,33	3.57	4 (12%)	45,52,52	1.05	1 (2%)
2	SO4	J	4020	-	4,4,4	1.52	1 (25%)	6,6,6	1.11	0
2	SO4	J	4019	-	4,4,4	1.51	1 (25%)	6,6,6	1.10	0
5	AGS	G	1	3,4	32,33,33	3.63	2 (6%)	45,52,52	1.07	1 (2%)
5	AGS	D	551	3,4	32,33,33	3.57	3 (9%)	45,52,52	1.01	1 (2%)
2	SO4	M	4013	-	4,4,4	1.56	1 (25%)	6,6,6	1.12	0
2	SO4	G	4002	-	4,4,4	1.51	1 (25%)	6,6,6	1.14	0
2	SO4	B	4009	-	4,4,4	1.50	1 (25%)	6,6,6	1.09	0

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
5	AGS	F	1	3,4	-	3/21/38/38	0/3/3/3
5	AGS	G	1	3,4	-	3/21/38/38	0/3/3/3
5	AGS	M	1	3,4	-	3/21/38/38	0/3/3/3
5	AGS	D	551	3,4	-	3/21/38/38	0/3/3/3
5	AGS	N	1	3,4	-	3/21/38/38	0/3/3/3
5	AGS	J	1	3,4	-	3/21/38/38	0/3/3/3
5	AGS	K	1	3,4	-	3/21/38/38	0/3/3/3
5	AGS	B	1	3,4	-	3/21/38/38	0/3/3/3
5	AGS	E	1	3,4	-	3/21/38/38	0/3/3/3
5	AGS	I	1	3,4	-	3/21/38/38	0/3/3/3
5	AGS	H	1	3,4	-	3/21/38/38	0/3/3/3
5	AGS	A	1	3,4	-	3/21/38/38	0/3/3/3
5	AGS	L	1	3,4	-	3/21/38/38	0/3/3/3
5	AGS	C	1	3,4	-	3/21/38/38	0/3/3/3

The worst 5 of 69 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	1	AGS	PG-S1G	-19.61	1.48	1.90
5	E	1	AGS	PG-S1G	-19.53	1.48	1.90
5	D	551	AGS	PG-S1G	-19.43	1.48	1.90
5	N	1	AGS	PG-S1G	-19.13	1.49	1.90
5	I	1	AGS	PG-S1G	-19.13	1.49	1.90

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1	AGS	O4'-C1'-N9	3.93	115.64	108.09
5	B	1	AGS	O4'-C1'-N9	3.69	115.17	108.09
5	C	1	AGS	O4'-C1'-N9	3.43	114.68	108.09
5	H	1	AGS	O4'-C1'-N9	3.39	114.59	108.09
5	L	1	AGS	O4'-C1'-N9	3.35	114.53	108.09

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1	AGS	PB-O3B-PG-O2G
5	A	1	AGS	PB-O3B-PG-O3G
5	B	1	AGS	PB-O3B-PG-O2G
5	B	1	AGS	PB-O3B-PG-O3G
5	C	1	AGS	PB-O3B-PG-O2G

There are no ring outliers.

15 monomers are involved in 58 short contacts:

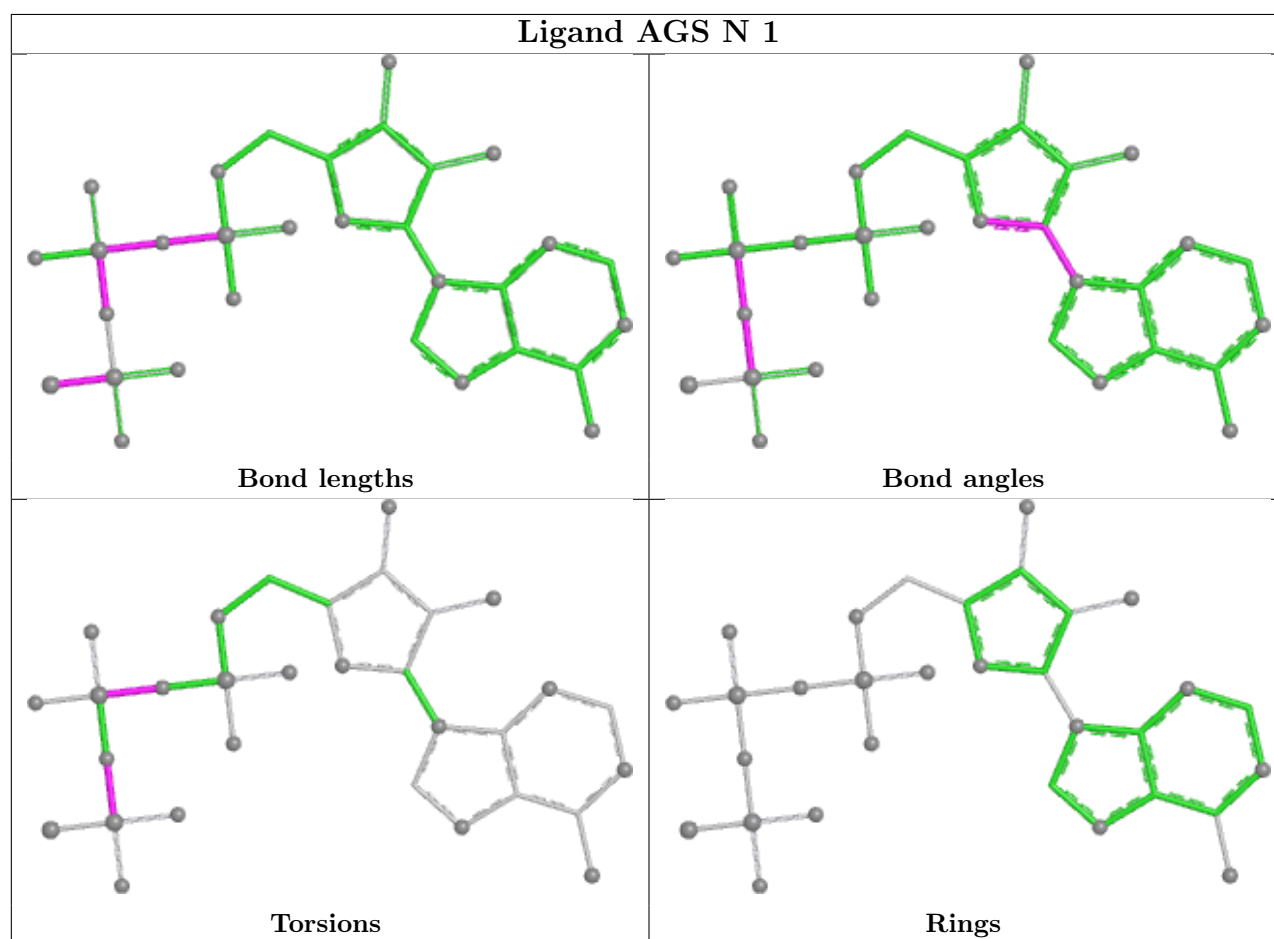
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	N	1	AGS	4	0
5	J	1	AGS	4	0
5	B	1	AGS	4	0
5	I	1	AGS	4	0
5	L	1	AGS	5	0
5	H	1	AGS	4	0
5	F	1	AGS	3	0
5	M	1	AGS	5	0
2	E	4005	SO4	1	0
5	K	1	AGS	5	0
5	E	1	AGS	4	0

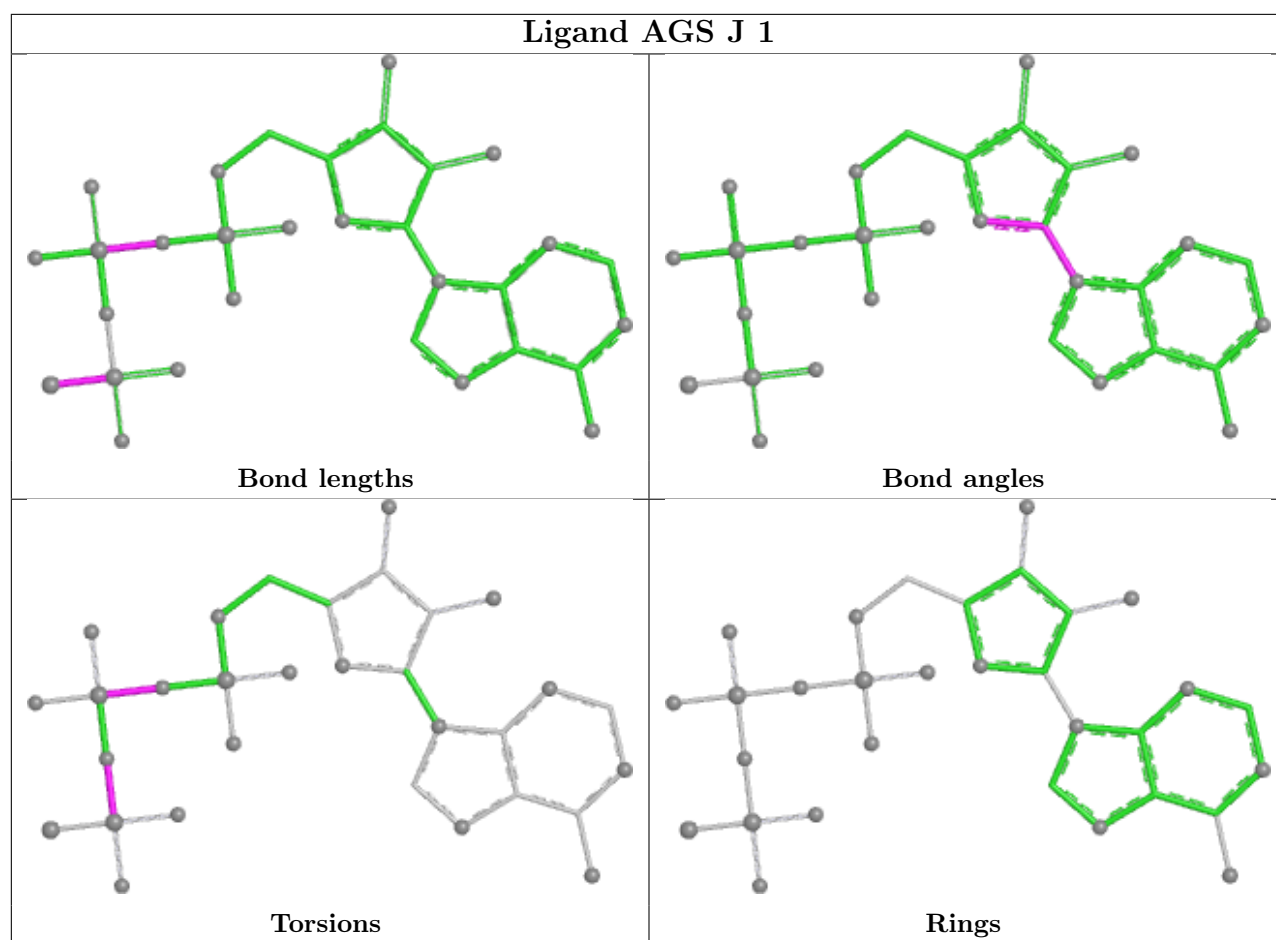
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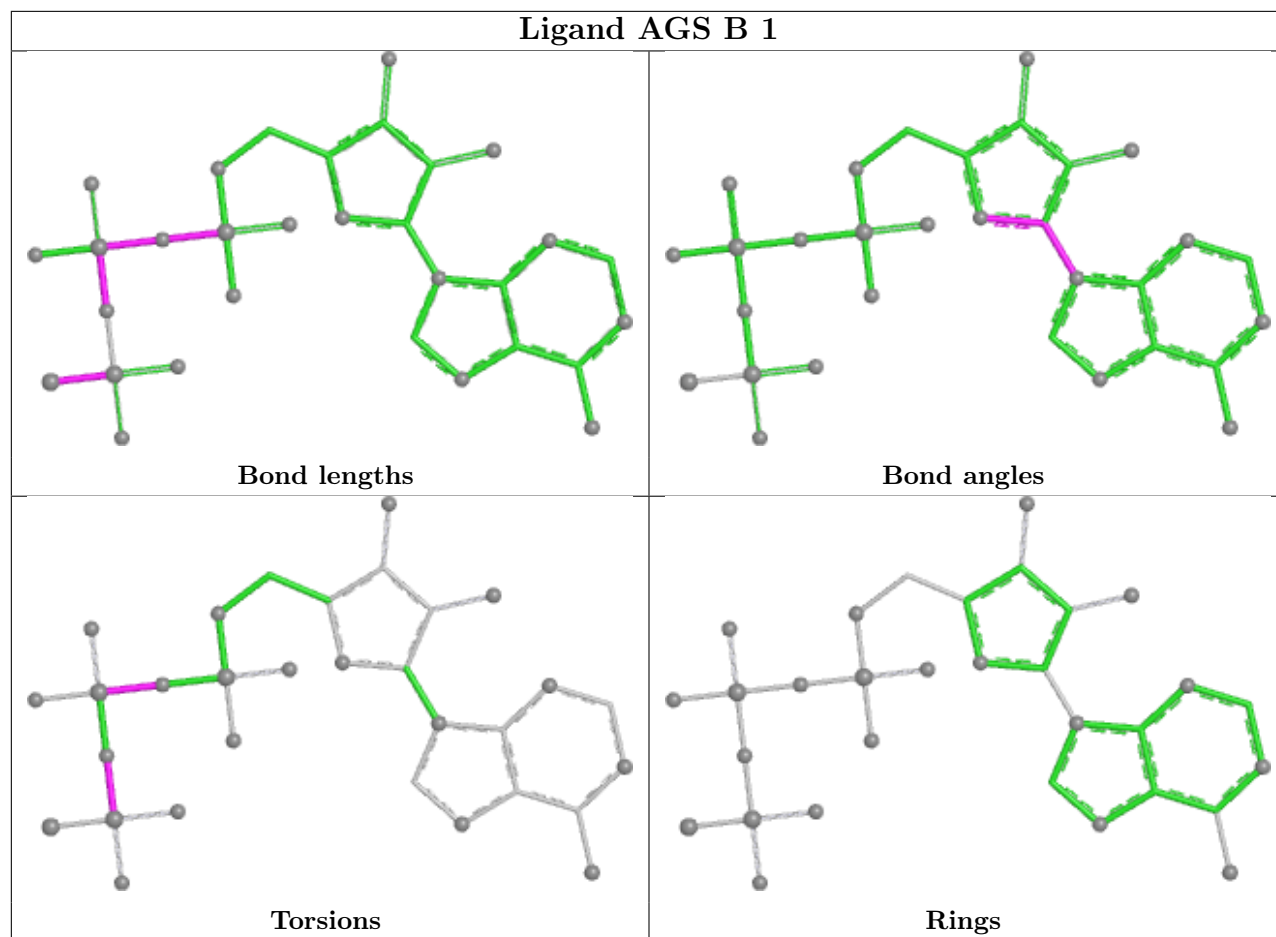
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1	AGS	3	0
5	C	1	AGS	3	0
5	G	1	AGS	5	0
5	D	551	AGS	4	0

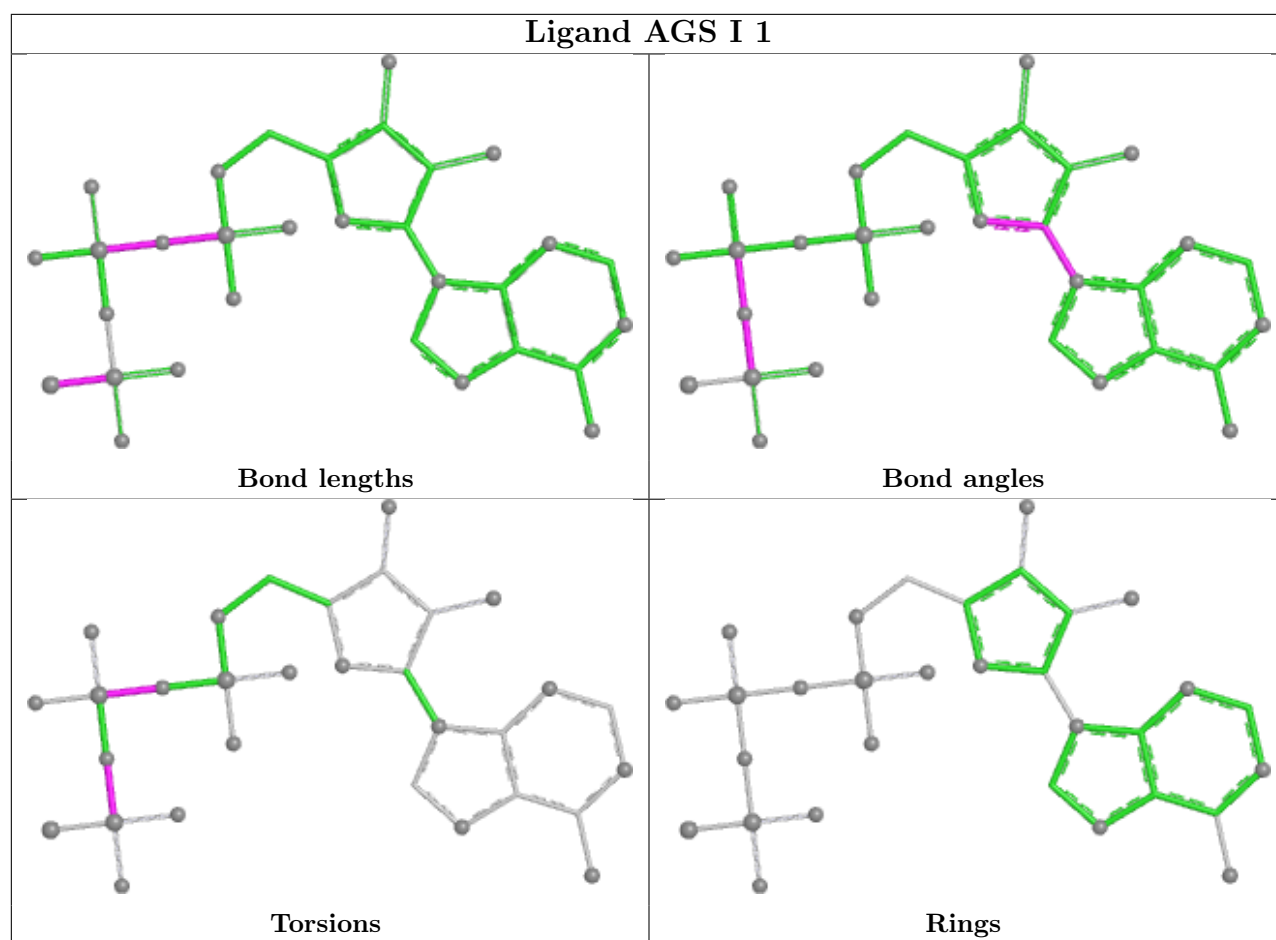
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

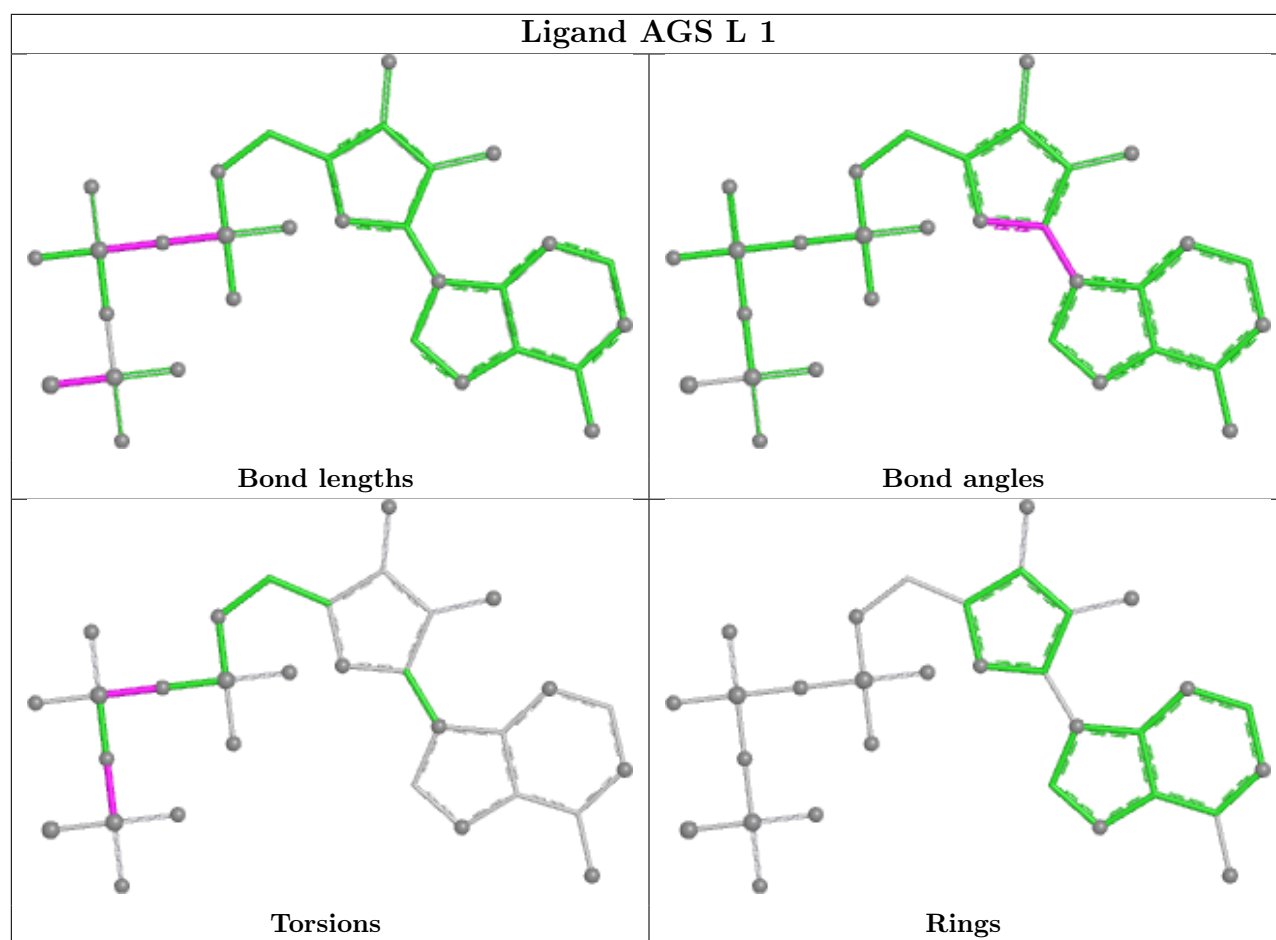


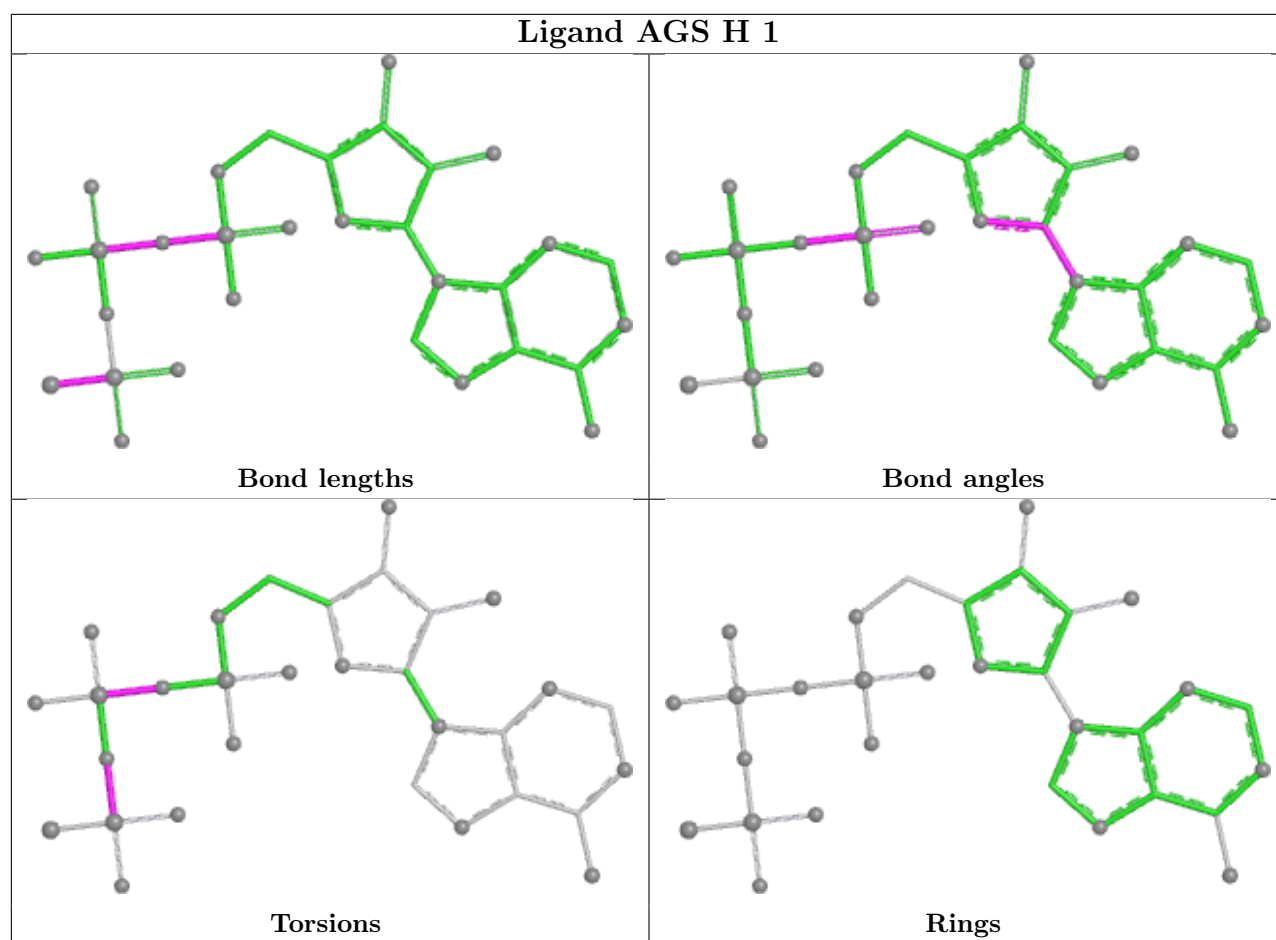


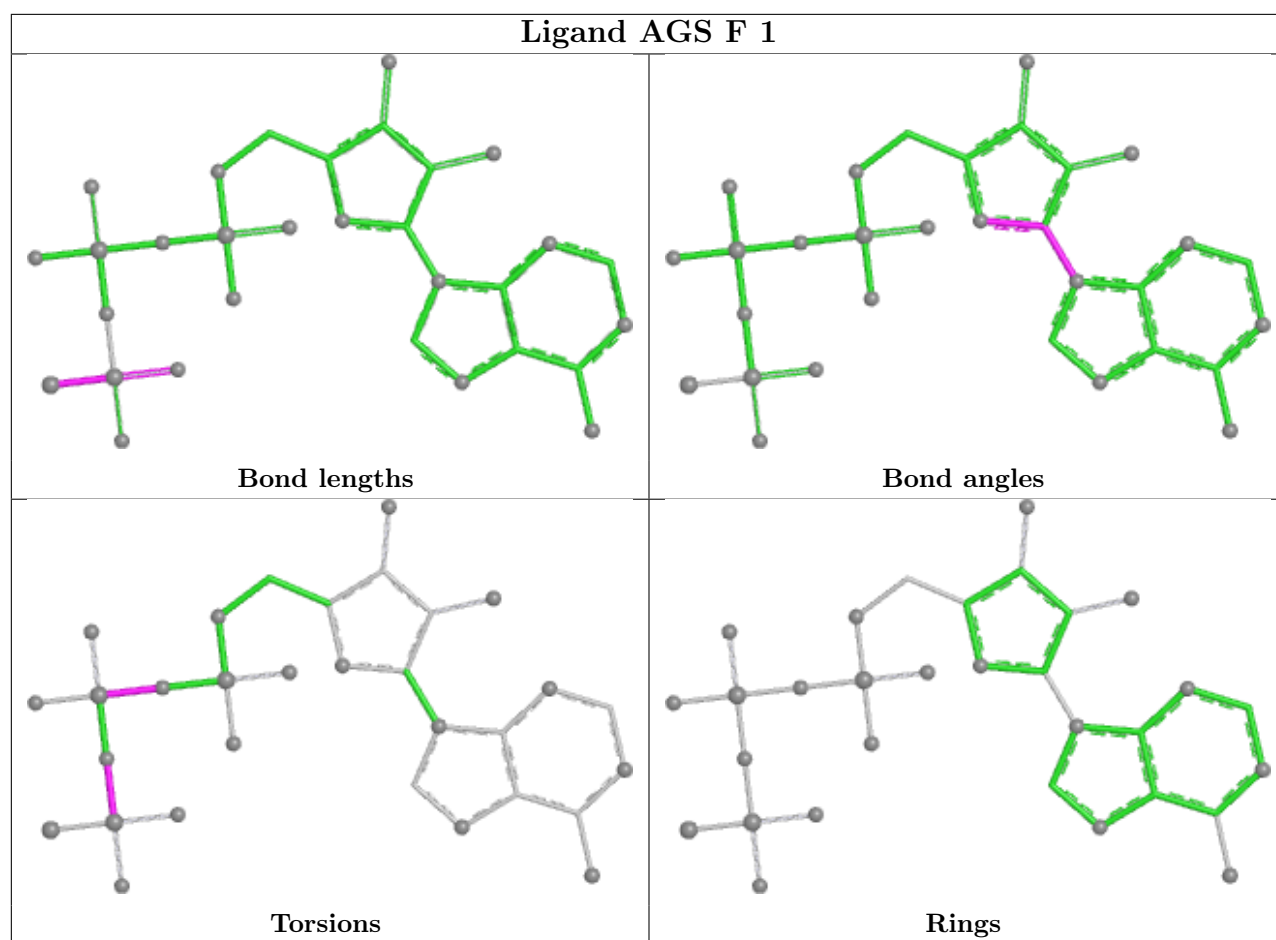
Ligand AGS B 1

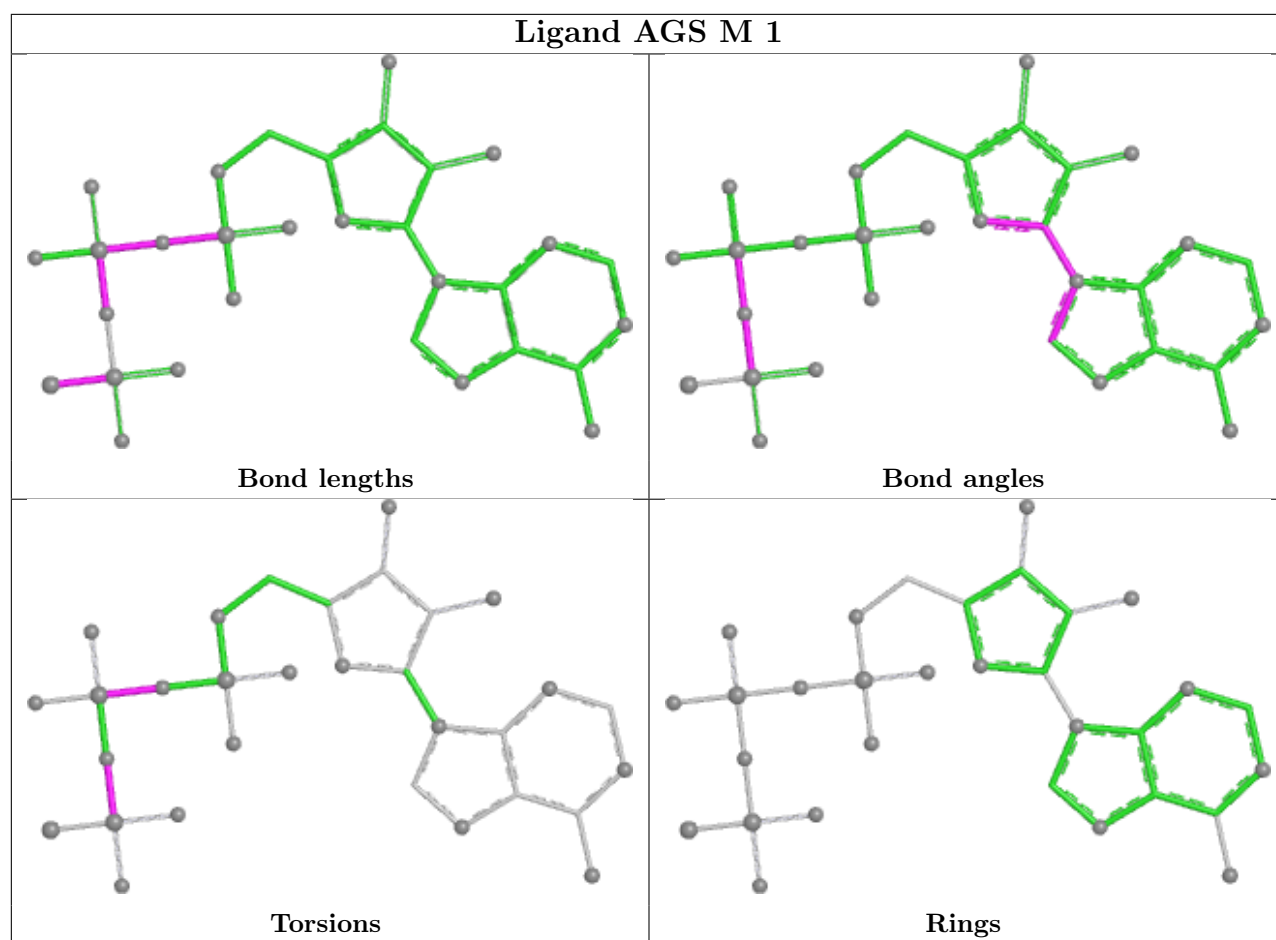




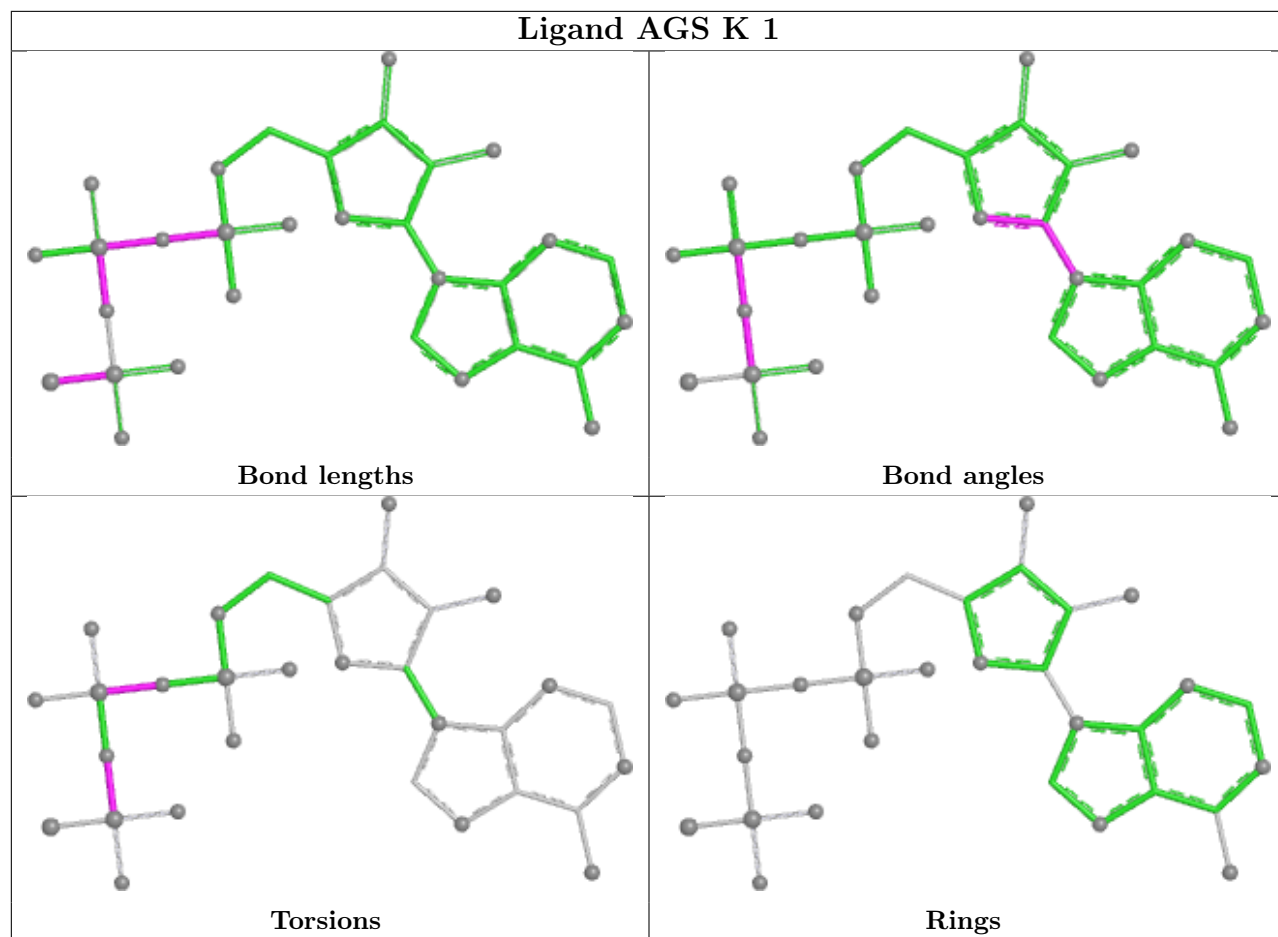




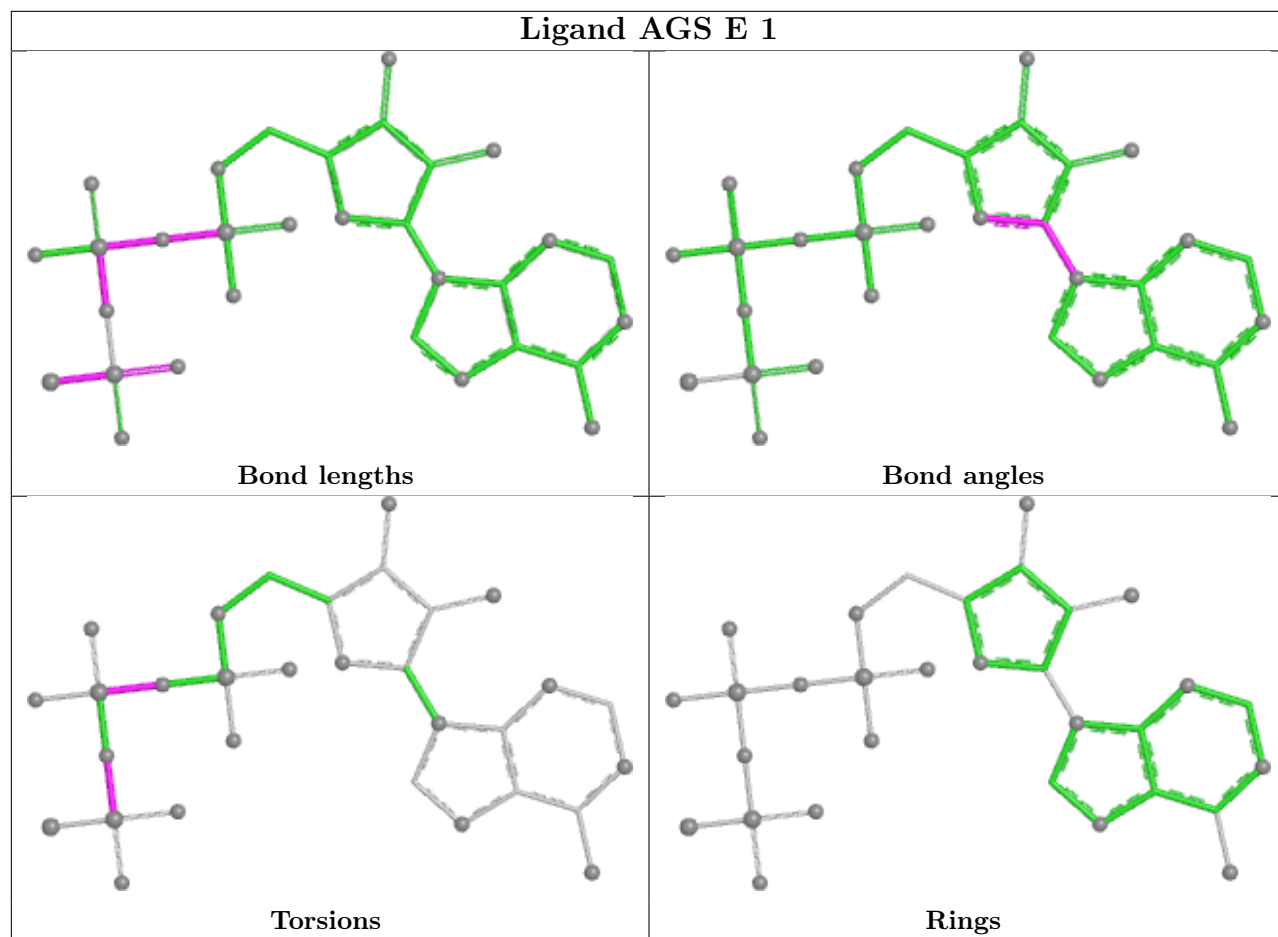




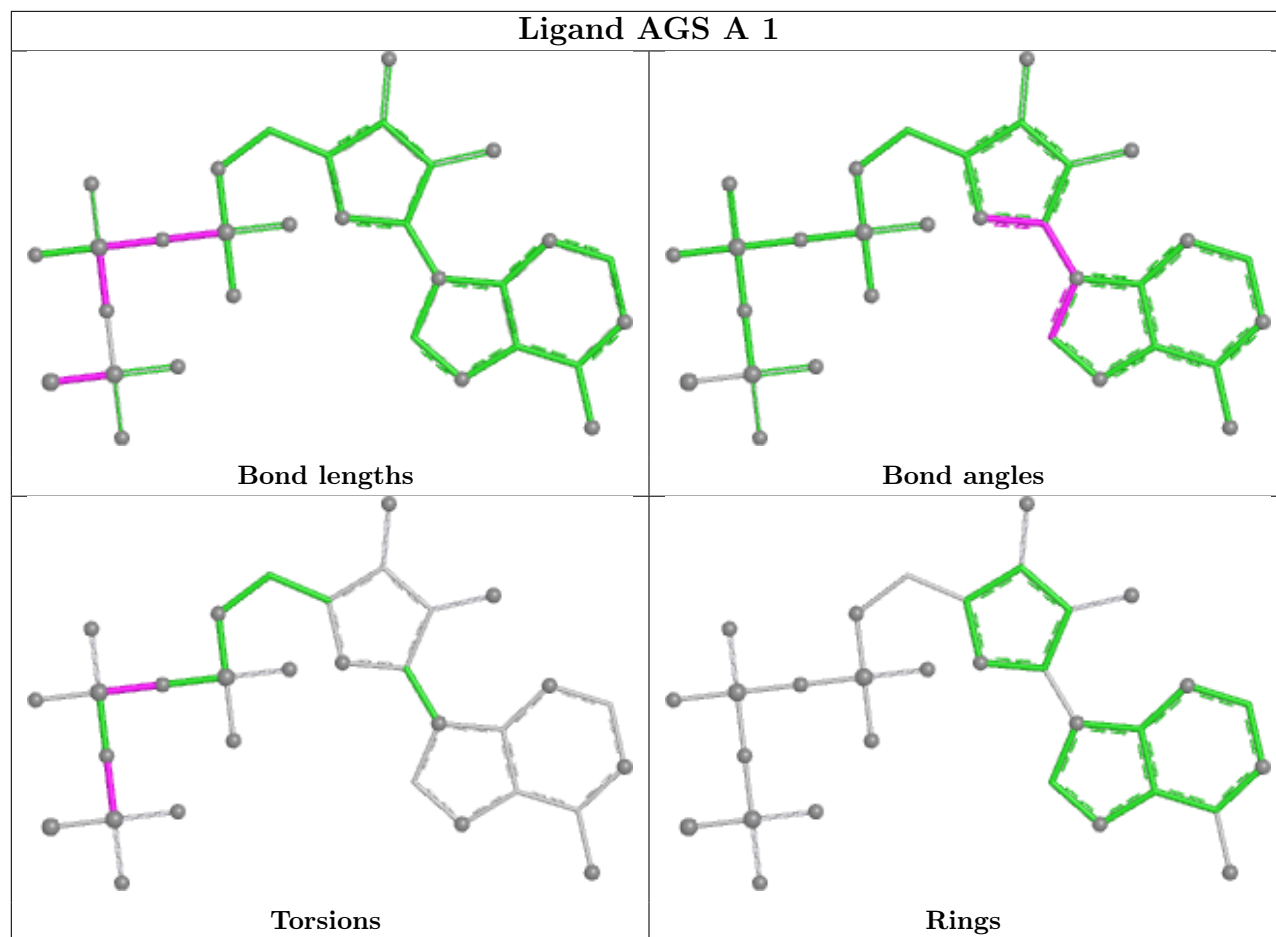
Ligand AGS K 1



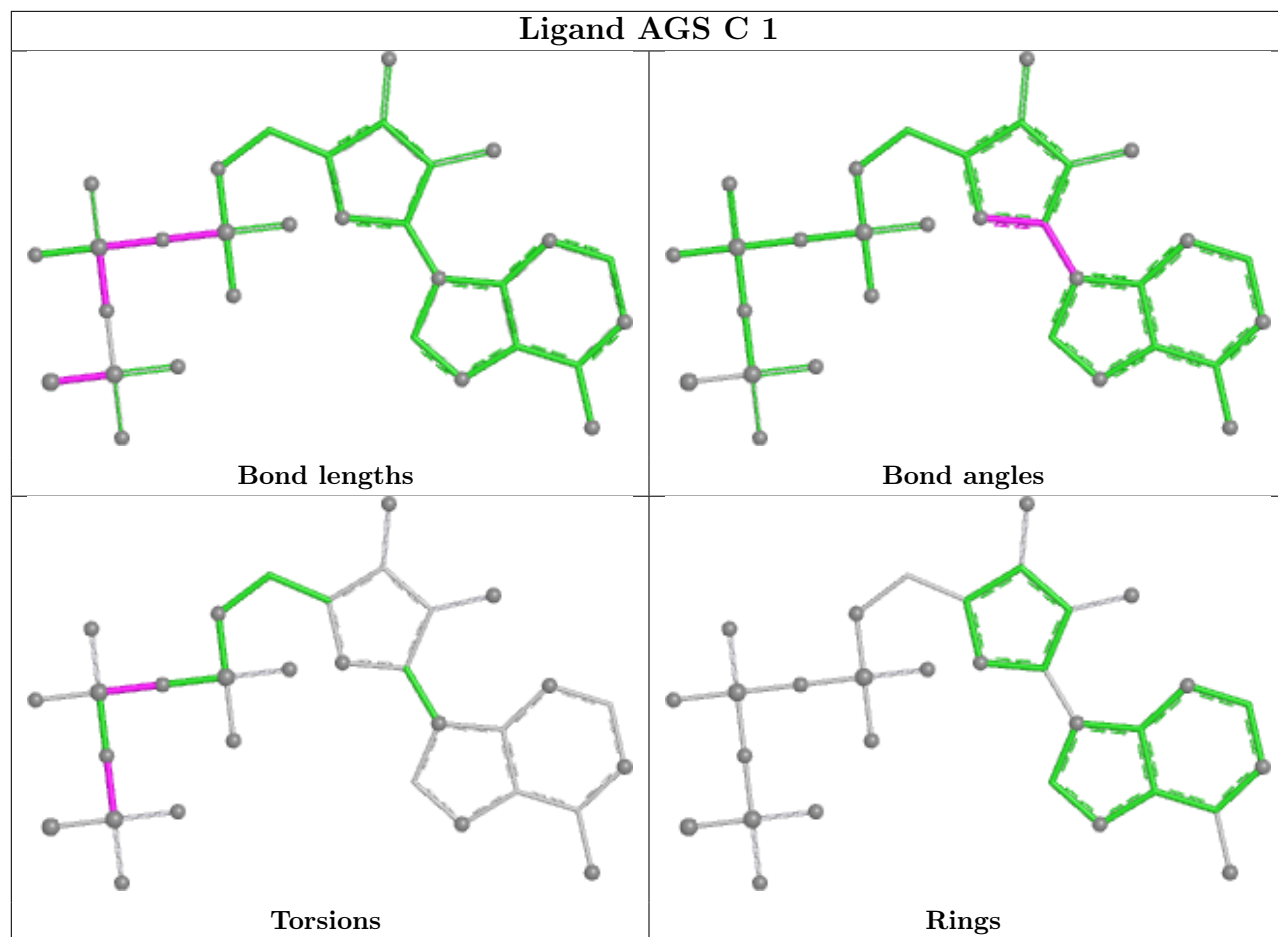
Ligand AGS E 1

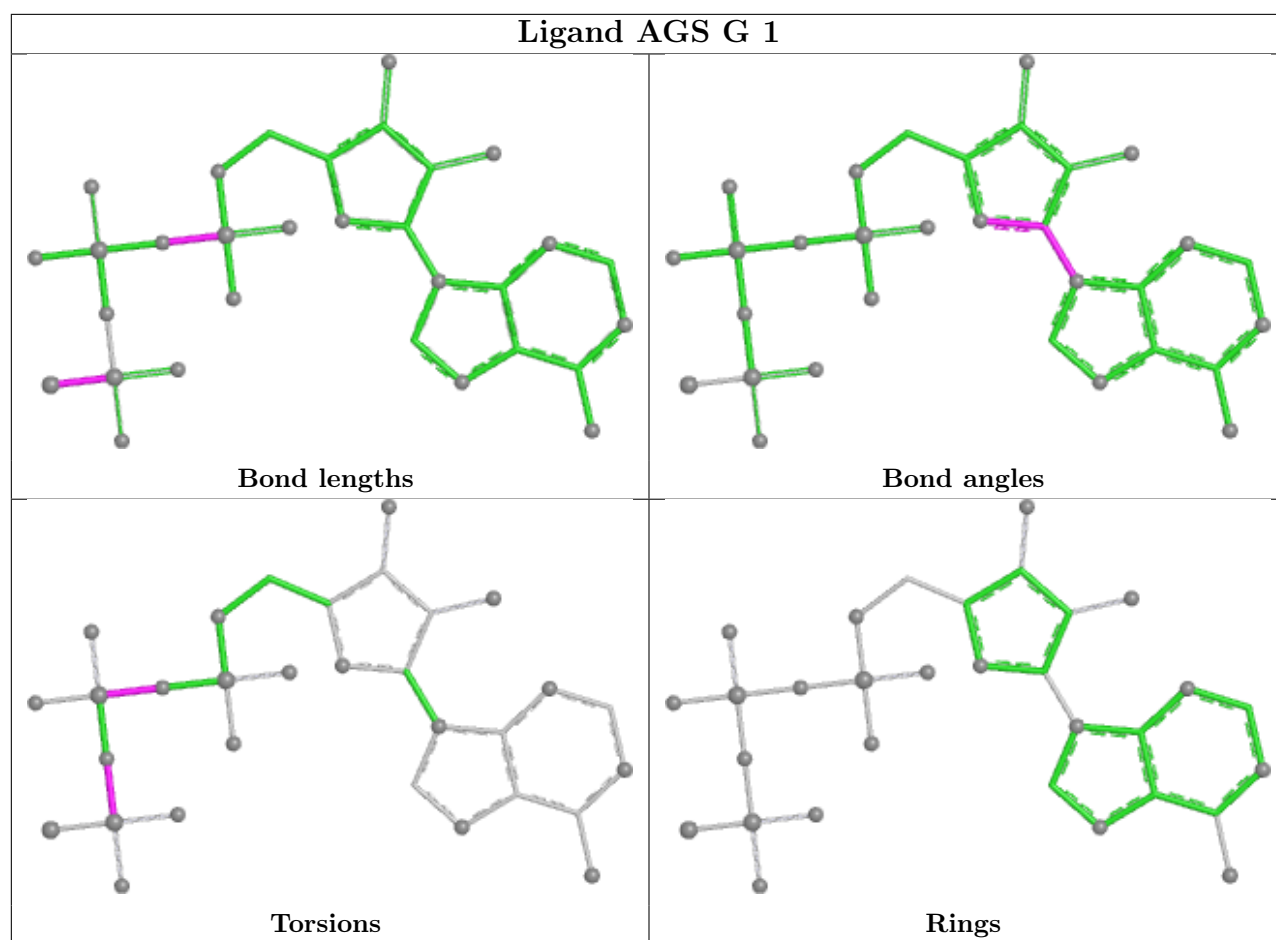


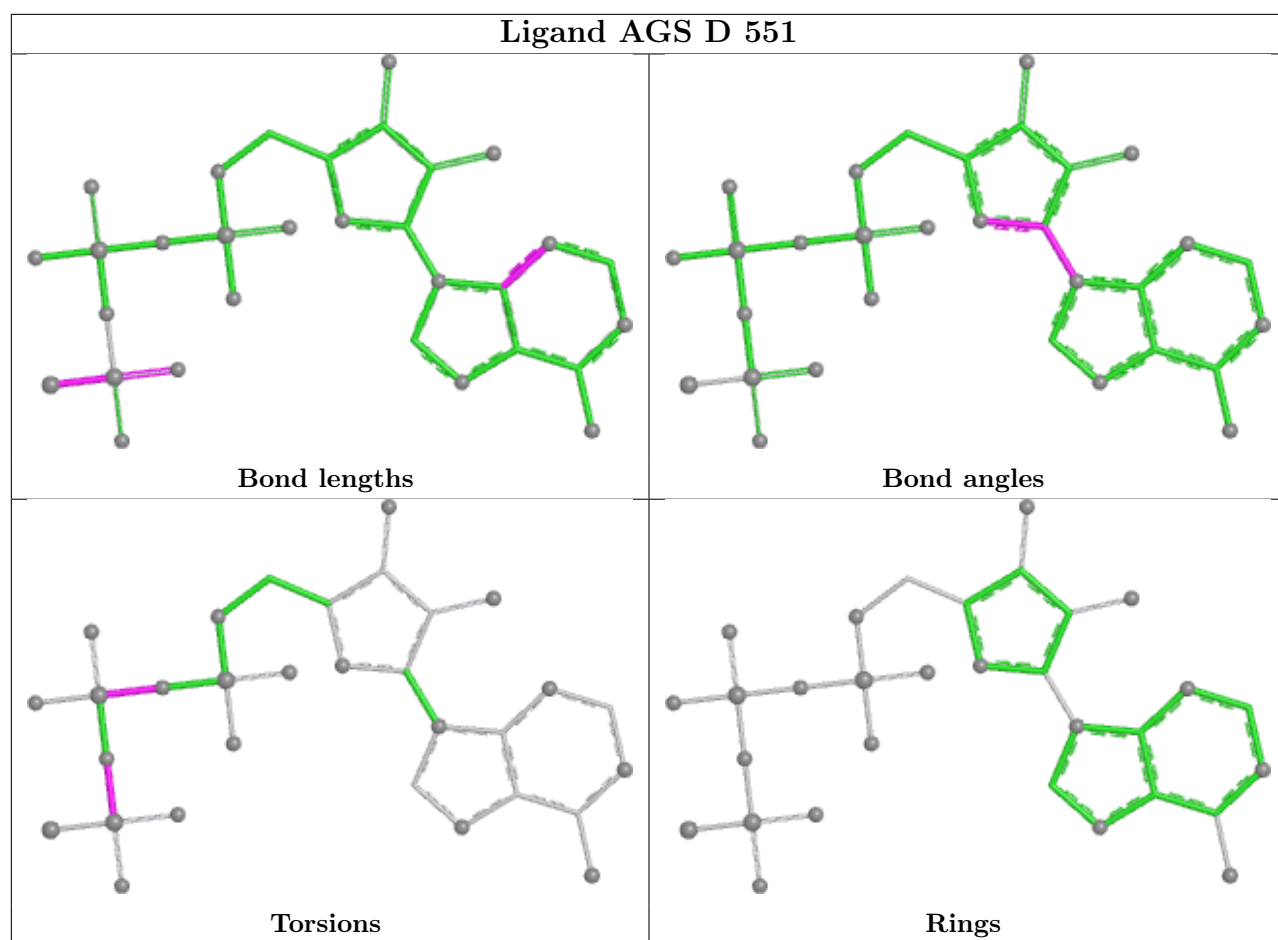
Ligand AGS A 1



Ligand AGS C 1







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	525/547 (95%)	0.97	106 (20%) 3 2	28, 64, 121, 132	0
1	B	525/547 (95%)	1.04	135 (25%) 1 1	24, 59, 149, 159	0
1	C	525/547 (95%)	1.27	147 (28%) 1 1	29, 71, 141, 152	0
1	D	525/547 (95%)	0.66	60 (11%) 10 9	25, 48, 99, 115	0
1	E	525/547 (95%)	0.90	123 (23%) 2 2	23, 55, 134, 145	0
1	F	525/547 (95%)	1.15	135 (25%) 1 1	27, 66, 150, 159	0
1	G	525/547 (95%)	0.81	92 (17%) 4 3	26, 50, 113, 126	0
1	H	525/547 (95%)	0.82	87 (16%) 4 4	26, 56, 118, 130	0
1	I	525/547 (95%)	1.00	112 (21%) 2 2	31, 69, 132, 143	0
1	J	525/547 (95%)	1.11	114 (21%) 2 2	31, 73, 138, 146	0
1	K	525/547 (95%)	1.32	149 (28%) 1 1	31, 78, 151, 159	0
1	L	525/547 (95%)	1.04	119 (22%) 2 2	29, 66, 136, 149	0
1	M	525/547 (95%)	1.29	157 (29%) 1 1	30, 77, 152, 160	0
1	N	525/547 (95%)	0.95	97 (18%) 3 3	28, 65, 118, 129	0
All	All	7350/7658 (95%)	1.02	1633 (22%) 2 2	23, 60, 140, 160	0

The worst 5 of 1633 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	233	MET	6.4
1	M	259	LEU	6.3
1	M	223	ALA	6.3
1	M	346	VAL	6.0
1	K	349	ILE	5.9

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	C	4012	5/5	0.64	0.20	141,141,141,142	0
2	SO4	H	4018	5/5	0.66	0.23	125,125,126,126	0
2	SO4	K	4022	5/5	0.71	0.20	145,146,146,146	0
2	SO4	N	4016	5/5	0.71	0.17	137,137,137,138	0
2	SO4	M	4014	5/5	0.72	0.17	142,142,143,143	0
2	SO4	J	4020	5/5	0.77	0.20	160,160,160,160	0
2	SO4	H	4017	5/5	0.78	0.24	145,146,146,146	0
2	SO4	M	4013	5/5	0.78	0.21	126,126,127,127	0
2	SO4	A	4008	5/5	0.79	0.18	150,150,150,150	0
2	SO4	E	4006	5/5	0.81	0.18	118,119,119,120	0
2	SO4	B	4010	5/5	0.82	0.19	137,137,137,138	0
2	SO4	N	4015	5/5	0.82	0.22	132,133,133,133	0
2	SO4	K	4021	5/5	0.82	0.24	137,138,139,139	0
2	SO4	F	4004	5/5	0.83	0.20	137,138,138,138	0
2	SO4	A	4007	5/5	0.85	0.20	128,129,129,129	0
2	SO4	L	4003	5/5	0.85	0.16	130,131,132,132	0
2	SO4	C	4011	5/5	0.86	0.20	137,137,137,138	0
2	SO4	B	4009	5/5	0.86	0.18	118,119,119,120	0
2	SO4	G	4002	5/5	0.88	0.21	128,128,129,129	0
2	SO4	E	4005	5/5	0.89	0.22	140,141,141,141	0
2	SO4	J	4019	5/5	0.90	0.18	123,124,124,124	0
2	SO4	A	4001	5/5	0.91	0.17	119,120,120,120	0
5	AGS	D	551	31/31	0.94	0.07	25,31,39,41	0
5	AGS	G	1	31/31	0.94	0.07	25,32,40,41	0
5	AGS	J	1	31/31	0.94	0.08	39,42,53,54	0
5	AGS	K	1	31/31	0.94	0.07	37,40,51,54	0
5	AGS	M	1	31/31	0.94	0.07	38,42,50,52	0

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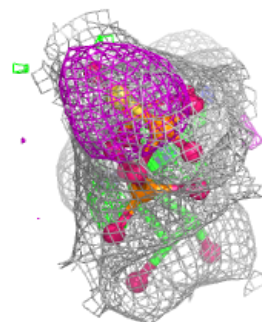
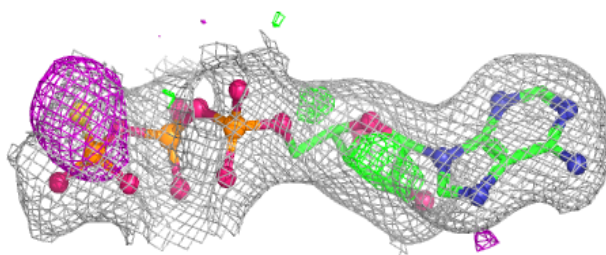
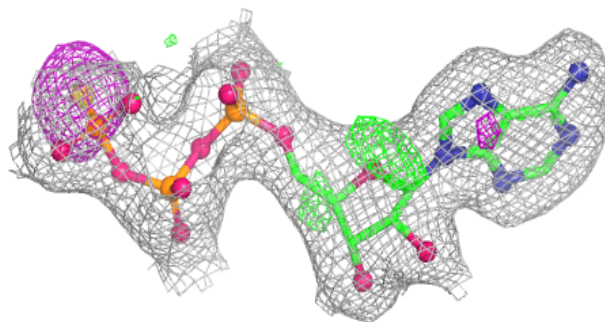
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	AGS	I	1	31/31	0.95	0.07	37,41,48,51	0
5	AGS	E	1	31/31	0.95	0.06	27,30,34,37	0
5	AGS	F	1	31/31	0.95	0.07	34,37,44,45	0
5	AGS	L	1	31/31	0.95	0.07	34,37,45,48	0
5	AGS	C	1	31/31	0.95	0.07	37,41,49,52	0
5	AGS	N	1	31/31	0.95	0.07	35,39,47,48	0
5	AGS	B	1	31/31	0.96	0.07	31,37,48,50	0
5	AGS	A	1	31/31	0.96	0.06	35,38,42,44	0
5	AGS	H	1	31/31	0.96	0.06	30,34,38,42	0
4	K	D	549	1/1	0.97	0.04	34,34,34,34	0
4	K	D	1	1/1	0.98	0.04	30,30,30,30	0
3	MG	G	550	1/1	0.98	0.05	29,29,29,29	0
4	K	E	549	1/1	0.98	0.06	31,31,31,31	0
4	K	E	4007	1/1	0.98	0.03	36,36,36,36	0
4	K	G	549	1/1	0.98	0.04	39,39,39,39	0
4	K	H	549	1/1	0.98	0.03	41,41,41,41	0
4	K	L	549	1/1	0.98	0.04	39,39,39,39	0
4	K	N	549	1/1	0.98	0.04	41,41,41,41	0
3	MG	L	550	1/1	0.98	0.03	31,31,31,31	0
4	K	B	549	1/1	0.98	0.04	38,38,38,38	0
4	K	C	549	1/1	0.98	0.03	45,45,45,45	0
4	K	M	549	1/1	0.99	0.02	45,45,45,45	0
3	MG	N	550	1/1	0.99	0.06	34,34,34,34	0
4	K	A	549	1/1	0.99	0.03	40,40,40,40	0
3	MG	C	550	1/1	0.99	0.02	36,36,36,36	0
3	MG	D	550	1/1	0.99	0.04	29,29,29,29	0
3	MG	E	550	1/1	0.99	0.02	24,24,24,24	0
3	MG	F	550	1/1	0.99	0.02	30,30,30,30	0
3	MG	A	550	1/1	0.99	0.06	31,31,31,31	0
3	MG	I	550	1/1	0.99	0.04	34,34,34,34	0
4	K	F	549	1/1	0.99	0.03	41,41,41,41	0
3	MG	J	550	1/1	0.99	0.03	37,37,37,37	0
3	MG	K	550	1/1	0.99	0.02	35,35,35,35	0
4	K	I	549	1/1	0.99	0.04	43,43,43,43	0
4	K	J	549	1/1	0.99	0.03	47,47,47,47	0
4	K	K	549	1/1	0.99	0.03	46,46,46,46	0
3	MG	B	550	1/1	0.99	0.04	31,31,31,31	0
3	MG	M	550	1/1	1.00	0.06	38,38,38,38	0
3	MG	H	550	1/1	1.00	0.04	26,26,26,26	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.

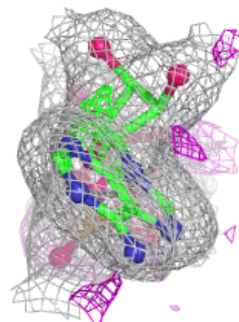
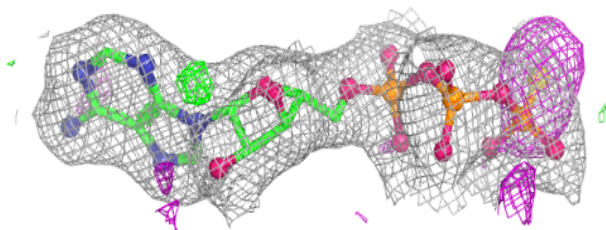
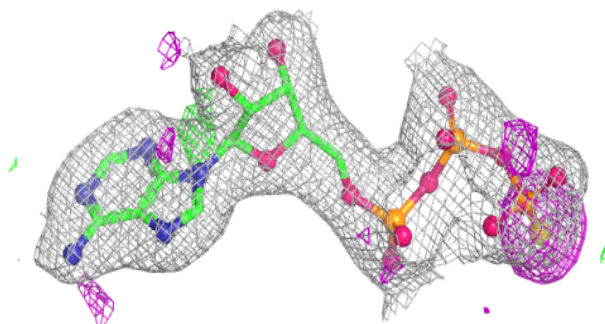
Electron density around AGS D 551:

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



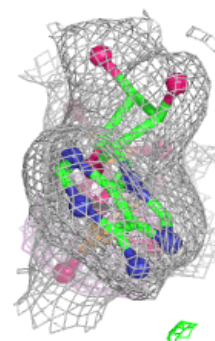
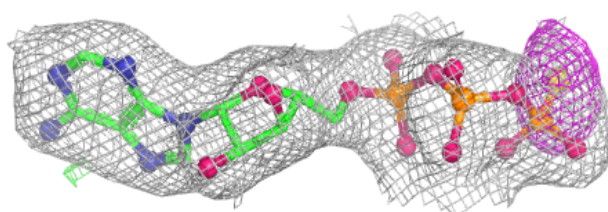
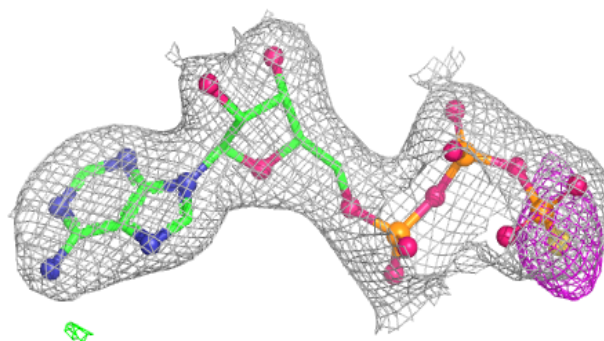
Electron density around AGS G 1:

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

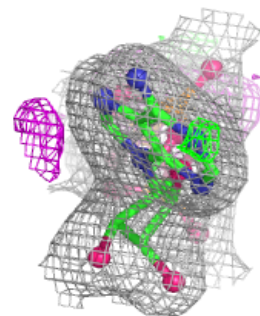
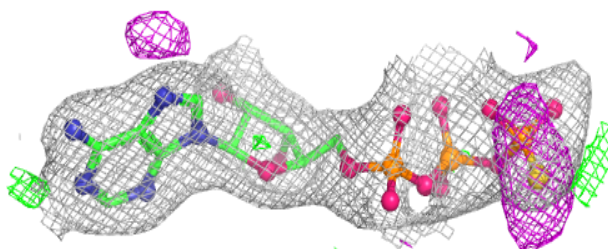
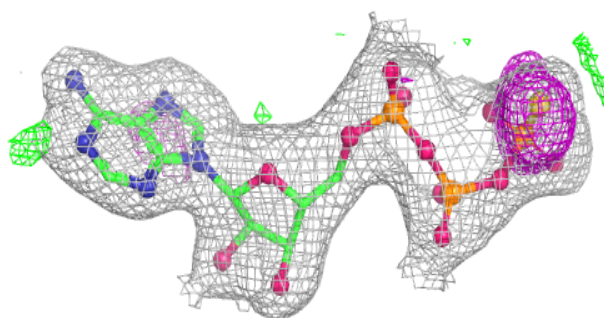


Electron density around AGS J 1:

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and green (positive)

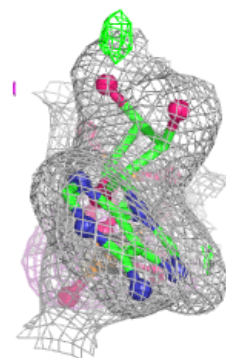
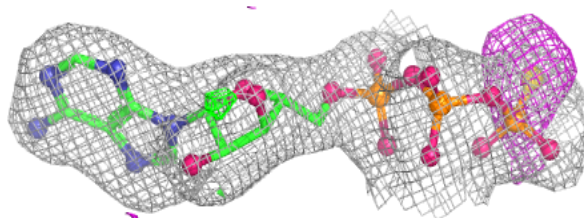
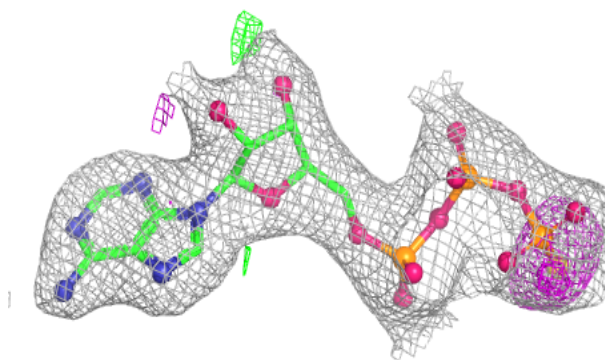
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 mF_o-DF_c (at 3 rmsd) in purple (negative)
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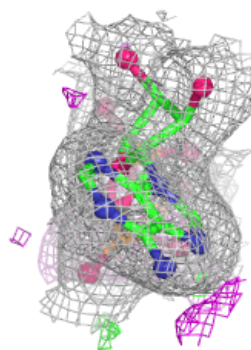
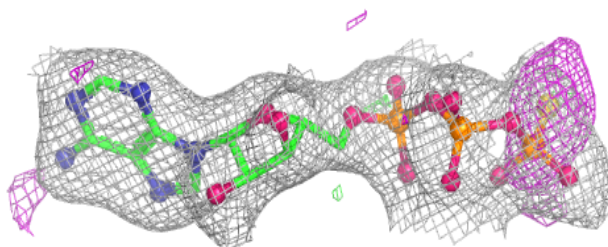
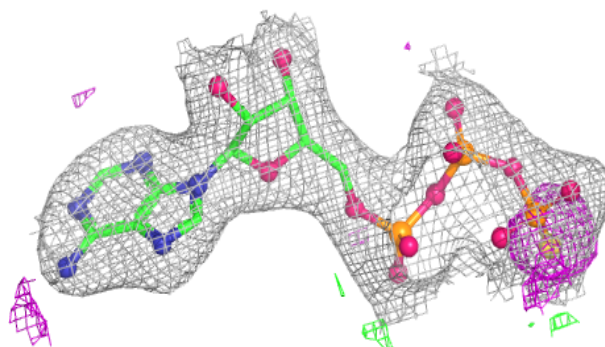


Electron density around AGS M 1:

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

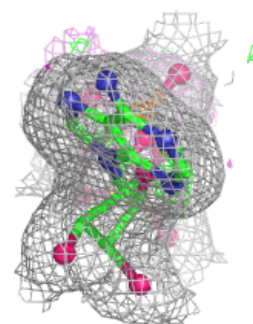
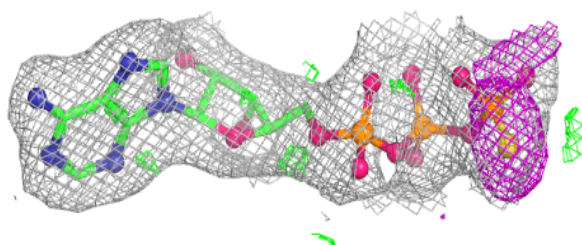
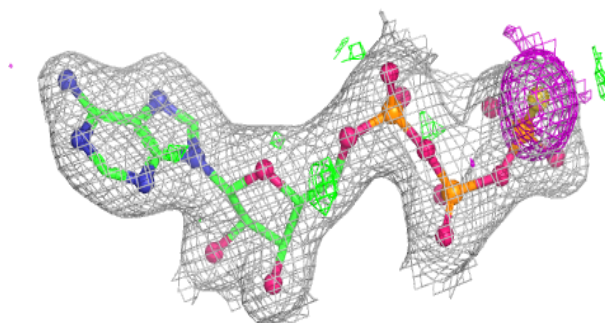
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and green (positive)

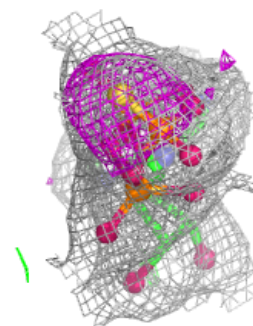
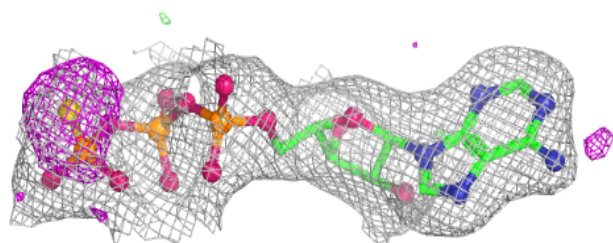
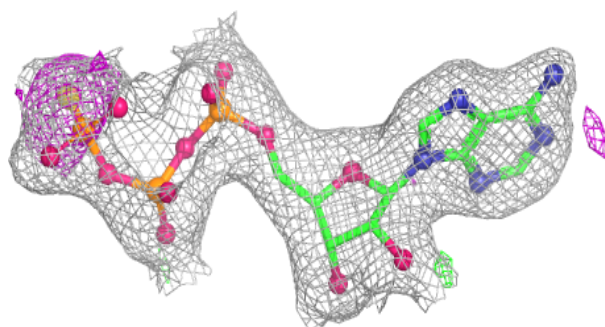


Electron density around AGS E 1:

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and green (positive)

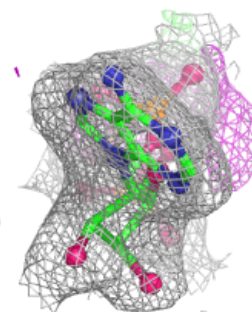
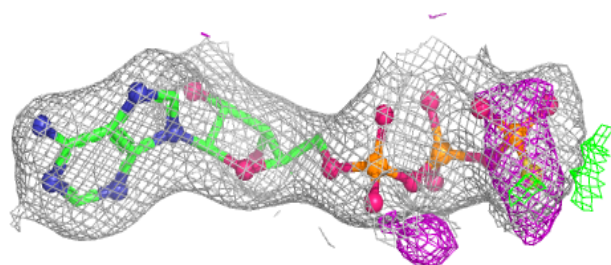
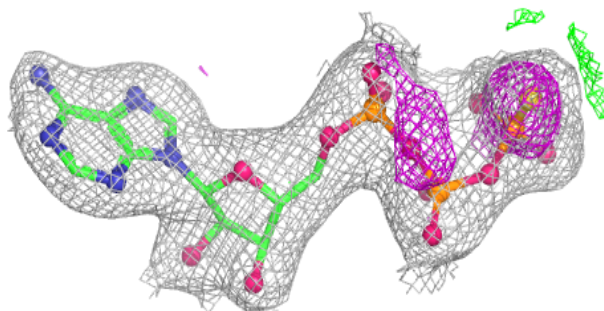
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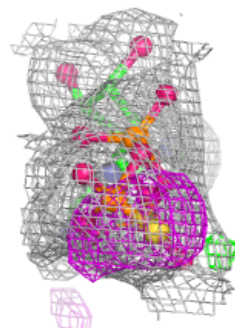
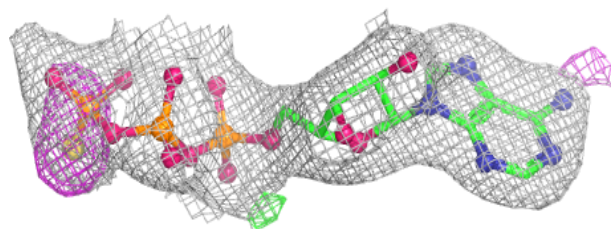
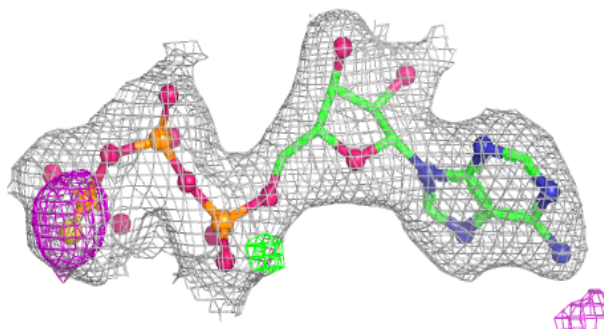


Electron density around AGS L 1:

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and green (positive)

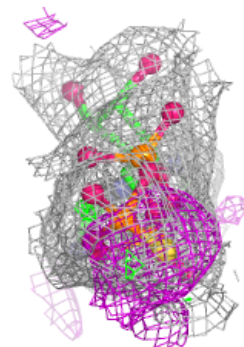
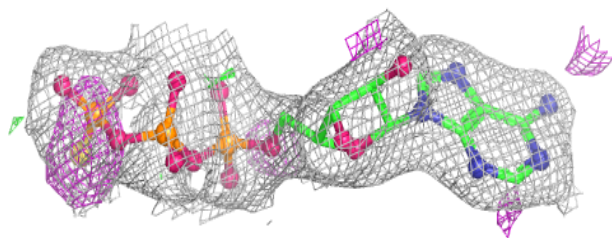
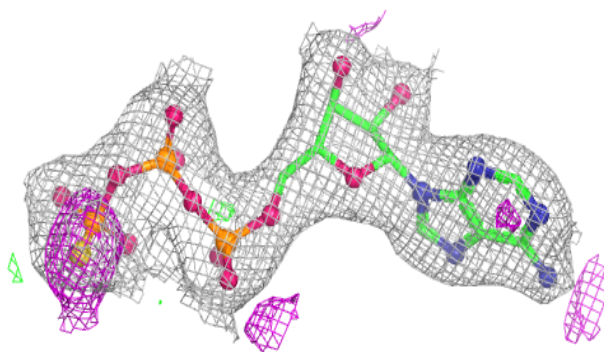
**Electron density around AGS C 1:**

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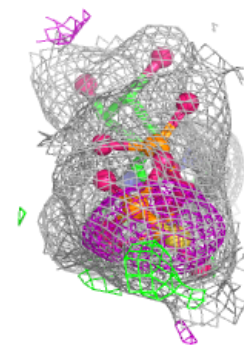
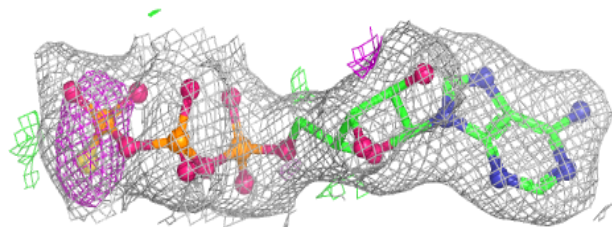
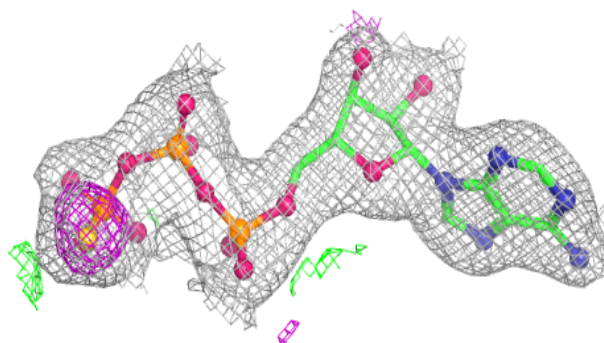


Electron density around AGS N 1:

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and green (positive)

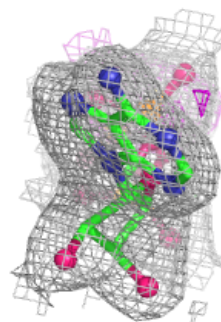
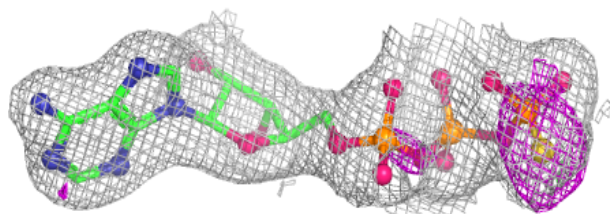
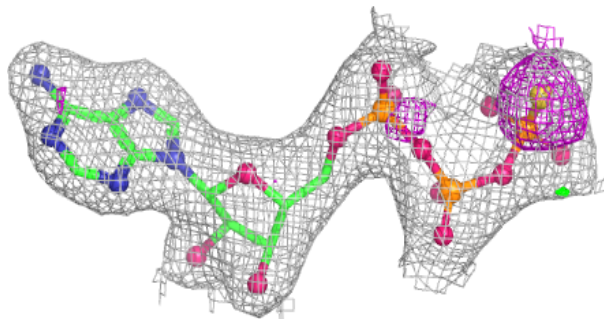
**Electron density around AGS B 1:**

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and green (positive)

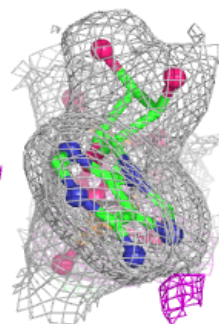
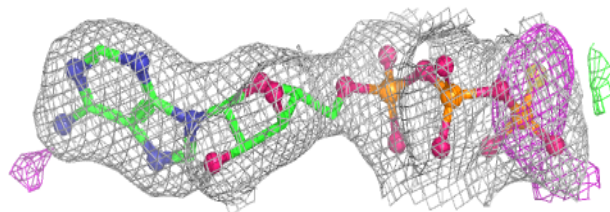
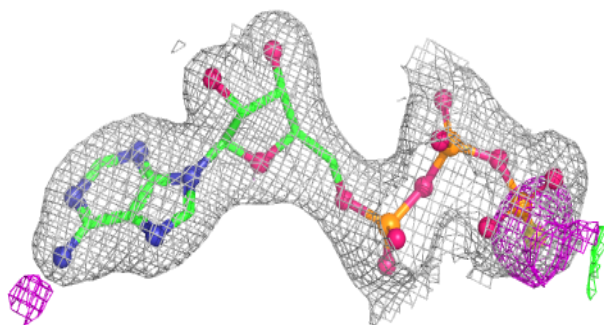


Electron density around AGS A 1:

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

**Electron density around AGS H 1:**

$2mF_o-DF_c$ (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.