



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 08:37 am BST

PDB ID : 5C18
Title : p97-delta709-728 in complex with ATP-gamma-S
Authors : Haenzelmann, P.; Schindelin, H.
Deposited on : 2015-06-13
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

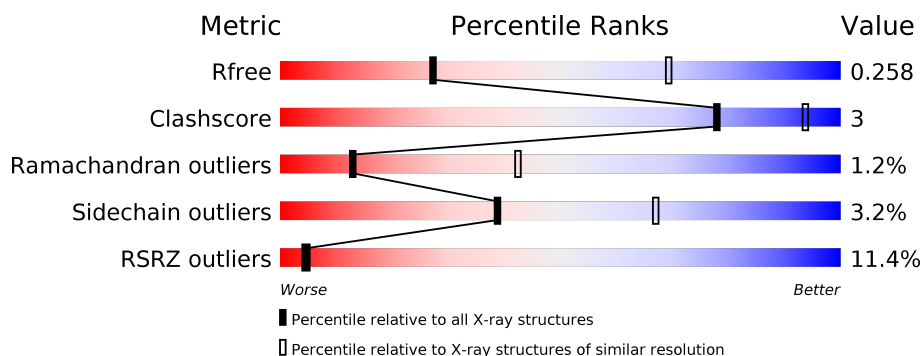
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 1149 (3.34-3.26) |
| Clashscore | 141614 | 1205 (3.34-3.26) |
| Ramachandran outliers | 138981 | 1183 (3.34-3.26) |
| Sidechain outliers | 138945 | 1182 (3.34-3.26) |
| RSRZ outliers | 127900 | 1115 (3.34-3.26) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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 | 785 | <div> <div>14%</div> <div> <div></div> <div>85%</div> <div>7%</div> <div>8%</div> </div> </div> |
| 1 | B | 785 | <div> <div>5%</div> <div> <div></div> <div>82%</div> <div>9%</div> <div>8%</div> </div> </div> |
| 1 | C | 785 | <div> <div>9%</div> <div> <div></div> <div>83%</div> <div>9%</div> <div>8%</div> </div> </div> |
| 1 | D | 785 | <div> <div>14%</div> <div> <div></div> <div>84%</div> <div>7%</div> <div>8%</div> </div> </div> |
| 1 | E | 785 | <div> <div>7%</div> <div> <div></div> <div>81%</div> <div>10%</div> <div>8%</div> </div> </div> |
| 1 | F | 785 | <div> <div>14%</div> <div> <div></div> <div>83%</div> <div>8%</div> <div>8%</div> </div> </div> |

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 69089 atoms, of which 34628 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Transitional endoplasmic reticulum ATPase.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|------|----|---------|---------|-------|
| 1 | A | 722 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 11409 | 3567 | 5741 | 1001 | 1070 | 30 | | | |
| 1 | B | 723 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 11420 | 3570 | 5746 | 1002 | 1072 | 30 | | | |
| 1 | C | 724 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 11427 | 3572 | 5749 | 1003 | 1073 | 30 | | | |
| 1 | D | 722 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 11409 | 3567 | 5741 | 1001 | 1070 | 30 | | | |
| 1 | E | 723 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 11418 | 3570 | 5745 | 1002 | 1071 | 30 | | | |
| 1 | F | 724 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 11430 | 3573 | 5750 | 1004 | 1073 | 30 | | | |

There are 120 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| A | ? | - | ARG | deletion | UNP P55072 |
| A | ? | - | GLU | deletion | UNP P55072 |
| A | ? | - | ARG | deletion | UNP P55072 |
| A | ? | - | GLU | deletion | UNP P55072 |
| A | ? | - | ARG | deletion | UNP P55072 |
| A | ? | - | GLN | deletion | UNP P55072 |
| A | ? | - | THR | deletion | UNP P55072 |
| A | ? | - | ASN | deletion | UNP P55072 |
| A | ? | - | PRO | deletion | UNP P55072 |
| A | ? | - | SER | deletion | UNP P55072 |
| A | ? | - | ALA | deletion | UNP P55072 |
| A | ? | - | MET | deletion | UNP P55072 |
| A | ? | - | GLU | deletion | UNP P55072 |
| A | ? | - | VAL | deletion | UNP P55072 |
| A | ? | - | GLU | deletion | UNP P55072 |
| A | ? | - | GLU | deletion | UNP P55072 |
| A | ? | - | ASP | deletion | UNP P55072 |

Continued on next page...

Continued from previous page...

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| A | ? | - | ASP | deletion | UNP P55072 |
| A | ? | - | PRO | deletion | UNP P55072 |
| A | ? | - | VAL | deletion | UNP P55072 |
| B | ? | - | ARG | deletion | UNP P55072 |
| B | ? | - | GLU | deletion | UNP P55072 |
| B | ? | - | ARG | deletion | UNP P55072 |
| B | ? | - | GLU | deletion | UNP P55072 |
| B | ? | - | ARG | deletion | UNP P55072 |
| B | ? | - | GLN | deletion | UNP P55072 |
| B | ? | - | THR | deletion | UNP P55072 |
| B | ? | - | ASN | deletion | UNP P55072 |
| B | ? | - | PRO | deletion | UNP P55072 |
| B | ? | - | SER | deletion | UNP P55072 |
| B | ? | - | ALA | deletion | UNP P55072 |
| B | ? | - | MET | deletion | UNP P55072 |
| B | ? | - | GLU | deletion | UNP P55072 |
| B | ? | - | VAL | deletion | UNP P55072 |
| B | ? | - | GLU | deletion | UNP P55072 |
| B | ? | - | GLU | deletion | UNP P55072 |
| B | ? | - | ASP | deletion | UNP P55072 |
| B | ? | - | ASP | deletion | UNP P55072 |
| B | ? | - | PRO | deletion | UNP P55072 |
| B | ? | - | VAL | deletion | UNP P55072 |
| C | ? | - | ARG | deletion | UNP P55072 |
| C | ? | - | GLU | deletion | UNP P55072 |
| C | ? | - | ARG | deletion | UNP P55072 |
| C | ? | - | GLU | deletion | UNP P55072 |
| C | ? | - | ARG | deletion | UNP P55072 |
| C | ? | - | GLN | deletion | UNP P55072 |
| C | ? | - | THR | deletion | UNP P55072 |
| C | ? | - | ASN | deletion | UNP P55072 |
| C | ? | - | PRO | deletion | UNP P55072 |
| C | ? | - | SER | deletion | UNP P55072 |
| C | ? | - | ALA | deletion | UNP P55072 |
| C | ? | - | MET | deletion | UNP P55072 |
| C | ? | - | GLU | deletion | UNP P55072 |
| C | ? | - | VAL | deletion | UNP P55072 |
| C | ? | - | GLU | deletion | UNP P55072 |
| C | ? | - | GLU | deletion | UNP P55072 |
| C | ? | - | ASP | deletion | UNP P55072 |
| C | ? | - | ASP | deletion | UNP P55072 |
| C | ? | - | PRO | deletion | UNP P55072 |

Continued on next page...

Continued from previous page...

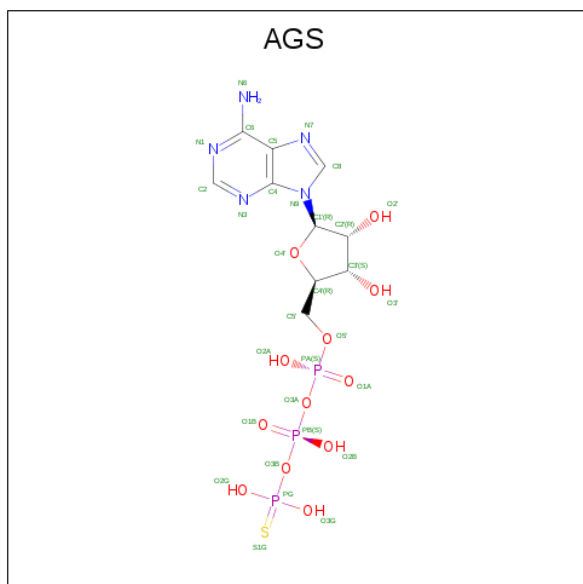
| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| C | ? | - | VAL | deletion | UNP P55072 |
| D | ? | - | ARG | deletion | UNP P55072 |
| D | ? | - | GLU | deletion | UNP P55072 |
| D | ? | - | ARG | deletion | UNP P55072 |
| D | ? | - | GLU | deletion | UNP P55072 |
| D | ? | - | ARG | deletion | UNP P55072 |
| D | ? | - | GLN | deletion | UNP P55072 |
| D | ? | - | THR | deletion | UNP P55072 |
| D | ? | - | ASN | deletion | UNP P55072 |
| D | ? | - | PRO | deletion | UNP P55072 |
| D | ? | - | SER | deletion | UNP P55072 |
| D | ? | - | ALA | deletion | UNP P55072 |
| D | ? | - | MET | deletion | UNP P55072 |
| D | ? | - | GLU | deletion | UNP P55072 |
| D | ? | - | VAL | deletion | UNP P55072 |
| D | ? | - | GLU | deletion | UNP P55072 |
| D | ? | - | GLU | deletion | UNP P55072 |
| D | ? | - | ASP | deletion | UNP P55072 |
| D | ? | - | ASP | deletion | UNP P55072 |
| D | ? | - | PRO | deletion | UNP P55072 |
| D | ? | - | VAL | deletion | UNP P55072 |
| E | ? | - | ARG | deletion | UNP P55072 |
| E | ? | - | GLU | deletion | UNP P55072 |
| E | ? | - | ARG | deletion | UNP P55072 |
| E | ? | - | GLU | deletion | UNP P55072 |
| E | ? | - | ARG | deletion | UNP P55072 |
| E | ? | - | GLN | deletion | UNP P55072 |
| E | ? | - | THR | deletion | UNP P55072 |
| E | ? | - | ASN | deletion | UNP P55072 |
| E | ? | - | PRO | deletion | UNP P55072 |
| E | ? | - | SER | deletion | UNP P55072 |
| E | ? | - | ALA | deletion | UNP P55072 |
| E | ? | - | MET | deletion | UNP P55072 |
| E | ? | - | GLU | deletion | UNP P55072 |
| E | ? | - | VAL | deletion | UNP P55072 |
| E | ? | - | GLU | deletion | UNP P55072 |
| E | ? | - | GLU | deletion | UNP P55072 |
| E | ? | - | ASP | deletion | UNP P55072 |
| E | ? | - | ASP | deletion | UNP P55072 |
| E | ? | - | PRO | deletion | UNP P55072 |
| E | ? | - | VAL | deletion | UNP P55072 |
| F | ? | - | ARG | deletion | UNP P55072 |

Continued on next page...

Continued from previous page...

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| F | ? | - | GLU | deletion | UNP P55072 |
| F | ? | - | ARG | deletion | UNP P55072 |
| F | ? | - | GLU | deletion | UNP P55072 |
| F | ? | - | ARG | deletion | UNP P55072 |
| F | ? | - | GLN | deletion | UNP P55072 |
| F | ? | - | THR | deletion | UNP P55072 |
| F | ? | - | ASN | deletion | UNP P55072 |
| F | ? | - | PRO | deletion | UNP P55072 |
| F | ? | - | SER | deletion | UNP P55072 |
| F | ? | - | ALA | deletion | UNP P55072 |
| F | ? | - | MET | deletion | UNP P55072 |
| F | ? | - | GLU | deletion | UNP P55072 |
| F | ? | - | VAL | deletion | UNP P55072 |
| F | ? | - | GLU | deletion | UNP P55072 |
| F | ? | - | GLU | deletion | UNP P55072 |
| F | ? | - | ASP | deletion | UNP P55072 |
| F | ? | - | ASP | deletion | UNP P55072 |
| F | ? | - | PRO | deletion | UNP P55072 |
| F | ? | - | VAL | deletion | UNP P55072 |

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



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

Continued on next page...

Continued from previous page...

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

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

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 4 | D | 1 | Total Cl 1 1 | 0 | 0 |
| 4 | E | 1 | Total Cl 1 1 | 0 | 0 |
| 4 | B | 1 | Total Cl 1 1 | 0 | 0 |
| 4 | C | 1 | Total Cl 1 1 | 0 | 0 |
| 4 | A | 1 | Total Cl 1 1 | 0 | 0 |
| 4 | F | 1 | Total Cl 1 1 | 0 | 0 |

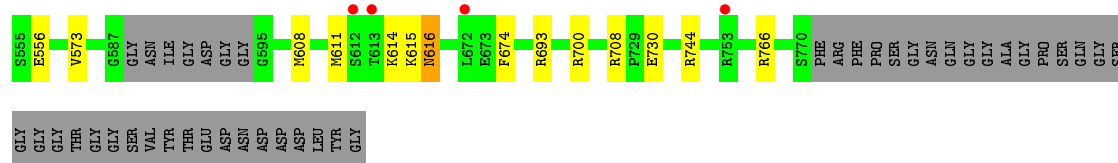
- Molecule 5 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 5 | A | 5 | Total O 5 5 | 0 | 0 |
| 5 | B | 5 | Total O 5 5 | 0 | 0 |
| 5 | C | 5 | Total O 5 5 | 0 | 0 |
| 5 | D | 5 | Total O 5 5 | 0 | 0 |
| 5 | E | 5 | Total O 5 5 | 0 | 0 |
| 5 | F | 5 | Total O 5 5 | 0 | 0 |

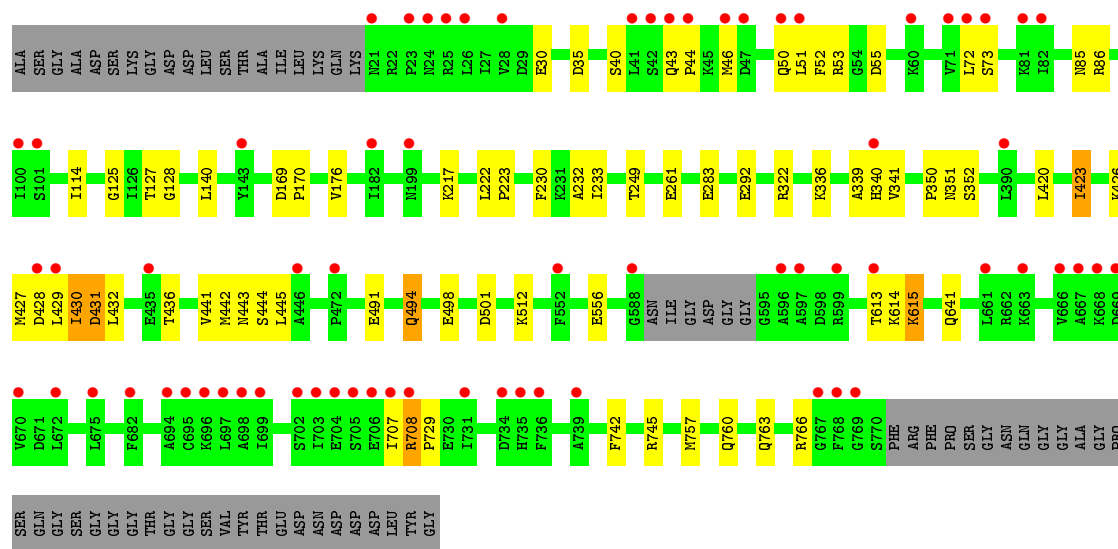
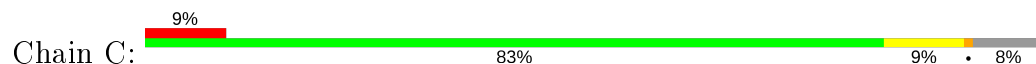
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 ($\text{RSRZ} > 2$). 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.

- Chain A:
-
- 14% 85% 7% 8%
- ALA
SER
GLY
ALA
ASP
SER
GLY
ASP
LEU
SER
THR
ALA
ILE
LYS
GLN
LYS
N21
R22
P23
N24
R25
L26
D29
V39
S40
L41
S42
Q43
P44
R45
M46
D47
E48
L49
Q50
L51
F52
R53
V57
L58
L59
R64
R65
V68
L72
S73
R82
R83
L84
N90
M91
L92
R93
D98
V99
I100
S101
I102
Q103
P104
R113
I114
H115
V116
L117
P118
I119
T127
L130
F131
E132
V133
Y134
L135
E141
P145
I151
G157
A160
V161
E162
F163
R164
P169
L174
I175
V176
I182
H183
C184
E185
G186
D187
P188
T193
D431
L432
E433
D434
E435
T436
L437
D438
A439
R442
H443
A446
V447
D450
E491
P500
D501
K502
F503
L504
K505
F506
P510
F552
E556
V573
G587
GLY
ASN
ILE
GLY
ASP
GLY
GLY
G595
M624
R635
P636
D649
S652
R653
L672
A676
L694
C695
R696
L697
R698
L699
R700
E701
S702
I703
E704
E705
E706
R707
R708
P729
E730
I731
R732
R733
D734
H735
F736
G769
SER
PHE
ARG
PHE
PRO
GLY
GLN
GLN
GLY
GLY
ALA
GLY
PRO
SER
GLN
GLY
SER
GLY
GLY
GLY
THR
GLY
GLY
VAL
TYR
THR
GLU
ASP
ASN
ASP
ASP
LEU

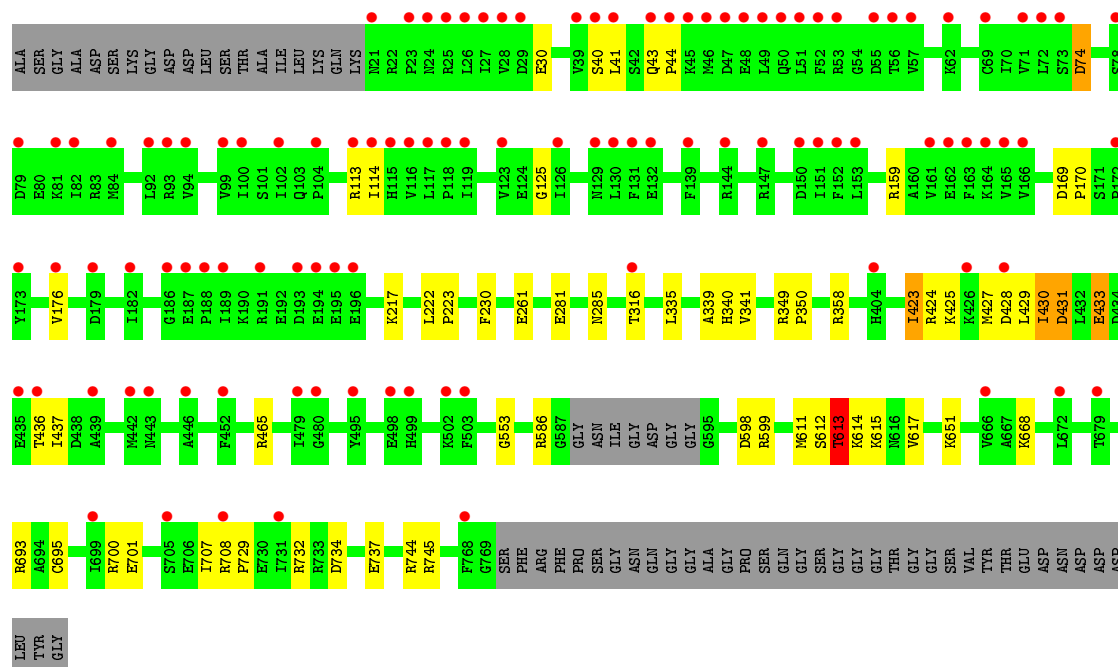
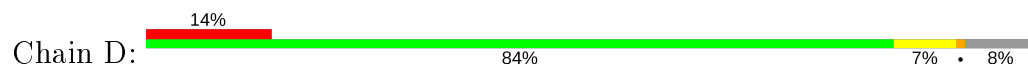
- [illegible]



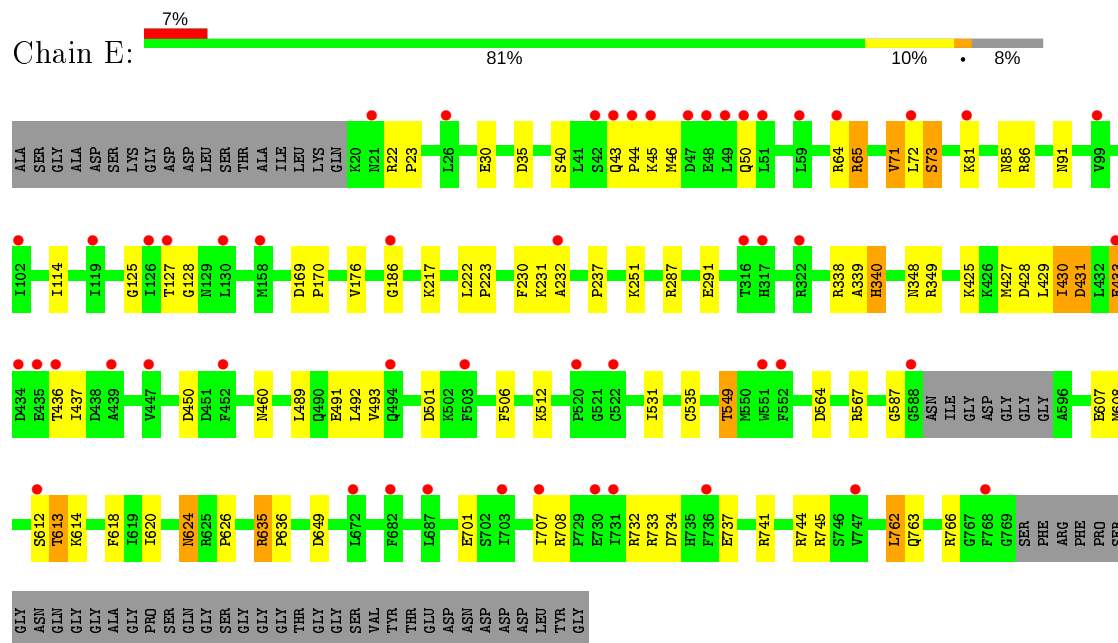
• Molecule 1: Transitional endoplasmic reticulum ATPase



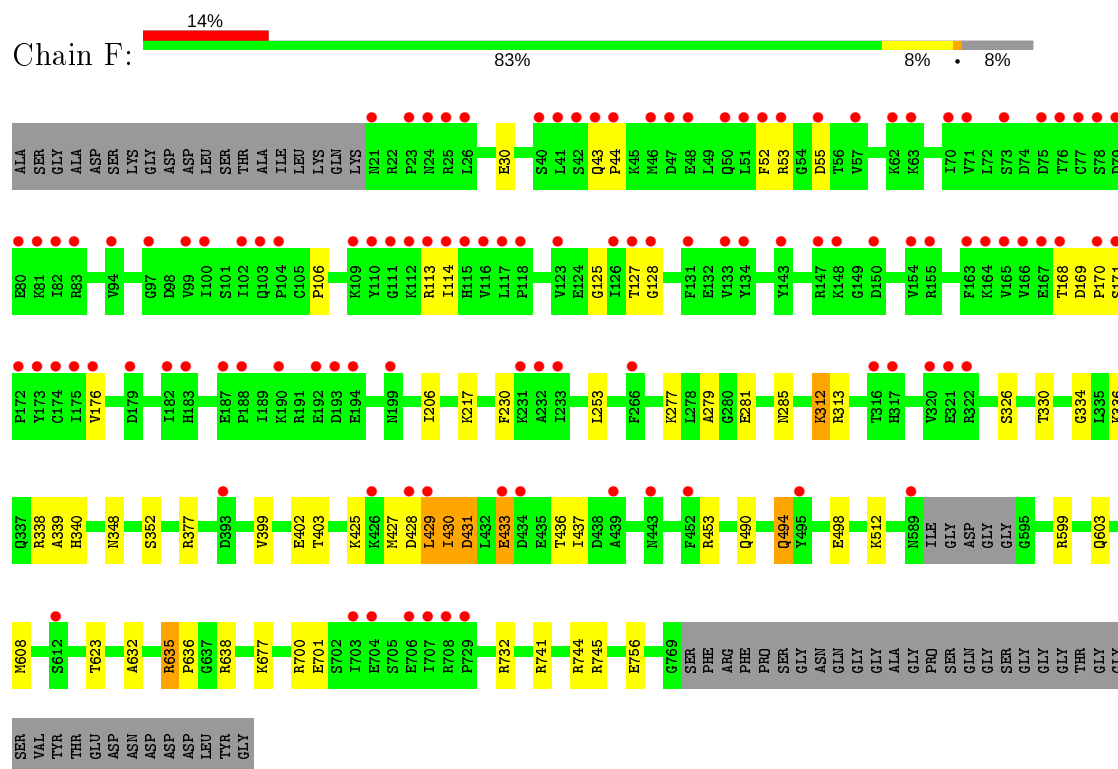
• Molecule 1: Transitional endoplasmic reticulum ATPase



• Molecule 1: Transitional endoplasmic reticulum ATPase



• Molecule 1: Transitional endoplasmic reticulum ATPase



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 140.33Å 180.06Å 255.61Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 19.99 – 3.30 49.18 – 3.30 | Depositor EDS |
| % Data completeness (in resolution range) | 100.0 (19.99-3.30) 100.0 (49.18-3.30) | Depositor EDS |
| R_{merge} | 0.18 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.79 (at 3.33Å) | Xtriage |
| Refinement program | PHENIX | Depositor |
| R, R_{free} | 0.211 , 0.249 0.222 , 0.258 | Depositor DCC |
| R_{free} test set | 4893 reflections (5.00%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 101.3 | Xtriage |
| Anisotropy | 0.324 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.38 , 77.8 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.92 | EDS |
| Total number of atoms | 69089 | wwPDB-VP |
| Average B, all atoms (Å ²) | 137.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% 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: MG, AGS, CL

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 | 0.22 | 0/5761 | 0.40 | 0/7778 |
| 1 | B | 0.22 | 0/5767 | 0.41 | 0/7786 |
| 1 | C | 0.23 | 0/5771 | 0.41 | 0/7791 |
| 1 | D | 0.22 | 0/5761 | 0.40 | 0/7778 |
| 1 | E | 0.22 | 0/5766 | 0.41 | 0/7785 |
| 1 | F | 0.22 | 0/5773 | 0.40 | 0/7794 |
| All | All | 0.22 | 0/34599 | 0.40 | 0/46712 |

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 | E | 0 | 1 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 1 | E | 339 | ALA | 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 | 5668 | 5741 | 5741 | 30 | 0 |
| 1 | B | 5674 | 5746 | 5746 | 39 | 0 |
| 1 | C | 5678 | 5749 | 5749 | 34 | 0 |
| 1 | D | 5668 | 5741 | 5741 | 32 | 0 |
| 1 | E | 5673 | 5745 | 5743 | 45 | 0 |
| 1 | F | 5680 | 5750 | 5750 | 32 | 0 |
| 2 | A | 62 | 26 | 24 | 2 | 0 |
| 2 | B | 62 | 26 | 24 | 3 | 0 |
| 2 | C | 62 | 26 | 24 | 0 | 0 |
| 2 | D | 62 | 26 | 24 | 0 | 0 |
| 2 | E | 62 | 26 | 24 | 2 | 0 |
| 2 | F | 62 | 26 | 24 | 2 | 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 |
| 4 | A | 1 | 0 | 0 | 0 | 0 |
| 4 | B | 1 | 0 | 0 | 0 | 0 |
| 4 | C | 1 | 0 | 0 | 0 | 0 |
| 4 | D | 1 | 0 | 0 | 0 | 0 |
| 4 | E | 1 | 0 | 0 | 0 | 0 |
| 4 | F | 1 | 0 | 0 | 0 | 0 |
| 5 | A | 5 | 0 | 0 | 0 | 0 |
| 5 | B | 5 | 0 | 0 | 2 | 0 |
| 5 | C | 5 | 0 | 0 | 0 | 0 |
| 5 | D | 5 | 0 | 0 | 0 | 0 |
| 5 | E | 5 | 0 | 0 | 1 | 0 |
| 5 | F | 5 | 0 | 0 | 1 | 0 |
| All | All | 34461 | 34628 | 34614 | 201 | 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 3.

All (201) 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:B:512:LYS:NZ | 1:B:608:MET:O | 2.14 | 0.81 |
| 1:F:313:ARG:NH2 | 1:F:326:SER:OG | 2.18 | 0.77 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:F:512:LYS:NZ | 1:F:608:MET:O | 2.20 | 0.75 |
| 1:A:653:ARG:NH2 | 1:A:676:ALA:O | 2.20 | 0.75 |
| 1:A:65:ARG:NH1 | 1:A:91:ASN:O | 2.19 | 0.75 |
| 1:F:338:ARG:O | 1:F:340:HIS:N | 2.22 | 0.73 |
| 1:E:701:GLU:OE2 | 1:E:732:ARG:NH1 | 2.22 | 0.72 |
| 1:E:30:GLU:OE2 | 1:E:217:LYS:NZ | 2.24 | 0.71 |
| 1:B:304:ASP:OD2 | 5:B:1001:HOH:O | 2.09 | 0.70 |
| 1:E:45:LYS:NZ | 1:E:81:LYS:O | 2.25 | 0.69 |
| 1:E:427:MET:O | 1:E:429:LEU:N | 2.26 | 0.69 |
| 1:A:399:VAL:O | 1:A:403:THR:OG1 | 2.09 | 0.68 |
| 1:B:30:GLU:OE2 | 1:B:217:LYS:NZ | 2.23 | 0.67 |
| 1:B:321:GLU:OE1 | 1:C:322:ARG:NH1 | 2.27 | 0.67 |
| 1:D:465:ARG:NH1 | 1:E:607:GLU:OE2 | 2.28 | 0.66 |
| 1:B:35:ASP:O | 1:B:85:ASN:ND2 | 2.28 | 0.66 |
| 1:E:512:LYS:NZ | 1:E:608:MET:O | 2.28 | 0.66 |
| 1:A:90:ASN:O | 1:A:93:ARG:NH1 | 2.30 | 0.65 |
| 1:B:399:VAL:O | 1:B:403:THR:OG1 | 2.09 | 0.65 |
| 1:C:339:ALA:O | 1:C:341:VAL:N | 2.29 | 0.65 |
| 2:A:901:AGS:S1G | 1:B:766:ARG:NH2 | 2.70 | 0.63 |
| 1:C:46:MET:SD | 1:C:73:SER:N | 2.72 | 0.63 |
| 1:D:700:ARG:NH1 | 1:E:491:GLU:OE2 | 2.31 | 0.63 |
| 1:C:35:ASP:O | 1:C:85:ASN:ND2 | 2.32 | 0.63 |
| 1:D:339:ALA:O | 1:D:341:VAL:N | 2.32 | 0.63 |
| 1:F:281:GLU:O | 1:F:285:ASN:ND2 | 2.32 | 0.62 |
| 2:B:901:AGS:S1G | 1:C:766:ARG:NH1 | 2.71 | 0.62 |
| 1:D:612:SER:O | 1:D:614:LYS:N | 2.33 | 0.61 |
| 1:E:46:MET:O | 1:E:50:GLN:N | 2.34 | 0.61 |
| 1:F:125:GLY:O | 1:F:436:THR:OG1 | 2.17 | 0.61 |
| 1:E:624:ASN:OD1 | 1:E:624:ASN:N | 2.34 | 0.60 |
| 1:D:430:ILE:HG23 | 1:D:431:ASP:H | 1.66 | 0.59 |
| 1:D:701:GLU:OE1 | 1:D:732:ARG:NH1 | 2.36 | 0.59 |
| 1:B:427:MET:O | 1:B:429:LEU:N | 2.36 | 0.59 |
| 1:F:399:VAL:O | 1:F:403:THR:OG1 | 2.10 | 0.59 |
| 1:A:358:ARG:NH1 | 1:A:366:GLU:OE2 | 2.36 | 0.59 |
| 1:D:465:ARG:NH2 | 1:E:564:ASP:OD1 | 2.36 | 0.58 |
| 1:A:430:ILE:HG23 | 1:A:431:ASP:H | 1.69 | 0.57 |
| 1:C:429:LEU:O | 1:C:431:ASP:N | 2.37 | 0.57 |
| 1:A:431:ASP:O | 1:A:433:GLU:N | 2.35 | 0.57 |
| 1:F:430:ILE:HG23 | 1:F:431:ASP:H | 1.70 | 0.57 |
| 1:B:431:ASP:O | 1:B:433:GLU:N | 2.38 | 0.57 |
| 1:C:423:ILE:O | 1:C:427:MET:N | 2.36 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:430:ILE:HG23 | 1:B:431:ASP:H | 1.70 | 0.56 |
| 1:A:98:ASP:OD2 | 1:A:225:ARG:NH2 | 2.38 | 0.56 |
| 1:A:251:LYS:NZ | 2:A:902:AGS:O3G | 2.39 | 0.56 |
| 1:B:125:GLY:O | 1:B:436:THR:OG1 | 2.10 | 0.56 |
| 1:F:427:MET:O | 1:F:429:LEU:N | 2.38 | 0.56 |
| 1:E:251:LYS:NZ | 2:E:902:AGS:O1B | 2.38 | 0.56 |
| 1:F:336:LYS:O | 1:F:338:ARG:NE | 2.39 | 0.56 |
| 1:E:35:ASP:O | 1:E:85:ASN:ND2 | 2.39 | 0.55 |
| 1:C:127:THR:OG1 | 1:C:128:GLY:N | 2.39 | 0.55 |
| 1:D:159:ARG:NH2 | 1:E:232:ALA:O | 2.36 | 0.55 |
| 1:D:427:MET:O | 1:D:429:LEU:N | 2.39 | 0.55 |
| 1:A:491:GLU:OE2 | 1:F:700:ARG:NH2 | 2.39 | 0.54 |
| 1:A:427:MET:SD | 1:A:430:ILE:HG21 | 2.48 | 0.54 |
| 1:D:427:MET:O | 1:D:430:ILE:N | 2.41 | 0.54 |
| 1:E:430:ILE:HG23 | 1:E:431:ASP:H | 1.73 | 0.54 |
| 1:F:312:LYS:N | 1:F:352:SER:O | 2.39 | 0.54 |
| 2:F:902:AGS:O1A | 5:F:1001:HOH:O | 2.19 | 0.54 |
| 1:A:624:ASN:N | 1:A:624:ASN:OD1 | 2.40 | 0.54 |
| 1:B:614:LYS:O | 1:B:616:ASN:N | 2.41 | 0.54 |
| 1:A:732:ARG:NE | 1:A:734:ASP:OD1 | 2.41 | 0.54 |
| 1:C:430:ILE:HG23 | 1:C:432:LEU:HG | 1.91 | 0.53 |
| 1:C:613:THR:O | 1:C:615:LYS:N | 2.41 | 0.53 |
| 1:F:431:ASP:O | 1:F:433:GLU:N | 2.38 | 0.52 |
| 2:E:902:AGS:O1A | 5:E:1001:HOH:O | 2.19 | 0.52 |
| 1:D:431:ASP:O | 1:D:433:GLU:N | 2.38 | 0.52 |
| 1:C:430:ILE:HG23 | 1:C:431:ASP:H | 1.76 | 0.51 |
| 1:B:700:ARG:NH2 | 1:C:491:GLU:OE2 | 2.43 | 0.51 |
| 1:F:632:ALA:O | 1:F:638:ARG:NH1 | 2.43 | 0.51 |
| 1:D:125:GLY:O | 1:D:436:THR:OG1 | 2.23 | 0.51 |
| 1:E:732:ARG:NH2 | 1:E:734:ASP:OD2 | 2.44 | 0.50 |
| 1:C:30:GLU:OE2 | 1:C:217:LYS:NZ | 2.32 | 0.50 |
| 1:F:30:GLU:OE2 | 1:F:217:LYS:NZ | 2.25 | 0.50 |
| 1:B:220:VAL:HG12 | 1:B:224:LEU:HD11 | 1.94 | 0.50 |
| 1:A:312:LYS:NZ | 1:A:351:ASN:O | 2.30 | 0.49 |
| 1:C:125:GLY:O | 1:C:436:THR:OG1 | 2.18 | 0.49 |
| 1:C:494:GLN:NE2 | 1:C:498:GLU:OE2 | 2.46 | 0.49 |
| 1:C:52:PHE:N | 1:C:55:ASP:OD2 | 2.45 | 0.49 |
| 1:E:431:ASP:O | 1:E:433:GLU:N | 2.42 | 0.49 |
| 1:E:72:LEU:O | 1:E:73:SER:OG | 2.28 | 0.49 |
| 1:E:125:GLY:O | 1:E:436:THR:OG1 | 2.17 | 0.49 |
| 1:F:169:ASP:HB3 | 1:F:170:PRO:HD3 | 1.94 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:701:GLU:OE1 | 1:F:732:ARG:NH2 | 2.45 | 0.49 |
| 1:C:427:MET:HG3 | 1:C:430:ILE:HG21 | 1.95 | 0.49 |
| 1:C:283:GLU:OE1 | 1:C:283:GLU:N | 2.42 | 0.48 |
| 1:F:402:GLU:OE1 | 1:F:453:ARG:NH1 | 2.47 | 0.48 |
| 1:A:348:ASN:OD1 | 1:A:348:ASN:N | 2.46 | 0.48 |
| 1:B:127:THR:OG1 | 1:B:128:GLY:N | 2.47 | 0.48 |
| 1:C:708:ARG:N | 1:C:729:PRO:HD3 | 2.28 | 0.48 |
| 1:C:140:LEU:O | 1:C:140:LEU:HD12 | 2.13 | 0.48 |
| 1:C:169:ASP:HB3 | 1:C:170:PRO:HD3 | 1.96 | 0.48 |
| 1:A:169:ASP:HB3 | 1:A:170:PRO:HD3 | 1.96 | 0.47 |
| 1:D:169:ASP:HB3 | 1:D:170:PRO:HD3 | 1.94 | 0.47 |
| 1:D:430:ILE:HD11 | 1:D:437:ILE:HD12 | 1.96 | 0.47 |
| 1:B:169:ASP:HB3 | 1:B:170:PRO:HD3 | 1.96 | 0.47 |
| 1:E:564:ASP:OD1 | 1:E:567:ARG:NH1 | 2.48 | 0.47 |
| 1:C:429:LEU:HD12 | 1:C:430:ILE:N | 2.29 | 0.47 |
| 1:C:427:MET:O | 1:C:429:LEU:N | 2.47 | 0.47 |
| 1:A:114:ILE:CD1 | 1:A:176:VAL:HG22 | 2.45 | 0.47 |
| 1:D:423:ILE:O | 1:D:425:LYS:N | 2.48 | 0.47 |
| 1:B:79:ASP:OD1 | 1:B:79:ASP:N | 2.48 | 0.47 |
| 1:C:114:ILE:CD1 | 1:C:176:VAL:HG22 | 2.44 | 0.47 |
| 1:B:159:ARG:NH2 | 1:C:232:ALA:O | 2.41 | 0.47 |
| 1:D:350:PRO:O | 1:D:358:ARG:NH2 | 2.45 | 0.47 |
| 1:E:114:ILE:CD1 | 1:E:176:VAL:HG22 | 2.44 | 0.47 |
| 1:B:222:LEU:HB2 | 1:B:223:PRO:HD3 | 1.97 | 0.46 |
| 1:A:321:GLU:OE2 | 1:B:322:ARG:NE | 2.48 | 0.46 |
| 1:A:429:LEU:HG | 1:A:430:ILE:N | 2.30 | 0.46 |
| 1:B:114:ILE:CD1 | 1:B:176:VAL:HG22 | 2.46 | 0.46 |
| 1:A:635:ARG:NH1 | 1:A:636:PRO:O | 2.49 | 0.46 |
| 1:D:732:ARG:NE | 1:D:734:ASP:OD1 | 2.41 | 0.46 |
| 1:E:127:THR:OG1 | 1:E:128:GLY:N | 2.48 | 0.46 |
| 1:D:30:GLU:OE2 | 1:D:217:LYS:NZ | 2.34 | 0.46 |
| 1:B:93:ARG:NH2 | 1:B:195:GLU:OE2 | 2.46 | 0.46 |
| 1:A:29:ASP:OD2 | 1:A:83:ARG:NH1 | 2.49 | 0.46 |
| 1:D:281:GLU:O | 1:D:285:ASN:ND2 | 2.44 | 0.45 |
| 1:D:613:THR:O | 1:D:615:LYS:N | 2.48 | 0.45 |
| 1:E:493:VAL:HG12 | 1:E:535:CYS:SG | 2.56 | 0.45 |
| 1:B:708:ARG:NH1 | 1:B:730:GLU:OE1 | 2.49 | 0.45 |
| 1:D:41:LEU:O | 1:D:74:ASP:N | 2.47 | 0.45 |
| 1:E:531:ILE:HD11 | 1:E:620:ILE:CD1 | 2.47 | 0.45 |
| 1:E:169:ASP:HB3 | 1:E:170:PRO:HD3 | 1.97 | 0.45 |
| 1:E:635:ARG:NE | 1:E:636:PRO:O | 2.48 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:277:LYS:NZ | 1:F:285:ASN:OD1 | 2.49 | 0.45 |
| 1:F:490:GLN:O | 1:F:494:GLN:N | 2.49 | 0.45 |
| 1:F:635:ARG:NE | 1:F:636:PRO:O | 2.47 | 0.45 |
| 1:C:501:ASP:N | 1:C:501:ASP:OD1 | 2.50 | 0.44 |
| 1:E:46:MET:HE2 | 1:E:71:VAL:HG12 | 1.99 | 0.44 |
| 1:B:484:ASP:OD1 | 1:B:484:ASP:N | 2.49 | 0.44 |
| 1:E:493:VAL:HG13 | 1:E:618:PHE:CD2 | 2.53 | 0.44 |
| 1:F:377:ARG:NE | 1:F:403:THR:O | 2.51 | 0.44 |
| 1:A:430:ILE:HD11 | 1:A:437:ILE:HD12 | 1.99 | 0.44 |
| 1:E:237:PRO:HG2 | 1:E:340:HIS:NE2 | 2.32 | 0.44 |
| 1:E:493:VAL:HG13 | 1:E:618:PHE:CE2 | 2.53 | 0.44 |
| 1:E:287:ARG:NH1 | 1:E:291:GLU:OE2 | 2.51 | 0.44 |
| 1:A:321:GLU:OE1 | 1:B:322:ARG:NH1 | 2.51 | 0.44 |
| 1:B:501:ASP:N | 1:B:501:ASP:OD1 | 2.50 | 0.44 |
| 1:F:114:ILE:CD1 | 1:F:176:VAL:HG22 | 2.48 | 0.44 |
| 1:F:52:PHE:N | 1:F:55:ASP:OD2 | 2.47 | 0.44 |
| 1:A:222:LEU:HB2 | 1:A:223:PRO:HD3 | 1.98 | 0.43 |
| 1:B:423:ILE:CD1 | 1:C:233:ILE:HD11 | 2.48 | 0.43 |
| 1:E:222:LEU:HB3 | 1:E:223:PRO:HD3 | 2.00 | 0.43 |
| 1:E:549:THR:CG2 | 1:F:603:GLN:HA | 2.48 | 0.43 |
| 1:C:46:MET:HA | 1:C:51:LEU:HD12 | 1.99 | 0.43 |
| 1:D:114:ILE:CD1 | 1:D:176:VAL:HG22 | 2.48 | 0.43 |
| 1:E:489:LEU:HB3 | 1:E:531:ILE:HG21 | 2.00 | 0.43 |
| 1:E:707:ILE:HG22 | 1:E:708:ARG:N | 2.33 | 0.43 |
| 1:C:427:MET:CG | 1:C:430:ILE:HG21 | 2.48 | 0.43 |
| 1:B:430:ILE:HD11 | 1:B:437:ILE:HD12 | 1.99 | 0.43 |
| 1:C:441:VAL:O | 1:C:444:SER:OG | 2.26 | 0.43 |
| 1:E:733:ARG:NH2 | 1:E:737:GLU:OE2 | 2.52 | 0.43 |
| 1:D:430:ILE:HG13 | 1:D:431:ASP:N | 2.33 | 0.43 |
| 1:E:65:ARG:NH1 | 1:E:91:ASN:O | 2.51 | 0.43 |
| 1:A:427:MET:O | 1:A:429:LEU:N | 2.52 | 0.42 |
| 1:B:27:ILE:HG22 | 1:B:28:VAL:N | 2.34 | 0.42 |
| 1:C:222:LEU:HB2 | 1:C:223:PRO:HD3 | 2.00 | 0.42 |
| 1:D:586:ARG:HD3 | 1:D:598:ASP:HA | 2.01 | 0.42 |
| 1:E:430:ILE:HD11 | 1:E:437:ILE:HD12 | 2.00 | 0.42 |
| 1:E:626:PRO:HB2 | 1:E:762:LEU:HD11 | 2.01 | 0.42 |
| 1:A:649:ASP:O | 1:A:652:SER:OG | 2.37 | 0.42 |
| 1:F:127:THR:OG1 | 1:F:128:GLY:N | 2.52 | 0.42 |
| 1:E:501:ASP:N | 1:E:501:ASP:OD1 | 2.52 | 0.42 |
| 1:F:206:ILE:HG12 | 1:F:253:LEU:HD22 | 2.01 | 0.42 |
| 1:B:693:ARG:NH2 | 1:C:641:GLN:OE1 | 2.51 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:494:GLN:NE2 | 1:F:498:GLU:OE2 | 2.51 | 0.42 |
| 1:D:695:CYS:HB3 | 1:E:506:PHE:CE2 | 2.55 | 0.42 |
| 1:B:708:ARG:O | 1:B:730:GLU:N | 2.51 | 0.42 |
| 1:F:168:THR:O | 1:F:171:SER:OG | 2.35 | 0.42 |
| 1:D:222:LEU:HB2 | 1:D:223:PRO:HD3 | 2.01 | 0.42 |
| 1:B:108:VAL:HG12 | 1:B:173:TYR:CD1 | 2.54 | 0.41 |
| 1:D:429:LEU:HD12 | 1:D:430:ILE:N | 2.35 | 0.41 |
| 1:D:611:MET:HE2 | 1:D:617:VAL:HG11 | 2.01 | 0.41 |
| 2:F:902:AGS:H8 | 2:F:902:AGS:H5'1 | 2.01 | 0.41 |
| 1:A:430:ILE:HG13 | 1:A:431:ASP:N | 2.35 | 0.41 |
| 1:E:430:ILE:HG13 | 1:E:431:ASP:N | 2.34 | 0.41 |
| 1:A:407:VAL:HG12 | 1:A:408:GLY:H | 1.85 | 0.41 |
| 1:E:22:ARG:HB3 | 1:E:23:PRO:HD2 | 2.01 | 0.41 |
| 1:D:707:ILE:HG22 | 1:D:708:ARG:N | 2.36 | 0.41 |
| 1:F:430:ILE:HD11 | 1:F:437:ILE:HD12 | 2.02 | 0.41 |
| 1:E:43:GLN:N | 1:E:44:PRO:CD | 2.84 | 0.41 |
| 1:F:43:GLN:N | 1:F:44:PRO:CD | 2.83 | 0.41 |
| 1:B:460:ASN:OD1 | 1:B:460:ASN:N | 2.52 | 0.41 |
| 1:C:43:GLN:N | 1:C:44:PRO:CD | 2.84 | 0.41 |
| 1:F:430:ILE:HG13 | 1:F:431:ASP:N | 2.35 | 0.41 |
| 1:B:225:ARG:C | 1:B:227:PRO:HD3 | 2.41 | 0.41 |
| 1:A:43:GLN:N | 1:A:44:PRO:CD | 2.84 | 0.41 |
| 1:B:312:LYS:N | 1:B:352:SER:O | 2.54 | 0.41 |
| 1:B:430:ILE:HG13 | 1:B:431:ASP:N | 2.36 | 0.41 |
| 1:D:553:GLY:HA2 | 1:D:599:ARG:NH2 | 2.36 | 0.41 |
| 1:A:403:THR:CG2 | 1:A:406:HIS:CG | 3.05 | 0.41 |
| 1:C:760:GLN:O | 1:C:763:GLN:NE2 | 2.54 | 0.40 |
| 1:D:695:CYS:HB3 | 1:E:506:PHE:HE2 | 1.86 | 0.40 |
| 1:F:330:THR:O | 1:F:334:GLY:N | 2.51 | 0.40 |
| 1:B:269:ILE:HG23 | 1:B:274:ILE:HD11 | 2.03 | 0.40 |
| 1:B:526:LEU:HD11 | 2:B:901:AGS:H2' | 2.04 | 0.40 |
| 1:E:734:ASP:OD1 | 1:E:734:ASP:N | 2.49 | 0.40 |
| 1:B:226:HIS:HB3 | 1:B:229:LEU:HD23 | 2.03 | 0.40 |
| 2:B:902:AGS:O2A | 5:B:1002:HOH:O | 2.21 | 0.40 |
| 1:D:43:GLN:N | 1:D:44:PRO:CD | 2.85 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1 | A | 718/785 (92%) | 682 (95%) | 31 (4%) | 5 (1%) | 22 | 54 |
| 1 | B | 719/785 (92%) | 667 (93%) | 44 (6%) | 8 (1%) | 14 | 45 |
| 1 | C | 720/785 (92%) | 673 (94%) | 35 (5%) | 12 (2%) | 9 | 35 |
| 1 | D | 718/785 (92%) | 673 (94%) | 37 (5%) | 8 (1%) | 14 | 45 |
| 1 | E | 719/785 (92%) | 668 (93%) | 41 (6%) | 10 (1%) | 11 | 38 |
| 1 | F | 720/785 (92%) | 668 (93%) | 44 (6%) | 8 (1%) | 14 | 45 |
| All | All | 4314/4710 (92%) | 4031 (93%) | 232 (5%) | 51 (1%) | 13 | 42 |

All (51) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 80 | GLU |
| 1 | B | 428 | ASP |
| 1 | B | 615 | LYS |
| 1 | C | 50 | GLN |
| 1 | C | 352 | SER |
| 1 | C | 430 | ILE |
| 1 | C | 431 | ASP |
| 1 | C | 707 | ILE |
| 1 | D | 428 | ASP |
| 1 | D | 430 | ILE |
| 1 | D | 613 | THR |
| 1 | E | 428 | ASP |
| 1 | F | 339 | ALA |
| 1 | F | 428 | ASP |
| 1 | A | 428 | ASP |
| 1 | A | 430 | ILE |
| 1 | B | 430 | ILE |
| 1 | C | 340 | HIS |
| 1 | C | 428 | ASP |
| 1 | D | 340 | HIS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 424 | ARG |
| 1 | D | 431 | ASP |
| 1 | E | 430 | ILE |
| 1 | F | 279 | ALA |
| 1 | F | 430 | ILE |
| 1 | B | 425 | LYS |
| 1 | C | 614 | LYS |
| 1 | E | 425 | LYS |
| 1 | E | 431 | ASP |
| 1 | F | 425 | LYS |
| 1 | A | 431 | ASP |
| 1 | B | 78 | SER |
| 1 | B | 431 | ASP |
| 1 | E | 613 | THR |
| 1 | E | 614 | LYS |
| 1 | F | 312 | LYS |
| 1 | F | 431 | ASP |
| 1 | A | 432 | LEU |
| 1 | C | 615 | LYS |
| 1 | E | 73 | SER |
| 1 | B | 143 | TYR |
| 1 | D | 423 | ILE |
| 1 | E | 612 | SER |
| 1 | F | 106 | PRO |
| 1 | C | 708 | ARG |
| 1 | D | 729 | PRO |
| 1 | C | 350 | PRO |
| 1 | C | 423 | ILE |
| 1 | E | 186 | GLY |
| 1 | E | 587 | GLY |
| 1 | A | 186 | GLY |

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.

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1 | A | 616/658 (94%) | 600 (97%) | 16 (3%) | 46 | 71 |
| 1 | B | 617/658 (94%) | 591 (96%) | 26 (4%) | 30 | 60 |
| 1 | C | 617/658 (94%) | 596 (97%) | 21 (3%) | 37 | 65 |
| 1 | D | 616/658 (94%) | 600 (97%) | 16 (3%) | 46 | 71 |
| 1 | E | 616/658 (94%) | 590 (96%) | 26 (4%) | 30 | 60 |
| 1 | F | 617/658 (94%) | 602 (98%) | 15 (2%) | 49 | 73 |
| All | All | 3699/3948 (94%) | 3579 (97%) | 120 (3%) | 39 | 67 |

All (120) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 53 | ARG |
| 1 | A | 57 | VAL |
| 1 | A | 230 | PHE |
| 1 | A | 313 | ARG |
| 1 | A | 338 | ARG |
| 1 | A | 348 | ASN |
| 1 | A | 349 | ARG |
| 1 | A | 420 | LEU |
| 1 | A | 428 | ASP |
| 1 | A | 431 | ASP |
| 1 | A | 433 | GLU |
| 1 | A | 450 | ASP |
| 1 | A | 556 | GLU |
| 1 | A | 573 | VAL |
| 1 | A | 624 | ASN |
| 1 | A | 672 | LEU |
| 1 | B | 40 | SER |
| 1 | B | 45 | LYS |
| 1 | B | 46 | MET |
| 1 | B | 47 | ASP |
| 1 | B | 52 | PHE |
| 1 | B | 55 | ASP |
| 1 | B | 86 | ARG |
| 1 | B | 90 | ASN |
| 1 | B | 115 | HIS |
| 1 | B | 173 | TYR |
| 1 | B | 185 | GLU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 199 | ASN |
| 1 | B | 222 | LEU |
| 1 | B | 224 | LEU |
| 1 | B | 225 | ARG |
| 1 | B | 337 | GLN |
| 1 | B | 429 | LEU |
| 1 | B | 433 | GLU |
| 1 | B | 442 | MET |
| 1 | B | 494 | GLN |
| 1 | B | 556 | GLU |
| 1 | B | 573 | VAL |
| 1 | B | 611 | MET |
| 1 | B | 616 | ASN |
| 1 | B | 674 | PHE |
| 1 | B | 744 | ARG |
| 1 | C | 40 | SER |
| 1 | C | 53 | ARG |
| 1 | C | 72 | LEU |
| 1 | C | 86 | ARG |
| 1 | C | 230 | PHE |
| 1 | C | 249 | THR |
| 1 | C | 261 | GLU |
| 1 | C | 292 | GLU |
| 1 | C | 336 | LYS |
| 1 | C | 351 | ASN |
| 1 | C | 420 | LEU |
| 1 | C | 426 | LYS |
| 1 | C | 442 | MET |
| 1 | C | 443 | ASN |
| 1 | C | 445 | LEU |
| 1 | C | 494 | GLN |
| 1 | C | 512 | LYS |
| 1 | C | 556 | GLU |
| 1 | C | 742 | PHE |
| 1 | C | 745 | ARG |
| 1 | C | 757 | MET |
| 1 | D | 40 | SER |
| 1 | D | 74 | ASP |
| 1 | D | 113 | ARG |
| 1 | D | 230 | PHE |
| 1 | D | 261 | GLU |
| 1 | D | 316 | THR |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 335 | LEU |
| 1 | D | 349 | ARG |
| 1 | D | 433 | GLU |
| 1 | D | 613 | THR |
| 1 | D | 651 | LYS |
| 1 | D | 668 | LYS |
| 1 | D | 693 | ARG |
| 1 | D | 737 | GLU |
| 1 | D | 744 | ARG |
| 1 | D | 745 | ARG |
| 1 | E | 40 | SER |
| 1 | E | 64 | ARG |
| 1 | E | 65 | ARG |
| 1 | E | 71 | VAL |
| 1 | E | 86 | ARG |
| 1 | E | 230 | PHE |
| 1 | E | 231 | LYS |
| 1 | E | 338 | ARG |
| 1 | E | 340 | HIS |
| 1 | E | 348 | ASN |
| 1 | E | 349 | ARG |
| 1 | E | 433 | GLU |
| 1 | E | 450 | ASP |
| 1 | E | 460 | ASN |
| 1 | E | 492 | LEU |
| 1 | E | 549 | THR |
| 1 | E | 613 | THR |
| 1 | E | 624 | ASN |
| 1 | E | 635 | ARG |
| 1 | E | 649 | ASP |
| 1 | E | 741 | ARG |
| 1 | E | 744 | ARG |
| 1 | E | 745 | ARG |
| 1 | E | 762 | LEU |
| 1 | E | 763 | GLN |
| 1 | E | 766 | ARG |
| 1 | F | 53 | ARG |
| 1 | F | 113 | ARG |
| 1 | F | 230 | PHE |
| 1 | F | 348 | ASN |
| 1 | F | 429 | LEU |
| 1 | F | 433 | GLU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | F | 494 | GLN |
| 1 | F | 599 | ARG |
| 1 | F | 623 | THR |
| 1 | F | 635 | ARG |
| 1 | F | 677 | LYS |
| 1 | F | 741 | ARG |
| 1 | F | 744 | ARG |
| 1 | F | 745 | ARG |
| 1 | F | 756 | GLU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 348 | ASN |
| 1 | B | 616 | ASN |
| 1 | D | 21 | ASN |

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 18 are monoatomic - leaving 12 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 | A | 901 | 3 | 26,33,33 | 1.56 | 8 (30%) | 26,52,52 | 1.84 | 6 (23%) |
| 2 | AGS | E | 901 | 3 | 26,33,33 | 1.54 | 8 (30%) | 26,52,52 | 1.82 | 5 (19%) |
| 2 | AGS | B | 901 | 3 | 26,33,33 | 1.58 | 8 (30%) | 26,52,52 | 1.64 | 5 (19%) |
| 2 | AGS | D | 901 | 3 | 26,33,33 | 1.53 | 8 (30%) | 26,52,52 | 1.76 | 6 (23%) |
| 2 | AGS | F | 901 | 3 | 26,33,33 | 1.55 | 7 (26%) | 26,52,52 | 1.67 | 3 (11%) |
| 2 | AGS | D | 902 | 3 | 26,33,33 | 1.59 | 8 (30%) | 26,52,52 | 1.68 | 5 (19%) |
| 2 | AGS | C | 902 | 3 | 26,33,33 | 1.58 | 8 (30%) | 26,52,52 | 1.67 | 3 (11%) |
| 2 | AGS | B | 902 | 3 | 26,33,33 | 1.62 | 8 (30%) | 26,52,52 | 1.54 | 4 (15%) |
| 2 | AGS | A | 902 | 3 | 26,33,33 | 1.59 | 8 (30%) | 26,52,52 | 1.53 | 3 (11%) |
| 2 | AGS | C | 901 | 3 | 26,33,33 | 1.55 | 8 (30%) | 26,52,52 | 1.76 | 5 (19%) |
| 2 | AGS | F | 902 | 3 | 26,33,33 | 1.58 | 8 (30%) | 26,52,52 | 1.61 | 4 (15%) |
| 2 | AGS | E | 902 | 3 | 26,33,33 | 1.58 | 7 (26%) | 26,52,52 | 1.60 | 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 | A | 901 | 3 | - | 3/17/38/38 | 0/3/3/3 |
| 2 | AGS | E | 901 | 3 | - | 7/17/38/38 | 0/3/3/3 |
| 2 | AGS | B | 901 | 3 | - | 5/17/38/38 | 0/3/3/3 |
| 2 | AGS | D | 901 | 3 | - | 10/17/38/38 | 0/3/3/3 |
| 2 | AGS | F | 901 | 3 | - | 2/17/38/38 | 0/3/3/3 |
| 2 | AGS | D | 902 | 3 | - | 2/17/38/38 | 0/3/3/3 |
| 2 | AGS | C | 902 | 3 | - | 3/17/38/38 | 0/3/3/3 |
| 2 | AGS | B | 902 | 3 | - | 7/17/38/38 | 0/3/3/3 |
| 2 | AGS | A | 902 | 3 | - | 3/17/38/38 | 0/3/3/3 |
| 2 | AGS | C | 901 | 3 | - | 10/17/38/38 | 0/3/3/3 |
| 2 | AGS | F | 902 | 3 | - | 4/17/38/38 | 0/3/3/3 |
| 2 | AGS | E | 902 | 3 | - | 2/17/38/38 | 0/3/3/3 |

All (94) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | A | 902 | AGS | C2'-C1' | -3.71 | 1.48 | 1.53 |
| 2 | B | 902 | AGS | C2'-C1' | -3.63 | 1.48 | 1.53 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | D | 902 | AGS | C2'-C1' | -3.62 | 1.48 | 1.53 |
| 2 | F | 902 | AGS | C2'-C1' | -3.51 | 1.48 | 1.53 |
| 2 | E | 902 | AGS | C2'-C1' | -3.51 | 1.48 | 1.53 |
| 2 | B | 901 | AGS | C2'-C1' | -3.39 | 1.48 | 1.53 |
| 2 | C | 902 | AGS | C2'-C1' | -3.30 | 1.48 | 1.53 |
| 2 | A | 901 | AGS | C2'-C1' | -3.29 | 1.48 | 1.53 |
| 2 | C | 901 | AGS | C2'-C1' | -3.25 | 1.48 | 1.53 |
| 2 | F | 901 | AGS | C2'-C1' | -3.24 | 1.48 | 1.53 |
| 2 | E | 901 | AGS | C2'-C1' | -3.18 | 1.48 | 1.53 |
| 2 | D | 901 | AGS | C2'-C1' | -3.02 | 1.49 | 1.53 |
| 2 | C | 901 | AGS | C6-N6 | 2.62 | 1.43 | 1.34 |
| 2 | A | 902 | AGS | C6-N6 | 2.59 | 1.43 | 1.34 |
| 2 | A | 901 | AGS | C6-N6 | 2.58 | 1.43 | 1.34 |
| 2 | E | 901 | AGS | C6-N6 | 2.58 | 1.43 | 1.34 |
| 2 | F | 901 | AGS | C6-N6 | 2.57 | 1.43 | 1.34 |
| 2 | B | 901 | AGS | C6-N6 | 2.57 | 1.43 | 1.34 |
| 2 | D | 902 | AGS | C6-N6 | 2.57 | 1.43 | 1.34 |
| 2 | B | 902 | AGS | C6-N6 | 2.57 | 1.43 | 1.34 |
| 2 | C | 902 | AGS | C6-N6 | 2.57 | 1.43 | 1.34 |
| 2 | F | 902 | AGS | C6-N6 | 2.56 | 1.43 | 1.34 |
| 2 | D | 901 | AGS | C6-N6 | 2.56 | 1.43 | 1.34 |
| 2 | E | 902 | AGS | C6-N6 | 2.56 | 1.43 | 1.34 |
| 2 | B | 902 | AGS | C2'-C3' | -2.55 | 1.46 | 1.53 |
| 2 | C | 902 | AGS | C2'-C3' | -2.55 | 1.46 | 1.53 |
| 2 | F | 901 | AGS | C2'-C3' | -2.55 | 1.46 | 1.53 |
| 2 | A | 901 | AGS | C2'-C3' | -2.51 | 1.46 | 1.53 |
| 2 | A | 902 | AGS | C2'-C3' | -2.47 | 1.46 | 1.53 |
| 2 | F | 902 | AGS | C2'-C3' | -2.44 | 1.46 | 1.53 |
| 2 | B | 901 | AGS | O4'-C4' | -2.44 | 1.39 | 1.45 |
| 2 | B | 901 | AGS | C2'-C3' | -2.44 | 1.46 | 1.53 |
| 2 | D | 902 | AGS | C2'-C3' | -2.44 | 1.46 | 1.53 |
| 2 | D | 901 | AGS | C2'-C3' | -2.40 | 1.46 | 1.53 |
| 2 | C | 902 | AGS | O4'-C4' | -2.38 | 1.39 | 1.45 |
| 2 | D | 901 | AGS | O4'-C4' | -2.36 | 1.39 | 1.45 |
| 2 | E | 902 | AGS | O4'-C4' | -2.35 | 1.39 | 1.45 |
| 2 | E | 902 | AGS | C2'-C3' | -2.35 | 1.46 | 1.53 |
| 2 | F | 902 | AGS | O4'-C4' | -2.35 | 1.39 | 1.45 |
| 2 | F | 901 | AGS | O4'-C4' | -2.34 | 1.39 | 1.45 |
| 2 | E | 901 | AGS | O4'-C4' | -2.34 | 1.39 | 1.45 |
| 2 | C | 901 | AGS | O4'-C4' | -2.33 | 1.39 | 1.45 |
| 2 | C | 901 | AGS | C2'-C3' | -2.32 | 1.47 | 1.53 |
| 2 | D | 902 | AGS | O4'-C4' | -2.31 | 1.39 | 1.45 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | A | 901 | AGS | O2'-C2' | -2.29 | 1.37 | 1.43 |
| 2 | E | 901 | AGS | C2'-C3' | -2.28 | 1.47 | 1.53 |
| 2 | A | 902 | AGS | O4'-C4' | -2.28 | 1.39 | 1.45 |
| 2 | A | 901 | AGS | O4'-C4' | -2.27 | 1.39 | 1.45 |
| 2 | B | 902 | AGS | O4'-C4' | -2.22 | 1.40 | 1.45 |
| 2 | B | 902 | AGS | O2'-C2' | -2.22 | 1.37 | 1.43 |
| 2 | D | 902 | AGS | O3'-C3' | -2.21 | 1.37 | 1.43 |
| 2 | B | 901 | AGS | PG-S1G | 2.20 | 1.95 | 1.90 |
| 2 | B | 902 | AGS | PG-S1G | 2.17 | 1.95 | 1.90 |
| 2 | F | 901 | AGS | O2'-C2' | -2.16 | 1.37 | 1.43 |
| 2 | D | 902 | AGS | PG-S1G | 2.16 | 1.95 | 1.90 |
| 2 | D | 902 | AGS | O2'-C2' | -2.16 | 1.37 | 1.43 |
| 2 | C | 901 | AGS | O2'-C2' | -2.16 | 1.37 | 1.43 |
| 2 | F | 902 | AGS | PG-S1G | 2.16 | 1.95 | 1.90 |
| 2 | B | 902 | AGS | O3'-C3' | -2.16 | 1.37 | 1.43 |
| 2 | C | 901 | AGS | C2-N3 | 2.16 | 1.35 | 1.32 |
| 2 | B | 901 | AGS | O2'-C2' | -2.15 | 1.37 | 1.43 |
| 2 | C | 902 | AGS | PG-S1G | 2.15 | 1.95 | 1.90 |
| 2 | B | 901 | AGS | O3'-C3' | -2.14 | 1.37 | 1.43 |
| 2 | F | 901 | AGS | O3'-C3' | -2.14 | 1.37 | 1.43 |
| 2 | E | 901 | AGS | O2'-C2' | -2.14 | 1.37 | 1.43 |
| 2 | A | 902 | AGS | O3'-C3' | -2.14 | 1.37 | 1.43 |
| 2 | D | 901 | AGS | PG-S1G | 2.13 | 1.95 | 1.90 |
| 2 | A | 902 | AGS | PG-S1G | 2.13 | 1.95 | 1.90 |
| 2 | E | 902 | AGS | PG-S1G | 2.13 | 1.95 | 1.90 |
| 2 | B | 902 | AGS | C2-N3 | 2.12 | 1.35 | 1.32 |
| 2 | C | 901 | AGS | O3'-C3' | -2.12 | 1.38 | 1.43 |
| 2 | A | 901 | AGS | O3'-C3' | -2.12 | 1.38 | 1.43 |
| 2 | E | 902 | AGS | O2'-C2' | -2.12 | 1.38 | 1.43 |
| 2 | F | 902 | AGS | O2'-C2' | -2.12 | 1.38 | 1.43 |
| 2 | C | 902 | AGS | O2'-C2' | -2.11 | 1.38 | 1.43 |
| 2 | C | 901 | AGS | PG-S1G | 2.11 | 1.95 | 1.90 |
| 2 | E | 901 | AGS | O3'-C3' | -2.11 | 1.38 | 1.43 |
| 2 | D | 901 | AGS | O2'-C2' | -2.11 | 1.38 | 1.43 |
| 2 | A | 902 | AGS | O2'-C2' | -2.10 | 1.38 | 1.43 |
| 2 | E | 902 | AGS | O3'-C3' | -2.10 | 1.38 | 1.43 |
| 2 | F | 901 | AGS | PG-S1G | 2.09 | 1.95 | 1.90 |
| 2 | C | 902 | AGS | O3'-C3' | -2.09 | 1.38 | 1.43 |
| 2 | F | 902 | AGS | O3'-C3' | -2.08 | 1.38 | 1.43 |
| 2 | D | 901 | AGS | O3'-C3' | -2.07 | 1.38 | 1.43 |
| 2 | B | 901 | AGS | C2-N3 | 2.06 | 1.35 | 1.32 |
| 2 | E | 901 | AGS | PG-S1G | 2.06 | 1.95 | 1.90 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 2 | F | 902 | AGS | C2-N3 | 2.06 | 1.35 | 1.32 |
| 2 | C | 902 | AGS | C2-N3 | 2.06 | 1.35 | 1.32 |
| 2 | A | 901 | AGS | PG-S1G | 2.05 | 1.95 | 1.90 |
| 2 | A | 902 | AGS | C2-N3 | 2.04 | 1.35 | 1.32 |
| 2 | E | 901 | AGS | C2-N3 | 2.03 | 1.35 | 1.32 |
| 2 | A | 901 | AGS | C2-N3 | 2.03 | 1.35 | 1.32 |
| 2 | D | 901 | AGS | C2-N3 | 2.01 | 1.35 | 1.32 |
| 2 | D | 902 | AGS | C2-N3 | 2.01 | 1.35 | 1.32 |

All (53) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | F | 901 | AGS | N3-C2-N1 | -5.59 | 119.94 | 128.68 |
| 2 | C | 902 | AGS | N3-C2-N1 | -5.56 | 120.00 | 128.68 |
| 2 | E | 901 | AGS | N3-C2-N1 | -5.55 | 120.00 | 128.68 |
| 2 | D | 902 | AGS | N3-C2-N1 | -5.54 | 120.01 | 128.68 |
| 2 | A | 901 | AGS | N3-C2-N1 | -5.52 | 120.06 | 128.68 |
| 2 | B | 901 | AGS | N3-C2-N1 | -5.51 | 120.07 | 128.68 |
| 2 | B | 902 | AGS | N3-C2-N1 | -5.48 | 120.11 | 128.68 |
| 2 | F | 902 | AGS | N3-C2-N1 | -5.48 | 120.11 | 128.68 |
| 2 | D | 901 | AGS | N3-C2-N1 | -5.48 | 120.11 | 128.68 |
| 2 | A | 902 | AGS | N3-C2-N1 | -5.47 | 120.13 | 128.68 |
| 2 | E | 902 | AGS | N3-C2-N1 | -5.45 | 120.16 | 128.68 |
| 2 | C | 901 | AGS | N3-C2-N1 | -5.45 | 120.16 | 128.68 |
| 2 | E | 901 | AGS | PA-O3A-PB | -4.19 | 118.43 | 132.83 |
| 2 | C | 902 | AGS | PA-O3A-PB | -4.15 | 118.58 | 132.83 |
| 2 | D | 902 | AGS | PA-O3A-PB | -4.07 | 118.84 | 132.83 |
| 2 | F | 902 | AGS | PA-O3A-PB | -3.95 | 119.26 | 132.83 |
| 2 | A | 902 | AGS | PA-O3A-PB | -3.91 | 119.41 | 132.83 |
| 2 | D | 901 | AGS | PA-O3A-PB | -3.86 | 119.59 | 132.83 |
| 2 | A | 901 | AGS | PA-O3A-PB | -3.85 | 119.63 | 132.83 |
| 2 | E | 902 | AGS | PA-O3A-PB | -3.80 | 119.78 | 132.83 |
| 2 | C | 901 | AGS | PA-O3A-PB | -3.66 | 120.27 | 132.83 |
| 2 | F | 901 | AGS | PA-O3A-PB | -3.60 | 120.46 | 132.83 |
| 2 | A | 901 | AGS | C3'-C2'-C1' | 3.38 | 106.07 | 100.98 |
| 2 | B | 901 | AGS | PA-O3A-PB | -3.30 | 121.52 | 132.83 |
| 2 | C | 901 | AGS | C3'-C2'-C1' | 3.27 | 105.90 | 100.98 |
| 2 | E | 901 | AGS | C3'-C2'-C1' | 3.08 | 105.61 | 100.98 |
| 2 | B | 902 | AGS | PA-O3A-PB | -2.97 | 122.65 | 132.83 |
| 2 | D | 901 | AGS | C3'-C2'-C1' | 2.74 | 105.11 | 100.98 |
| 2 | F | 901 | AGS | O2G-PG-O3B | 2.54 | 113.10 | 104.64 |
| 2 | D | 901 | AGS | O2G-PG-O3B | 2.41 | 112.70 | 104.64 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | B | 901 | AGS | O2G-PG-O3B | 2.32 | 112.38 | 104.64 |
| 2 | A | 901 | AGS | O4'-C4'-C3' | 2.30 | 109.67 | 105.11 |
| 2 | E | 901 | AGS | O2G-PG-O3B | 2.30 | 112.32 | 104.64 |
| 2 | C | 901 | AGS | O4'-C4'-C3' | 2.30 | 109.66 | 105.11 |
| 2 | D | 902 | AGS | C3'-C2'-C1' | 2.28 | 104.41 | 100.98 |
| 2 | C | 902 | AGS | C4-C5-N7 | -2.24 | 107.06 | 109.40 |
| 2 | B | 902 | AGS | C4-C5-N7 | -2.21 | 107.09 | 109.40 |
| 2 | B | 902 | AGS | O2G-PG-O3B | 2.19 | 111.94 | 104.64 |
| 2 | A | 901 | AGS | C4-C5-N7 | -2.18 | 107.13 | 109.40 |
| 2 | D | 902 | AGS | C4-C5-N7 | -2.18 | 107.13 | 109.40 |
| 2 | F | 902 | AGS | C4-C5-N7 | -2.16 | 107.15 | 109.40 |
| 2 | E | 901 | AGS | O4'-C4'-C3' | 2.14 | 109.35 | 105.11 |
| 2 | E | 902 | AGS | O4'-C4'-C3' | 2.13 | 109.34 | 105.11 |
| 2 | A | 902 | AGS | C4-C5-N7 | -2.13 | 107.18 | 109.40 |
| 2 | A | 901 | AGS | O2G-PG-O3B | 2.13 | 111.74 | 104.64 |
| 2 | B | 901 | AGS | C3'-C2'-C1' | 2.09 | 104.13 | 100.98 |
| 2 | C | 901 | AGS | C4-C5-N7 | -2.07 | 107.24 | 109.40 |
| 2 | E | 902 | AGS | C4-C5-N7 | -2.07 | 107.24 | 109.40 |
| 2 | D | 902 | AGS | O4'-C4'-C3' | 2.07 | 109.21 | 105.11 |
| 2 | D | 901 | AGS | O4'-C4'-C3' | 2.07 | 109.20 | 105.11 |
| 2 | B | 901 | AGS | C4-C5-N7 | -2.06 | 107.25 | 109.40 |
| 2 | D | 901 | AGS | C4-C5-N7 | -2.06 | 107.25 | 109.40 |
| 2 | F | 902 | AGS | O4'-C4'-C3' | 2.05 | 109.17 | 105.11 |

There are no chirality outliers.

All (58) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 2 | E | 901 | AGS | PB-O3B-PG-O2G |
| 2 | E | 901 | AGS | PB-O3B-PG-O3G |
| 2 | E | 901 | AGS | C5'-O5'-PA-O2A |
| 2 | E | 901 | AGS | C5'-O5'-PA-O3A |
| 2 | E | 901 | AGS | O4'-C4'-C5'-O5' |
| 2 | D | 902 | AGS | O4'-C4'-C5'-O5' |
| 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 | A | 901 | AGS | PB-O3B-PG-O2G |
| 2 | A | 901 | AGS | PB-O3B-PG-O3G |
| 2 | B | 901 | AGS | PB-O3B-PG-O2G |
| 2 | B | 901 | AGS | PB-O3B-PG-O3G |
| 2 | B | 902 | AGS | PB-O3B-PG-O2G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 2 | B | 902 | AGS | PB-O3B-PG-O3G |
| 2 | B | 902 | AGS | C5'-O5'-PA-O1A |
| 2 | B | 902 | AGS | C5'-O5'-PA-O3A |
| 2 | C | 901 | AGS | PB-O3B-PG-O2G |
| 2 | C | 901 | AGS | C5'-O5'-PA-O2A |
| 2 | C | 902 | AGS | C5'-O5'-PA-O2A |
| 2 | C | 902 | AGS | C5'-O5'-PA-O3A |
| 2 | D | 901 | AGS | PB-O3B-PG-O2G |
| 2 | D | 901 | AGS | PB-O3B-PG-O3G |
| 2 | D | 901 | AGS | C5'-O5'-PA-O2A |
| 2 | D | 901 | AGS | C5'-O5'-PA-O3A |
| 2 | F | 901 | AGS | PB-O3B-PG-O2G |
| 2 | F | 901 | AGS | PB-O3B-PG-O3G |
| 2 | E | 901 | AGS | C3'-C4'-C5'-O5' |
| 2 | D | 902 | AGS | C3'-C4'-C5'-O5' |
| 2 | E | 902 | AGS | O4'-C4'-C5'-O5' |
| 2 | B | 902 | AGS | O4'-C4'-C5'-O5' |
| 2 | B | 902 | AGS | C3'-C4'-C5'-O5' |
| 2 | C | 901 | AGS | O4'-C4'-C5'-O5' |
| 2 | C | 901 | AGS | C3'-C4'-C5'-O5' |
| 2 | D | 901 | AGS | O4'-C4'-C5'-O5' |
| 2 | F | 902 | AGS | O4'-C4'-C5'-O5' |
| 2 | D | 901 | AGS | C3'-C4'-C5'-O5' |
| 2 | A | 902 | AGS | O4'-C4'-C5'-O5' |
| 2 | A | 902 | AGS | C3'-C4'-C5'-O5' |
| 2 | E | 902 | AGS | C3'-C4'-C5'-O5' |
| 2 | B | 901 | AGS | O4'-C4'-C5'-O5' |
| 2 | A | 902 | AGS | PA-O3A-PB-O1B |
| 2 | B | 901 | AGS | C3'-C4'-C5'-O5' |
| 2 | C | 901 | AGS | C5'-O5'-PA-O3A |
| 2 | C | 901 | AGS | C5'-O5'-PA-O1A |
| 2 | C | 902 | AGS | C5'-O5'-PA-O1A |
| 2 | D | 901 | AGS | C5'-O5'-PA-O1A |
| 2 | E | 901 | AGS | PG-O3B-PB-O2B |
| 2 | C | 901 | AGS | PG-O3B-PB-O2B |
| 2 | D | 901 | AGS | PG-O3B-PB-O2B |
| 2 | B | 901 | AGS | PA-O3A-PB-O2B |
| 2 | C | 901 | AGS | PB-O3A-PA-O2A |
| 2 | D | 901 | AGS | PB-O3A-PA-O2A |
| 2 | B | 902 | AGS | PG-O3B-PB-O1B |
| 2 | C | 901 | AGS | PB-O3B-PG-O3G |
| 2 | C | 901 | AGS | PB-O3A-PA-O1A |

Continued on next page...

Continued from previous page...

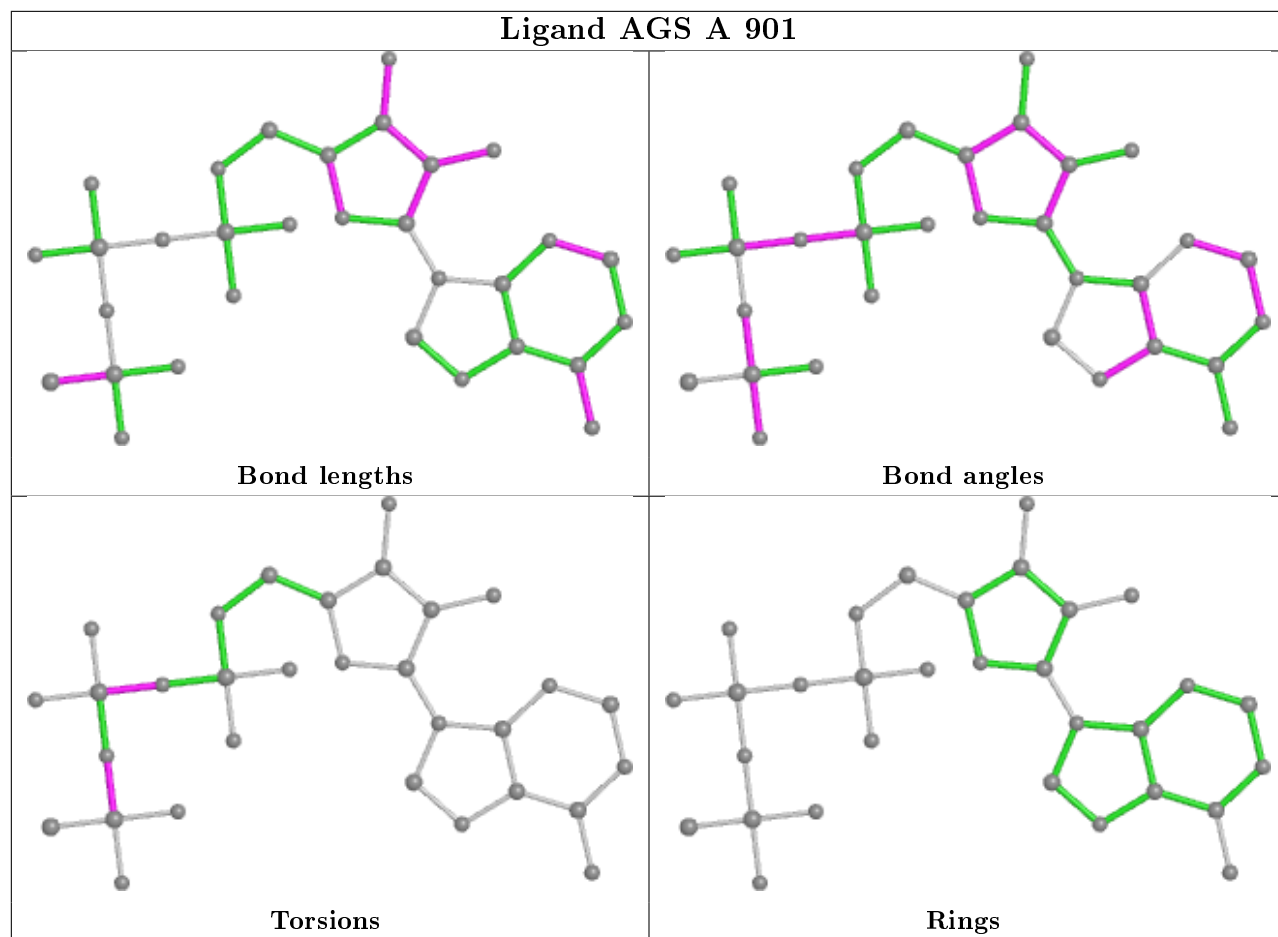
| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|---------------|
| 2 | A | 901 | AGS | PA-O3A-PB-O1B |
| 2 | D | 901 | AGS | PB-O3A-PA-O1A |

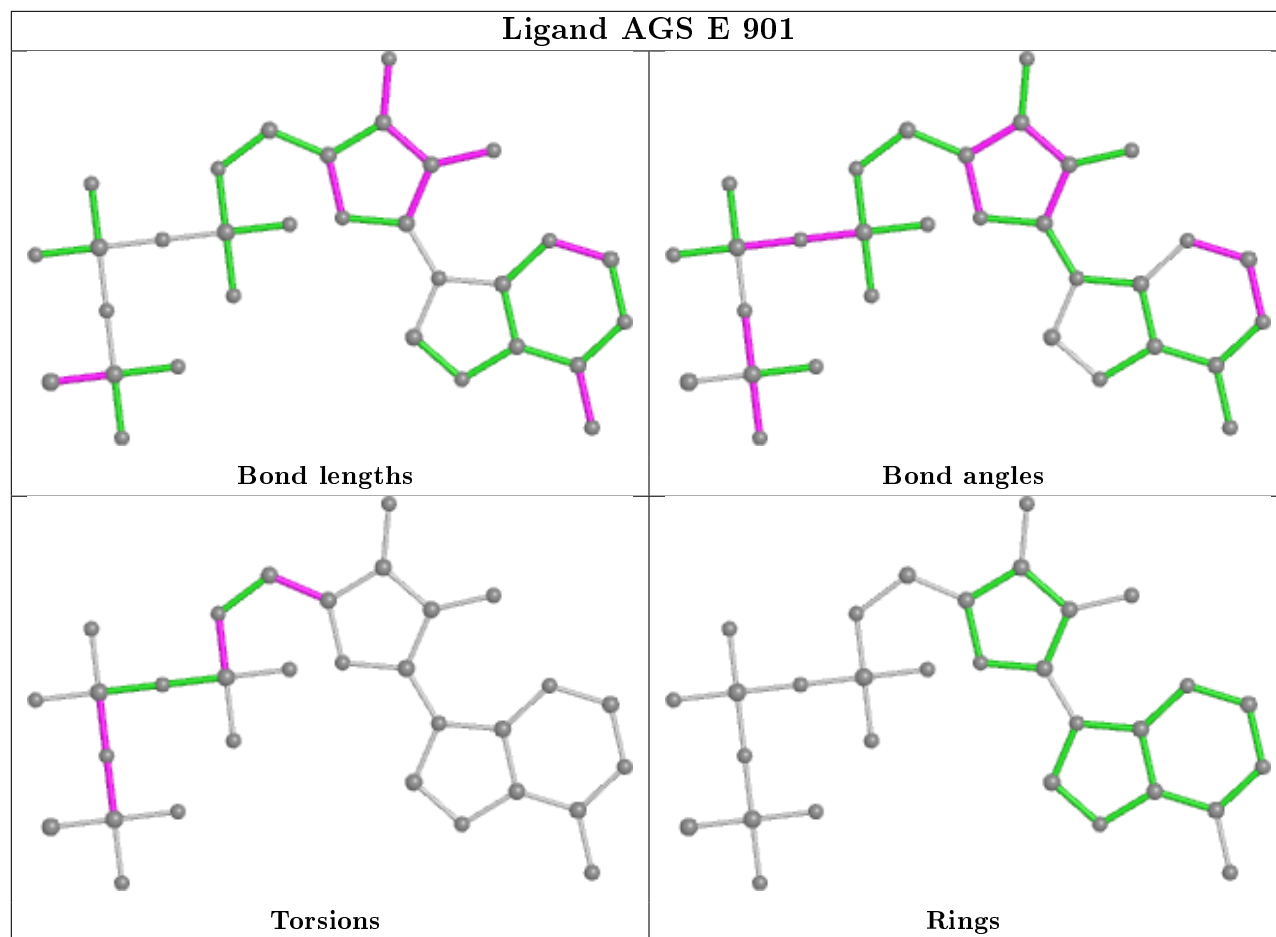
There are no ring outliers.

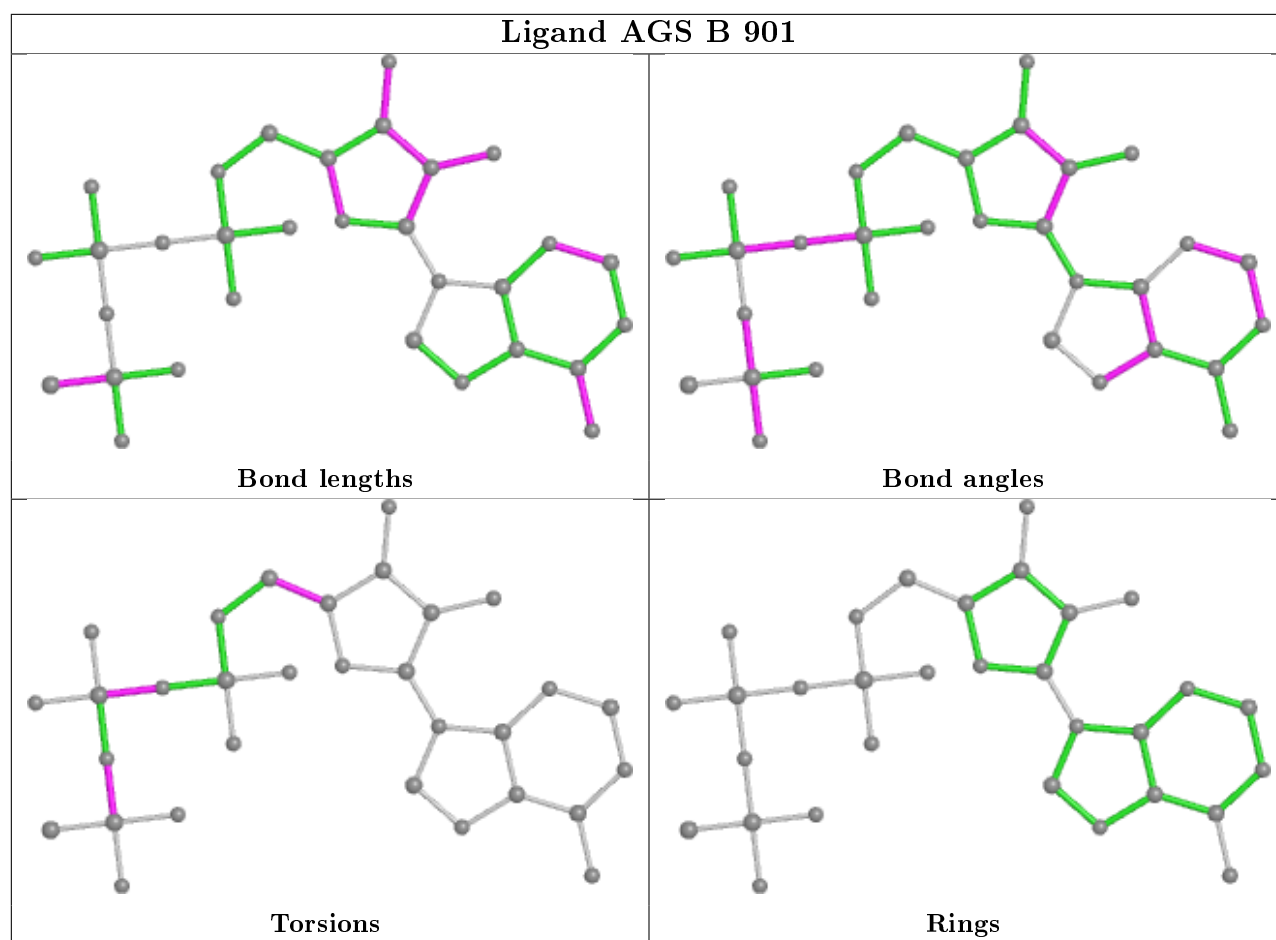
6 monomers are involved in 9 short contacts:

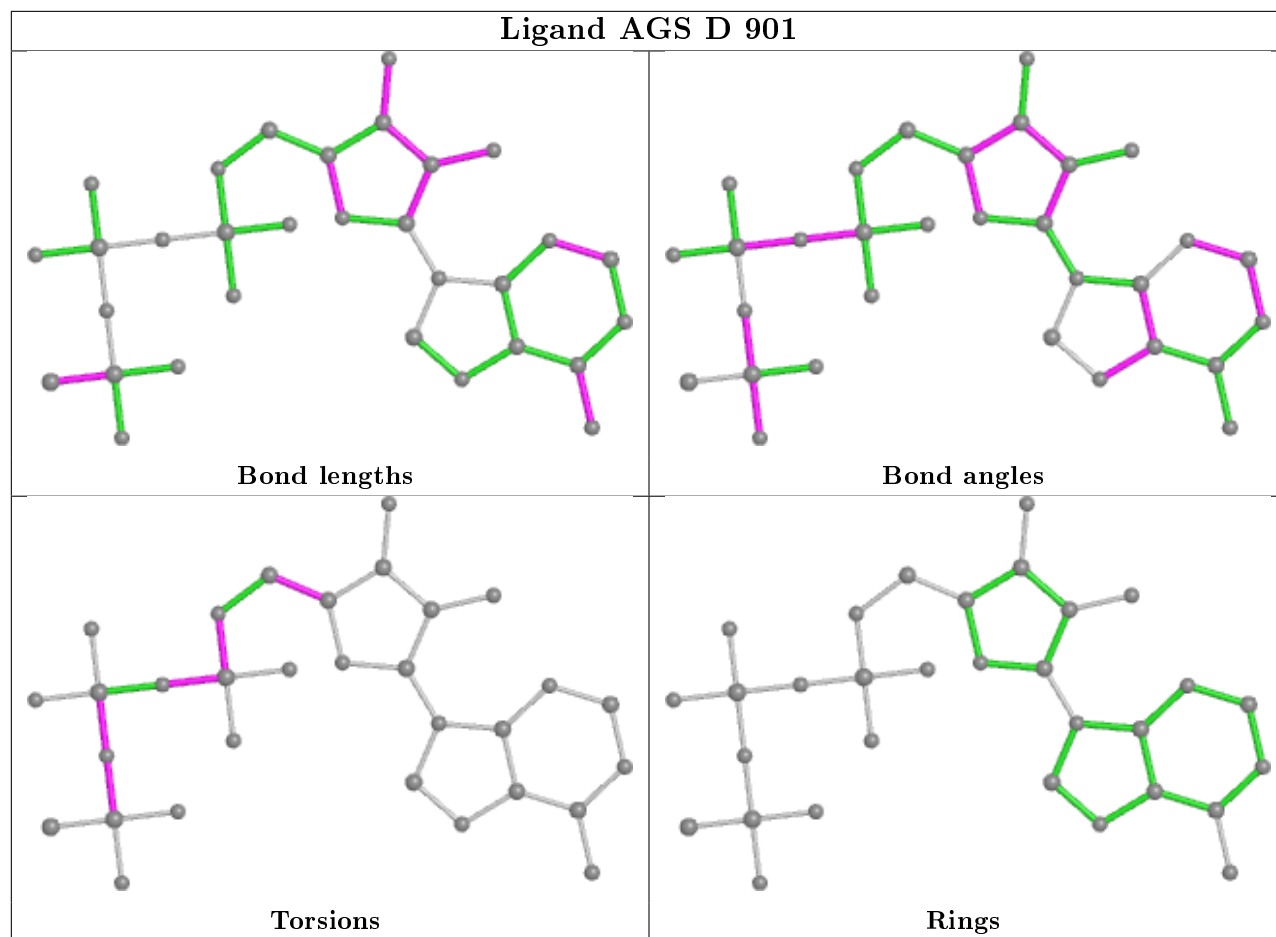
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2 | A | 901 | AGS | 1 | 0 |
| 2 | B | 901 | AGS | 2 | 0 |
| 2 | B | 902 | AGS | 1 | 0 |
| 2 | A | 902 | AGS | 1 | 0 |
| 2 | F | 902 | AGS | 2 | 0 |
| 2 | E | 902 | AGS | 2 | 0 |

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 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.

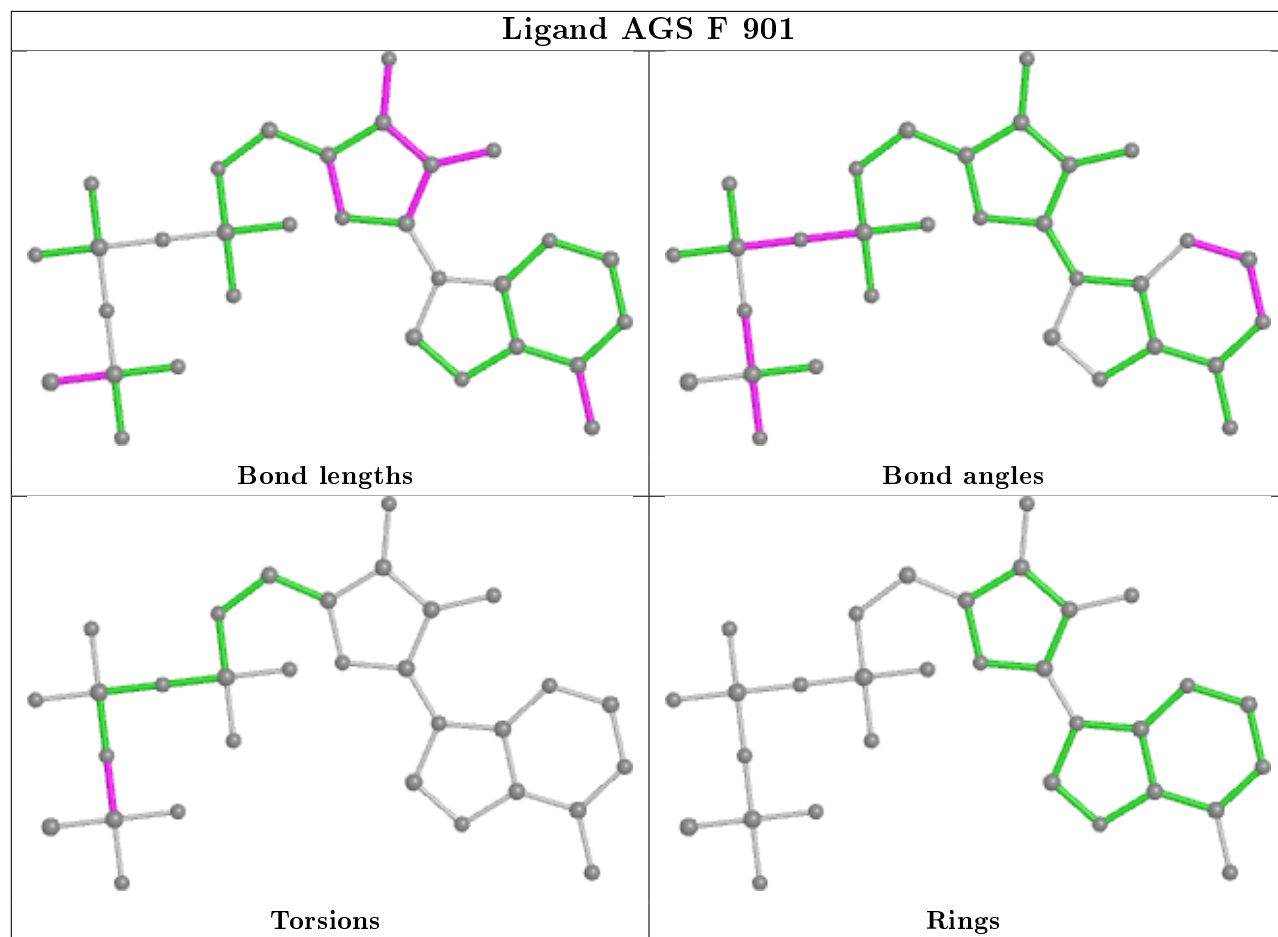


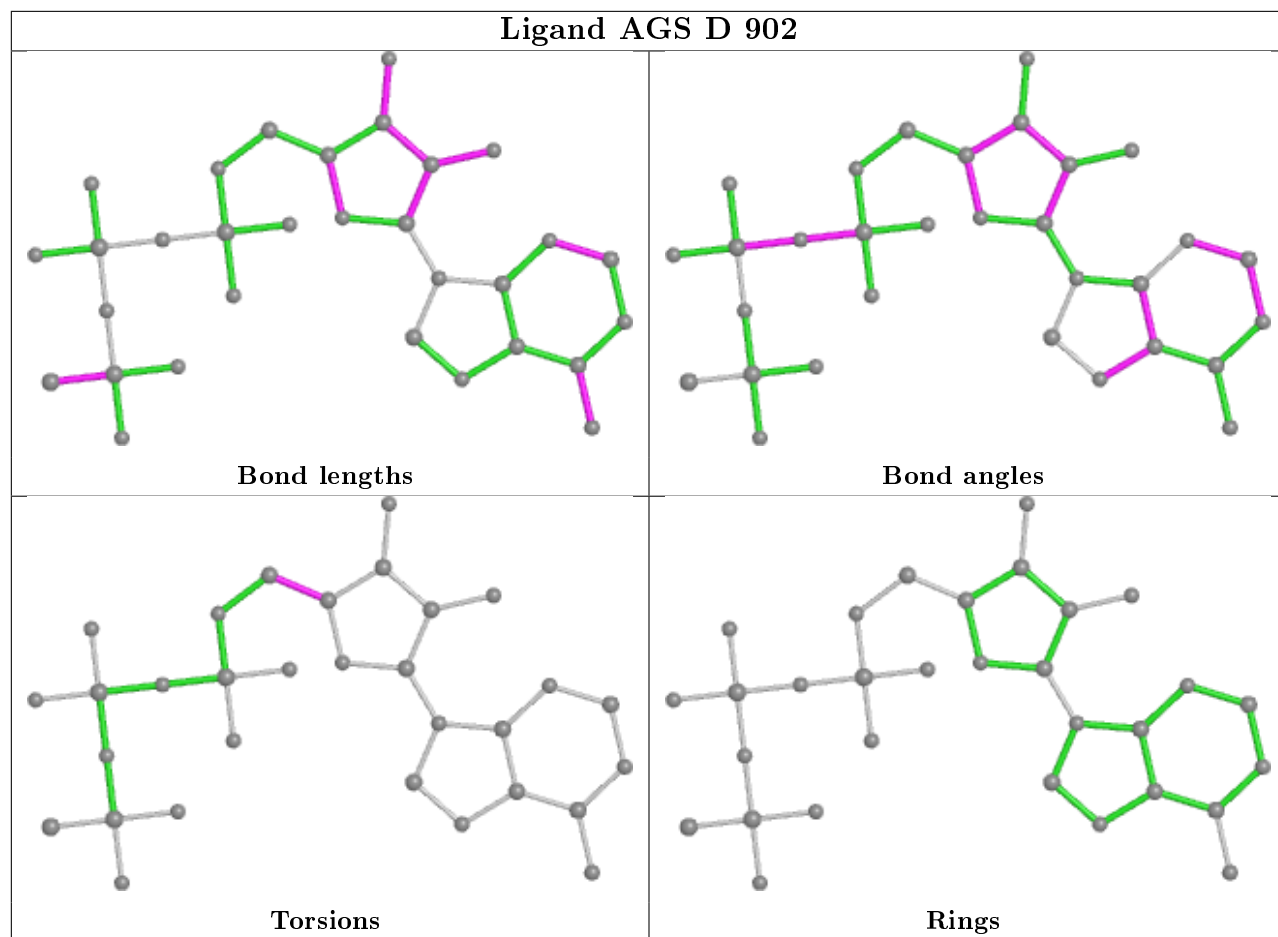


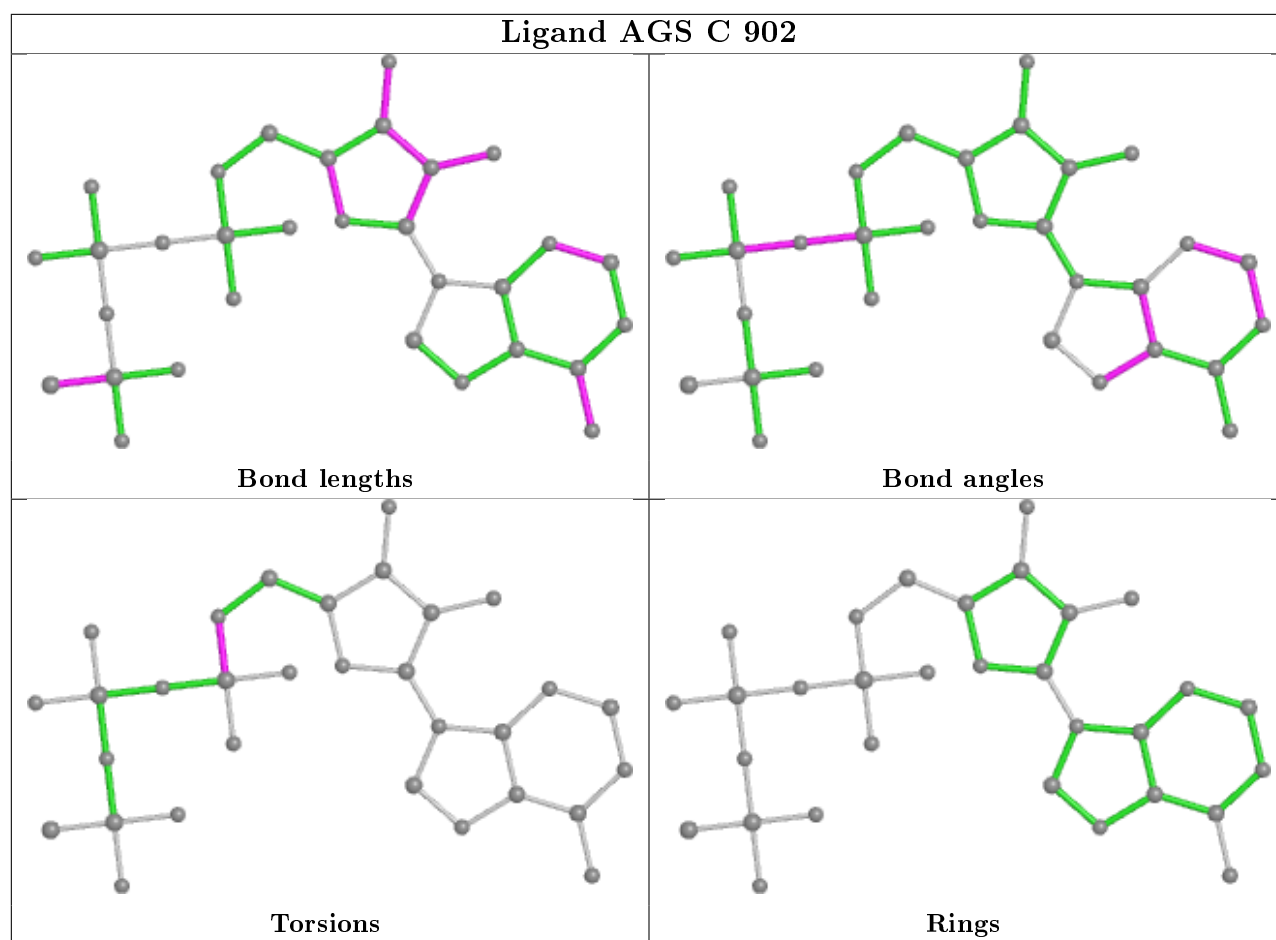


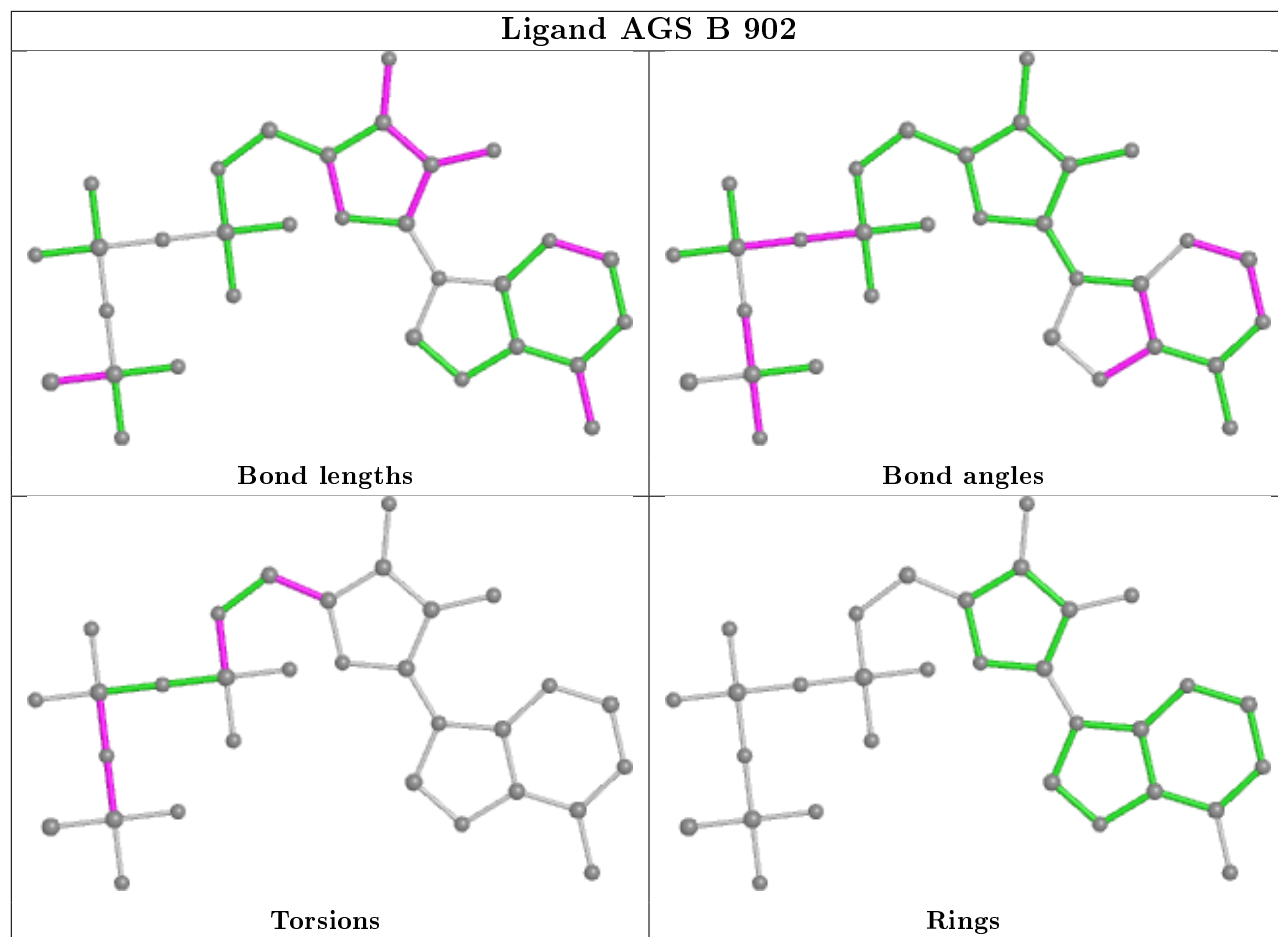


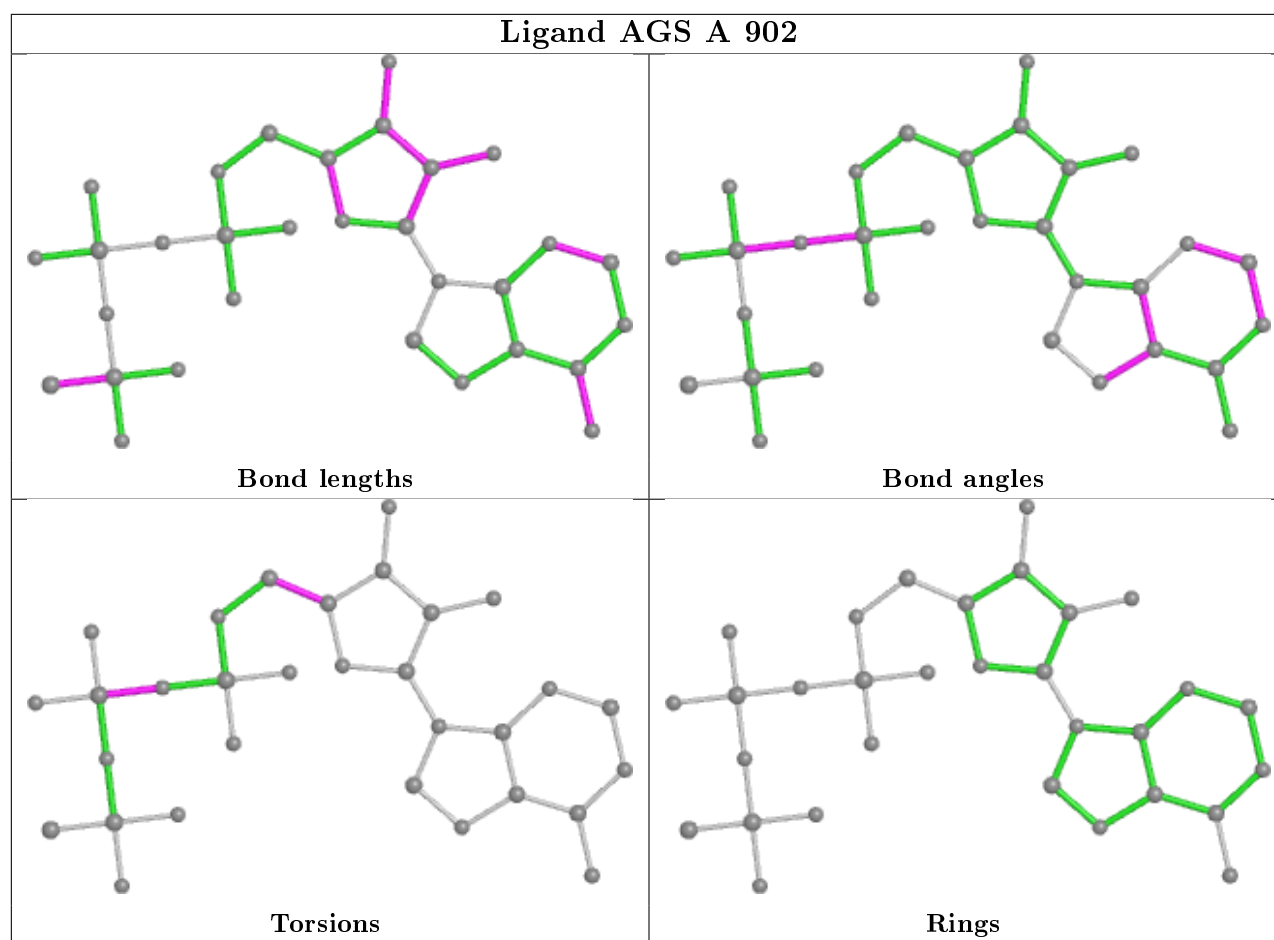
Ligand AGS F 901

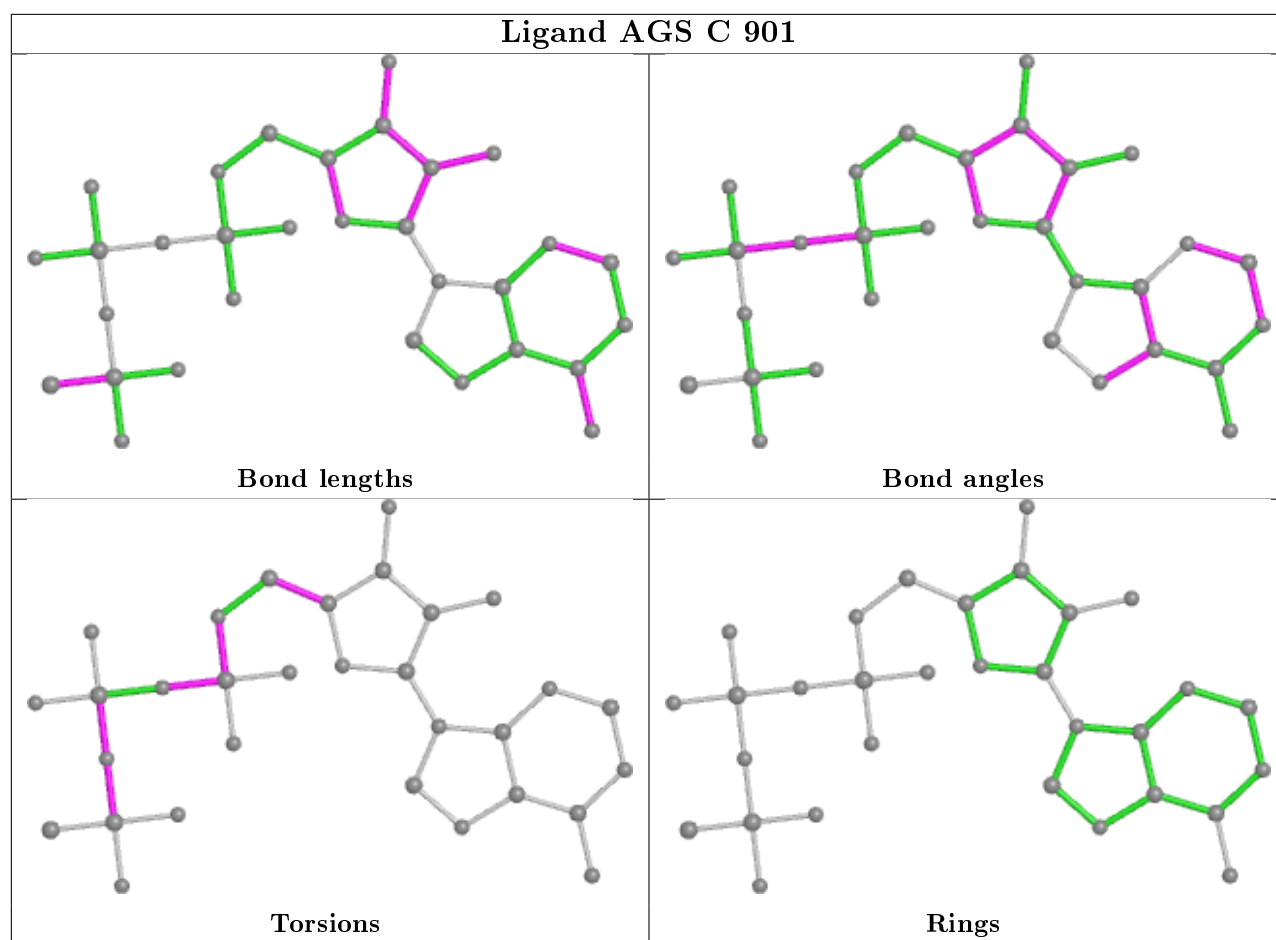


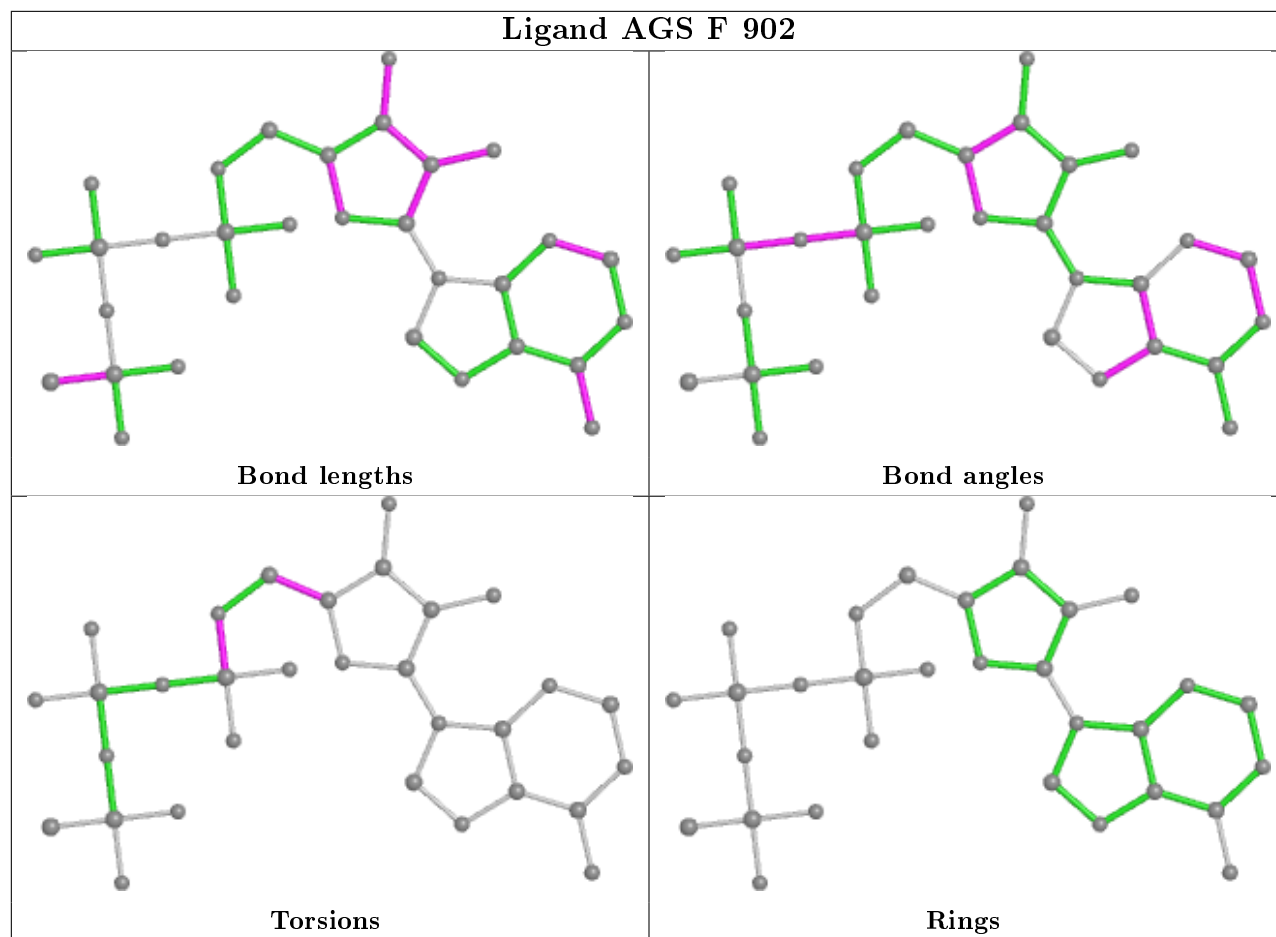


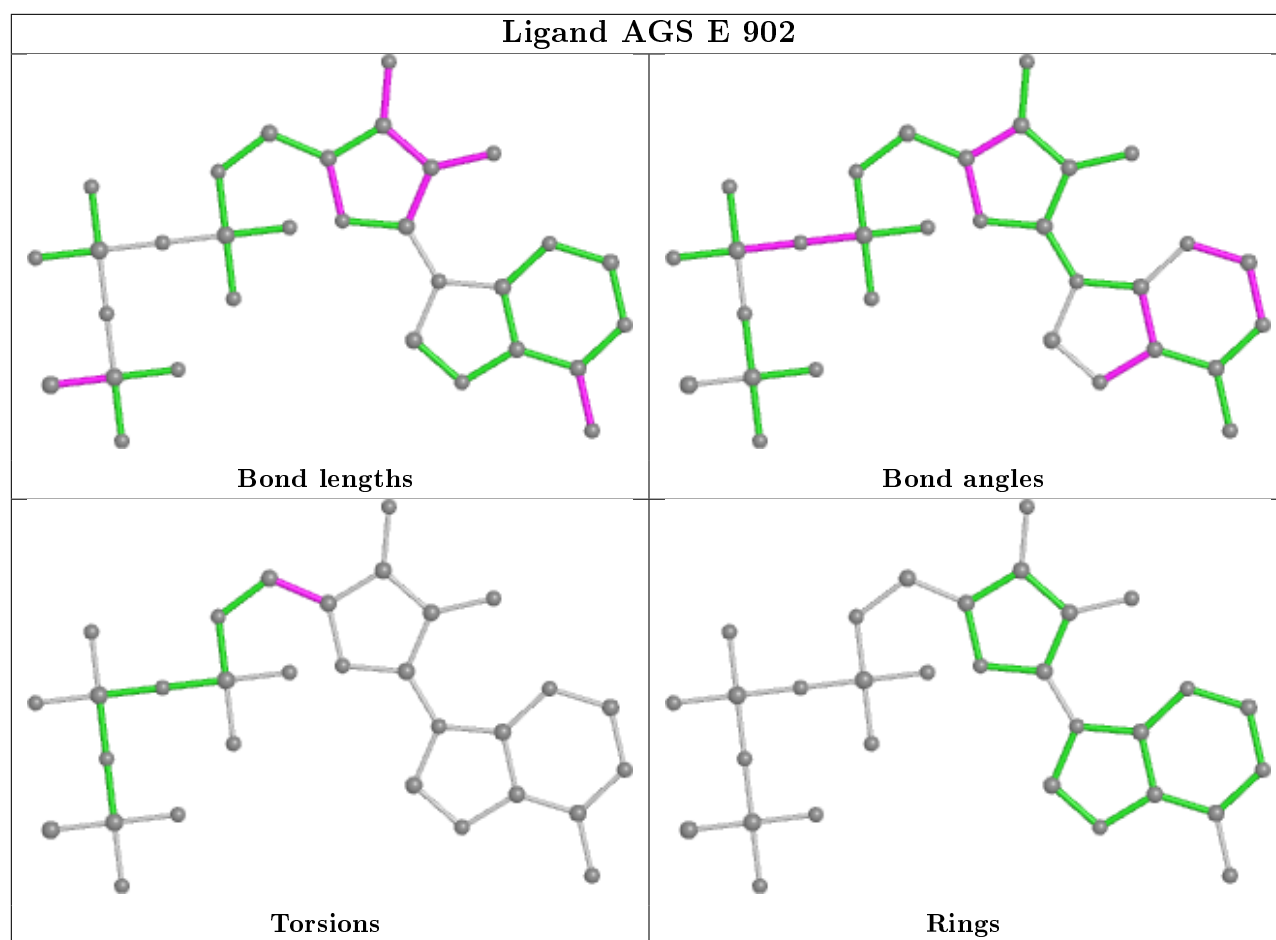












5.7 Other polymers [i](#)

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 | 722/785 (91%) | 0.94 | 112 (15%) 2 2 | 53, 121, 220, 294 | 0 |
| 1 | B | 723/785 (92%) | 0.55 | 40 (5%) 25 23 | 53, 108, 176, 299 | 0 |
| 1 | C | 724/785 (92%) | 0.60 | 69 (9%) 8 8 | 42, 113, 191, 278 | 0 |
| 1 | D | 722/785 (91%) | 0.83 | 108 (14%) 2 2 | 53, 135, 220, 266 | 0 |
| 1 | E | 723/785 (92%) | 0.59 | 52 (7%) 15 15 | 63, 113, 181, 272 | 0 |
| 1 | F | 724/785 (92%) | 0.93 | 113 (15%) 2 2 | 47, 122, 233, 304 | 0 |
| All | All | 4338/4710 (92%) | 0.74 | 494 (11%) 5 4 | 42, 117, 213, 304 | 0 |

All (494) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | F | 116 | VAL | 11.9 |
| 1 | F | 24 | ASN | 9.8 |
| 1 | F | 114 | ILE | 8.9 |
| 1 | F | 102 | ILE | 7.5 |
| 1 | D | 46 | MET | 7.4 |
| 1 | A | 435 | GLU | 7.1 |
| 1 | A | 117 | LEU | 7.0 |
| 1 | D | 26 | LEU | 7.0 |
| 1 | A | 23 | PRO | 6.9 |
| 1 | F | 164 | LYS | 6.9 |
| 1 | F | 174 | CYS | 6.7 |
| 1 | A | 21 | ASN | 6.5 |
| 1 | D | 173 | TYR | 6.3 |
| 1 | D | 41 | LEU | 6.2 |
| 1 | D | 40 | SER | 6.1 |
| 1 | F | 117 | LEU | 6.0 |
| 1 | F | 76 | THR | 6.0 |
| 1 | A | 134 | TYR | 5.8 |
| 1 | D | 71 | VAL | 5.7 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 114 | ILE | 5.7 |
| 1 | C | 23 | PRO | 5.5 |
| 1 | D | 21 | ASN | 5.5 |
| 1 | A | 174 | CYS | 5.4 |
| 1 | A | 26 | LEU | 5.4 |
| 1 | E | 317 | HIS | 5.4 |
| 1 | F | 166 | VAL | 5.4 |
| 1 | A | 53 | ARG | 5.3 |
| 1 | D | 43 | GLN | 5.2 |
| 1 | A | 175 | ILE | 5.2 |
| 1 | B | 552 | PHE | 5.2 |
| 1 | F | 134 | TYR | 5.1 |
| 1 | D | 57 | VAL | 5.1 |
| 1 | A | 390 | LEU | 5.1 |
| 1 | F | 103 | GLN | 5.1 |
| 1 | F | 173 | TYR | 5.0 |
| 1 | F | 41 | LEU | 5.0 |
| 1 | D | 116 | VAL | 5.0 |
| 1 | F | 589 | ASN | 5.0 |
| 1 | C | 21 | ASN | 5.0 |
| 1 | D | 25 | ARG | 4.9 |
| 1 | D | 53 | ARG | 4.9 |
| 1 | A | 47 | ASP | 4.9 |
| 1 | B | 445 | LEU | 4.8 |
| 1 | D | 162 | GLU | 4.8 |
| 1 | F | 111 | GLY | 4.8 |
| 1 | D | 114 | ILE | 4.8 |
| 1 | F | 194 | GLU | 4.8 |
| 1 | F | 94 | VAL | 4.8 |
| 1 | F | 52 | PHE | 4.8 |
| 1 | D | 24 | ASN | 4.7 |
| 1 | A | 116 | VAL | 4.7 |
| 1 | F | 183 | HIS | 4.7 |
| 1 | F | 707 | ILE | 4.7 |
| 1 | B | 21 | ASN | 4.6 |
| 1 | D | 94 | VAL | 4.6 |
| 1 | A | 433 | GLU | 4.6 |
| 1 | F | 115 | HIS | 4.6 |
| 1 | F | 21 | ASN | 4.6 |
| 1 | D | 188 | PRO | 4.5 |
| 1 | F | 43 | GLN | 4.5 |
| 1 | D | 117 | LEU | 4.4 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | A | 703 | ILE | 4.4 |
| 1 | C | 26 | LEU | 4.4 |
| 1 | E | 72 | LEU | 4.4 |
| 1 | D | 165 | VAL | 4.3 |
| 1 | D | 672 | LEU | 4.3 |
| 1 | F | 182 | ILE | 4.3 |
| 1 | A | 186 | GLY | 4.3 |
| 1 | B | 102 | ILE | 4.3 |
| 1 | F | 44 | PRO | 4.3 |
| 1 | D | 47 | ASP | 4.3 |
| 1 | B | 44 | PRO | 4.3 |
| 1 | D | 442 | MET | 4.3 |
| 1 | A | 44 | PRO | 4.3 |
| 1 | D | 69 | CYS | 4.2 |
| 1 | C | 694 | ALA | 4.2 |
| 1 | E | 433 | GLU | 4.2 |
| 1 | F | 187 | GLU | 4.2 |
| 1 | D | 194 | GLU | 4.2 |
| 1 | C | 73 | SER | 4.1 |
| 1 | D | 708 | ARG | 4.1 |
| 1 | C | 699 | ILE | 4.1 |
| 1 | D | 118 | PRO | 4.1 |
| 1 | F | 113 | ARG | 4.1 |
| 1 | D | 23 | PRO | 4.1 |
| 1 | A | 130 | LEU | 4.1 |
| 1 | A | 729 | PRO | 4.1 |
| 1 | D | 52 | PHE | 4.0 |
| 1 | A | 182 | ILE | 4.0 |
| 1 | C | 72 | LEU | 4.0 |
| 1 | D | 56 | THR | 4.0 |
| 1 | A | 436 | THR | 4.0 |
| 1 | D | 187 | GLU | 4.0 |
| 1 | C | 43 | GLN | 4.0 |
| 1 | E | 50 | GLN | 4.0 |
| 1 | F | 175 | ILE | 4.0 |
| 1 | C | 666 | VAL | 4.0 |
| 1 | A | 702 | SER | 3.9 |
| 1 | A | 316 | THR | 3.9 |
| 1 | F | 172 | PRO | 3.9 |
| 1 | A | 735 | HIS | 3.9 |
| 1 | D | 480 | GLY | 3.9 |
| 1 | B | 551 | TRP | 3.9 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | F | 128 | GLY | 3.8 |
| 1 | F | 452 | PHE | 3.8 |
| 1 | A | 72 | LEU | 3.8 |
| 1 | A | 731 | ILE | 3.8 |
| 1 | D | 163 | PHE | 3.8 |
| 1 | A | 187 | GLU | 3.8 |
| 1 | C | 702 | SER | 3.8 |
| 1 | C | 697 | LEU | 3.8 |
| 1 | F | 109 | LYS | 3.8 |
| 1 | F | 179 | ASP | 3.7 |
| 1 | D | 164 | LYS | 3.7 |
| 1 | A | 41 | LEU | 3.7 |
| 1 | C | 672 | LEU | 3.7 |
| 1 | B | 47 | ASP | 3.7 |
| 1 | F | 63 | LYS | 3.7 |
| 1 | A | 57 | VAL | 3.7 |
| 1 | A | 25 | ARG | 3.7 |
| 1 | D | 182 | ILE | 3.7 |
| 1 | F | 77 | CYS | 3.7 |
| 1 | D | 439 | ALA | 3.6 |
| 1 | F | 40 | SER | 3.6 |
| 1 | D | 502 | LYS | 3.6 |
| 1 | E | 49 | LEU | 3.6 |
| 1 | D | 150 | ASP | 3.6 |
| 1 | A | 185 | GLU | 3.6 |
| 1 | D | 51 | LEU | 3.6 |
| 1 | A | 102 | ILE | 3.6 |
| 1 | D | 731 | ILE | 3.6 |
| 1 | B | 502 | LYS | 3.6 |
| 1 | D | 104 | PRO | 3.6 |
| 1 | E | 731 | ILE | 3.6 |
| 1 | F | 57 | VAL | 3.6 |
| 1 | B | 506 | PHE | 3.6 |
| 1 | F | 23 | PRO | 3.6 |
| 1 | A | 434 | ASP | 3.6 |
| 1 | D | 82 | ILE | 3.5 |
| 1 | F | 82 | ILE | 3.5 |
| 1 | D | 316 | THR | 3.5 |
| 1 | A | 127 | THR | 3.5 |
| 1 | A | 188 | PRO | 3.5 |
| 1 | E | 435 | GLU | 3.5 |
| 1 | E | 126 | ILE | 3.5 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 50 | GLN | 3.5 |
| 1 | D | 55 | ASP | 3.5 |
| 1 | C | 44 | PRO | 3.5 |
| 1 | C | 731 | ILE | 3.5 |
| 1 | F | 434 | ASP | 3.5 |
| 1 | C | 81 | LYS | 3.5 |
| 1 | F | 165 | VAL | 3.5 |
| 1 | C | 703 | ILE | 3.5 |
| 1 | A | 705 | SER | 3.5 |
| 1 | E | 26 | LEU | 3.5 |
| 1 | D | 129 | ASN | 3.4 |
| 1 | F | 48 | GLU | 3.4 |
| 1 | D | 191 | ARG | 3.4 |
| 1 | E | 64 | ARG | 3.4 |
| 1 | D | 73 | SER | 3.4 |
| 1 | F | 73 | SER | 3.4 |
| 1 | A | 52 | PHE | 3.4 |
| 1 | C | 736 | PHE | 3.4 |
| 1 | E | 434 | ASP | 3.4 |
| 1 | E | 447 | VAL | 3.4 |
| 1 | A | 40 | SER | 3.4 |
| 1 | F | 71 | VAL | 3.4 |
| 1 | F | 167 | GLU | 3.4 |
| 1 | E | 44 | PRO | 3.3 |
| 1 | A | 736 | PHE | 3.3 |
| 1 | D | 100 | ILE | 3.3 |
| 1 | F | 612 | SER | 3.3 |
| 1 | A | 176 | VAL | 3.3 |
| 1 | F | 26 | LEU | 3.3 |
| 1 | F | 170 | PRO | 3.3 |
| 1 | C | 428 | ASP | 3.3 |
| 1 | A | 446 | ALA | 3.3 |
| 1 | D | 102 | ILE | 3.3 |
| 1 | D | 495 | TYR | 3.3 |
| 1 | A | 389 | LYS | 3.3 |
| 1 | C | 682 | PHE | 3.3 |
| 1 | A | 184 | CYS | 3.3 |
| 1 | F | 50 | GLN | 3.3 |
| 1 | C | 552 | PHE | 3.3 |
| 1 | E | 552 | PHE | 3.3 |
| 1 | A | 43 | GLN | 3.3 |
| 1 | F | 316 | THR | 3.3 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | C | 705 | SER | 3.2 |
| 1 | A | 708 | ARG | 3.2 |
| 1 | C | 42 | SER | 3.2 |
| 1 | D | 189 | ILE | 3.2 |
| 1 | D | 99 | VAL | 3.2 |
| 1 | F | 62 | LYS | 3.2 |
| 1 | B | 337 | GLN | 3.2 |
| 1 | A | 501 | ASP | 3.2 |
| 1 | A | 145 | PRO | 3.2 |
| 1 | D | 153 | LEU | 3.2 |
| 1 | C | 708 | ARG | 3.2 |
| 1 | F | 233 | ILE | 3.1 |
| 1 | D | 50 | GLN | 3.1 |
| 1 | F | 75 | ASP | 3.1 |
| 1 | A | 183 | HIS | 3.1 |
| 1 | A | 193 | ASP | 3.1 |
| 1 | A | 699 | ILE | 3.1 |
| 1 | E | 81 | LYS | 3.1 |
| 1 | A | 113 | ARG | 3.1 |
| 1 | D | 131 | PHE | 3.1 |
| 1 | E | 43 | GLN | 3.1 |
| 1 | F | 426 | LYS | 3.1 |
| 1 | A | 82 | ILE | 3.1 |
| 1 | A | 707 | ILE | 3.1 |
| 1 | B | 134 | TYR | 3.0 |
| 1 | F | 100 | ILE | 3.0 |
| 1 | A | 506 | PHE | 3.0 |
| 1 | D | 172 | PRO | 3.0 |
| 1 | D | 193 | ASP | 3.0 |
| 1 | A | 432 | LEU | 3.0 |
| 1 | C | 675 | LEU | 3.0 |
| 1 | F | 78 | SER | 3.0 |
| 1 | D | 119 | ILE | 3.0 |
| 1 | A | 100 | ILE | 3.0 |
| 1 | C | 695 | CYS | 3.0 |
| 1 | C | 698 | ALA | 3.0 |
| 1 | D | 426 | LYS | 3.0 |
| 1 | E | 747 | VAL | 3.0 |
| 1 | E | 439 | ALA | 2.9 |
| 1 | B | 230 | PHE | 2.9 |
| 1 | A | 162 | GLU | 2.9 |
| 1 | C | 706 | GLU | 2.9 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | F | 231 | LYS | 2.9 |
| 1 | D | 499 | HIS | 2.9 |
| 1 | D | 78 | SER | 2.9 |
| 1 | F | 443 | ASN | 2.9 |
| 1 | A | 68 | VAL | 2.9 |
| 1 | F | 47 | ASP | 2.9 |
| 1 | C | 143 | TYR | 2.9 |
| 1 | C | 41 | LEU | 2.9 |
| 1 | C | 71 | VAL | 2.9 |
| 1 | C | 707 | ILE | 2.9 |
| 1 | B | 446 | ALA | 2.9 |
| 1 | B | 41 | LEU | 2.9 |
| 1 | F | 322 | ARG | 2.9 |
| 1 | D | 92 | LEU | 2.9 |
| 1 | F | 46 | MET | 2.9 |
| 1 | F | 70 | ILE | 2.8 |
| 1 | F | 148 | LYS | 2.8 |
| 1 | F | 168 | THR | 2.8 |
| 1 | C | 735 | HIS | 2.8 |
| 1 | D | 161 | VAL | 2.8 |
| 1 | F | 176 | VAL | 2.8 |
| 1 | B | 105 | CYS | 2.8 |
| 1 | A | 104 | PRO | 2.8 |
| 1 | F | 393 | ASP | 2.8 |
| 1 | A | 439 | ALA | 2.8 |
| 1 | C | 472 | PRO | 2.8 |
| 1 | A | 103 | GLN | 2.8 |
| 1 | D | 503 | PHE | 2.8 |
| 1 | A | 64 | ARG | 2.8 |
| 1 | C | 668 | LYS | 2.8 |
| 1 | D | 147 | ARG | 2.8 |
| 1 | C | 670 | VAL | 2.8 |
| 1 | D | 28 | VAL | 2.8 |
| 1 | D | 166 | VAL | 2.8 |
| 1 | D | 176 | VAL | 2.8 |
| 1 | F | 123 | VAL | 2.7 |
| 1 | C | 100 | ILE | 2.7 |
| 1 | A | 161 | VAL | 2.7 |
| 1 | C | 82 | ILE | 2.7 |
| 1 | A | 22 | ARG | 2.7 |
| 1 | D | 452 | PHE | 2.7 |
| 1 | A | 428 | ASP | 2.7 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | C | 25 | ARG | 2.7 |
| 1 | A | 83 | ARG | 2.7 |
| 1 | F | 706 | GLU | 2.7 |
| 1 | F | 131 | PHE | 2.7 |
| 1 | A | 151 | ILE | 2.7 |
| 1 | B | 554 | GLU | 2.7 |
| 1 | F | 104 | PRO | 2.7 |
| 1 | F | 232 | ALA | 2.7 |
| 1 | B | 672 | LEU | 2.7 |
| 1 | B | 126 | ILE | 2.7 |
| 1 | E | 551 | TRP | 2.6 |
| 1 | E | 452 | PHE | 2.6 |
| 1 | C | 182 | ILE | 2.6 |
| 1 | C | 51 | LEU | 2.6 |
| 1 | E | 682 | PHE | 2.6 |
| 1 | E | 99 | VAL | 2.6 |
| 1 | F | 25 | ARG | 2.6 |
| 1 | F | 150 | ASP | 2.6 |
| 1 | E | 232 | ALA | 2.6 |
| 1 | B | 553 | GLY | 2.6 |
| 1 | E | 45 | LYS | 2.6 |
| 1 | F | 439 | ALA | 2.6 |
| 1 | A | 51 | LEU | 2.6 |
| 1 | C | 596 | ALA | 2.6 |
| 1 | B | 503 | PHE | 2.6 |
| 1 | A | 706 | GLU | 2.6 |
| 1 | C | 669 | ASP | 2.6 |
| 1 | D | 123 | VAL | 2.6 |
| 1 | E | 520 | PRO | 2.6 |
| 1 | C | 429 | LEU | 2.6 |
| 1 | C | 50 | GLN | 2.6 |
| 1 | D | 93 | ARG | 2.5 |
| 1 | E | 730 | GLU | 2.5 |
| 1 | F | 729 | PRO | 2.5 |
| 1 | C | 667 | ALA | 2.5 |
| 1 | D | 132 | GLU | 2.5 |
| 1 | A | 315 | LYS | 2.5 |
| 1 | C | 696 | LYS | 2.5 |
| 1 | A | 237 | PRO | 2.5 |
| 1 | A | 502 | LYS | 2.5 |
| 1 | E | 322 | ARG | 2.5 |
| 1 | D | 44 | PRO | 2.5 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 504 | LEU | 2.5 |
| 1 | B | 58 | LEU | 2.5 |
| 1 | E | 672 | LEU | 2.5 |
| 1 | A | 694 | ALA | 2.5 |
| 1 | C | 47 | ASP | 2.5 |
| 1 | E | 522 | CYS | 2.5 |
| 1 | A | 388 | MET | 2.5 |
| 1 | B | 28 | VAL | 2.5 |
| 1 | D | 79 | ASP | 2.5 |
| 1 | D | 498 | GLU | 2.5 |
| 1 | E | 130 | LEU | 2.5 |
| 1 | E | 687 | LEU | 2.4 |
| 1 | E | 21 | ASN | 2.4 |
| 1 | E | 47 | ASP | 2.4 |
| 1 | A | 234 | GLY | 2.4 |
| 1 | A | 160 | ALA | 2.4 |
| 1 | A | 500 | PRO | 2.4 |
| 1 | F | 112 | LYS | 2.4 |
| 1 | A | 267 | PHE | 2.4 |
| 1 | D | 446 | ALA | 2.4 |
| 1 | F | 147 | ARG | 2.4 |
| 1 | D | 113 | ARG | 2.4 |
| 1 | E | 51 | LEU | 2.4 |
| 1 | A | 131 | PHE | 2.4 |
| 1 | F | 703 | ILE | 2.4 |
| 1 | B | 340 | HIS | 2.4 |
| 1 | F | 193 | ASP | 2.4 |
| 1 | A | 46 | MET | 2.4 |
| 1 | A | 157 | GLY | 2.4 |
| 1 | A | 552 | PHE | 2.4 |
| 1 | B | 613 | THR | 2.4 |
| 1 | A | 119 | ILE | 2.4 |
| 1 | D | 29 | ASP | 2.4 |
| 1 | A | 92 | LEU | 2.4 |
| 1 | B | 24 | ASN | 2.4 |
| 1 | E | 707 | ILE | 2.4 |
| 1 | F | 99 | VAL | 2.4 |
| 1 | A | 701 | GLU | 2.4 |
| 1 | B | 82 | ILE | 2.4 |
| 1 | F | 83 | ARG | 2.4 |
| 1 | D | 48 | GLU | 2.4 |
| 1 | C | 597 | ALA | 2.4 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | E | 436 | THR | 2.4 |
| 1 | E | 158 | MET | 2.3 |
| 1 | B | 612 | SER | 2.3 |
| 1 | F | 433 | GLU | 2.3 |
| 1 | E | 316 | THR | 2.3 |
| 1 | F | 428 | ASP | 2.3 |
| 1 | B | 435 | GLU | 2.3 |
| 1 | C | 739 | ALA | 2.3 |
| 1 | D | 39 | VAL | 2.3 |
| 1 | E | 186 | GLY | 2.3 |
| 1 | A | 48 | GLU | 2.3 |
| 1 | F | 495 | TYR | 2.3 |
| 1 | F | 97 | GLY | 2.3 |
| 1 | E | 588 | GLY | 2.3 |
| 1 | E | 48 | GLU | 2.3 |
| 1 | F | 192 | GLU | 2.3 |
| 1 | B | 198 | LEU | 2.3 |
| 1 | C | 390 | LEU | 2.3 |
| 1 | F | 79 | ASP | 2.3 |
| 1 | F | 127 | THR | 2.3 |
| 1 | C | 446 | ALA | 2.3 |
| 1 | A | 695 | CYS | 2.3 |
| 1 | E | 42 | SER | 2.3 |
| 1 | E | 127 | THR | 2.3 |
| 1 | A | 164 | LYS | 2.3 |
| 1 | C | 101 | SER | 2.3 |
| 1 | F | 55 | ASP | 2.3 |
| 1 | A | 59 | LEU | 2.3 |
| 1 | A | 396 | LEU | 2.3 |
| 1 | B | 390 | LEU | 2.3 |
| 1 | B | 114 | ILE | 2.3 |
| 1 | D | 404 | HIS | 2.3 |
| 1 | F | 53 | ARG | 2.3 |
| 1 | F | 188 | PRO | 2.3 |
| 1 | A | 101 | SER | 2.3 |
| 1 | B | 232 | ALA | 2.3 |
| 1 | C | 340 | HIS | 2.3 |
| 1 | F | 110 | TYR | 2.3 |
| 1 | D | 130 | LEU | 2.3 |
| 1 | A | 394 | VAL | 2.3 |
| 1 | F | 171 | SER | 2.3 |
| 1 | A | 84 | MET | 2.2 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | E | 119 | ILE | 2.2 |
| 1 | B | 434 | ASP | 2.2 |
| 1 | D | 27 | ILE | 2.2 |
| 1 | A | 39 | VAL | 2.2 |
| 1 | D | 196 | GLU | 2.2 |
| 1 | D | 151 | ILE | 2.2 |
| 1 | D | 699 | ILE | 2.2 |
| 1 | F | 429 | LEU | 2.2 |
| 1 | A | 704 | GLU | 2.2 |
| 1 | D | 435 | GLU | 2.2 |
| 1 | C | 46 | MET | 2.2 |
| 1 | E | 503 | PHE | 2.2 |
| 1 | F | 154 | VAL | 2.2 |
| 1 | F | 199 | ASN | 2.2 |
| 1 | A | 73 | SER | 2.2 |
| 1 | F | 133 | VAL | 2.2 |
| 1 | D | 186 | GLY | 2.2 |
| 1 | A | 135 | LEU | 2.2 |
| 1 | D | 436 | THR | 2.2 |
| 1 | F | 126 | ILE | 2.2 |
| 1 | B | 433 | GLU | 2.2 |
| 1 | A | 696 | LYS | 2.2 |
| 1 | A | 336 | LYS | 2.2 |
| 1 | C | 60 | LYS | 2.2 |
| 1 | D | 62 | LYS | 2.2 |
| 1 | F | 155 | ARG | 2.2 |
| 1 | A | 447 | VAL | 2.2 |
| 1 | D | 126 | ILE | 2.2 |
| 1 | D | 144 | ARG | 2.2 |
| 1 | F | 81 | LYS | 2.2 |
| 1 | D | 705 | SER | 2.2 |
| 1 | A | 141 | GLU | 2.2 |
| 1 | A | 730 | GLU | 2.2 |
| 1 | C | 767 | GLY | 2.2 |
| 1 | A | 503 | PHE | 2.1 |
| 1 | D | 45 | LYS | 2.1 |
| 1 | D | 84 | MET | 2.1 |
| 1 | D | 115 | HIS | 2.1 |
| 1 | F | 321 | GLU | 2.1 |
| 1 | D | 152 | PHE | 2.1 |
| 1 | F | 190 | LYS | 2.1 |
| 1 | F | 266 | PHE | 2.1 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | C | 435 | GLU | 2.1 |
| 1 | D | 49 | LEU | 2.1 |
| 1 | D | 768 | PHE | 2.1 |
| 1 | E | 736 | PHE | 2.1 |
| 1 | F | 163 | PHE | 2.1 |
| 1 | B | 499 | HIS | 2.1 |
| 1 | D | 443 | ASN | 2.1 |
| 1 | C | 663 | LYS | 2.1 |
| 1 | C | 768 | PHE | 2.1 |
| 1 | F | 143 | TYR | 2.1 |
| 1 | C | 588 | GLY | 2.1 |
| 1 | D | 72 | LEU | 2.1 |
| 1 | D | 179 | ASP | 2.1 |
| 1 | D | 479 | ILE | 2.1 |
| 1 | D | 666 | VAL | 2.1 |
| 1 | A | 442 | MET | 2.1 |
| 1 | A | 443 | ASN | 2.1 |
| 1 | B | 439 | ALA | 2.1 |
| 1 | B | 479 | ILE | 2.1 |
| 1 | D | 428 | ASP | 2.1 |
| 1 | D | 139 | PHE | 2.1 |
| 1 | B | 36 | ASN | 2.1 |
| 1 | C | 613 | THR | 2.1 |
| 1 | D | 81 | LYS | 2.1 |
| 1 | F | 320 | VAL | 2.1 |
| 1 | E | 102 | ILE | 2.1 |
| 1 | E | 768 | PHE | 2.0 |
| 1 | F | 317 | HIS | 2.1 |
| 1 | A | 391 | ALA | 2.0 |
| 1 | A | 510 | PRO | 2.0 |
| 1 | C | 199 | ASN | 2.0 |
| 1 | C | 599 | ARG | 2.0 |
| 1 | E | 494 | GLN | 2.0 |
| 1 | E | 612 | SER | 2.0 |
| 1 | A | 132 | GLU | 2.0 |
| 1 | D | 195 | GLU | 2.0 |
| 1 | F | 80 | GLU | 2.0 |
| 1 | E | 59 | LEU | 2.0 |
| 1 | A | 431 | ASP | 2.0 |
| 1 | C | 734 | ASP | 2.0 |
| 1 | C | 704 | GLU | 2.0 |
| 1 | F | 42 | SER | 2.0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 698 | ALA | 2.0 |
| 1 | B | 96 | LEU | 2.0 |
| 1 | B | 753 | ARG | 2.0 |
| 1 | C | 661 | LEU | 2.0 |
| 1 | F | 51 | LEU | 2.0 |
| 1 | F | 708 | ARG | 2.0 |
| 1 | D | 679 | THR | 2.0 |
| 1 | F | 704 | GLU | 2.0 |
| 1 | C | 769 | GLY | 2.0 |
| 1 | E | 703 | ILE | 2.0 |
| 1 | F | 118 | PRO | 2.0 |
| 1 | C | 24 | ASN | 2.0 |
| 1 | C | 28 | 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 carbohydrates 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(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3 | MG | D | 903 | 1/1 | 0.84 | 0.13 | 170,170,170,170 | 0 |
| 4 | CL | F | 905 | 1/1 | 0.86 | 0.31 | 98,98,98,98 | 0 |
| 4 | CL | C | 905 | 1/1 | 0.86 | 0.20 | 117,117,117,117 | 0 |
| 4 | CL | D | 905 | 1/1 | 0.87 | 0.24 | 99,99,99,99 | 0 |
| 4 | CL | B | 905 | 1/1 | 0.88 | 0.23 | 92,92,92,92 | 0 |
| 4 | CL | E | 905 | 1/1 | 0.89 | 0.28 | 93,93,93,93 | 0 |
| 2 | AGS | E | 901 | 31/31 | 0.91 | 0.26 | 76,88,120,170 | 0 |
| 4 | CL | A | 905 | 1/1 | 0.91 | 0.28 | 87,87,87,87 | 0 |
| 3 | MG | A | 903 | 1/1 | 0.94 | 0.12 | 186,186,186,186 | 0 |
| 2 | AGS | B | 901 | 31/31 | 0.94 | 0.24 | 57,88,112,122 | 0 |

Continued on next page...

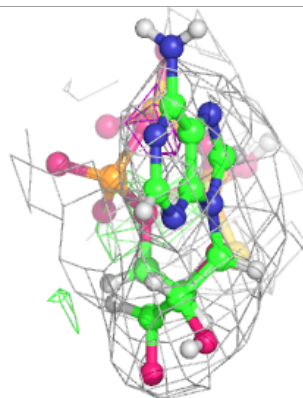
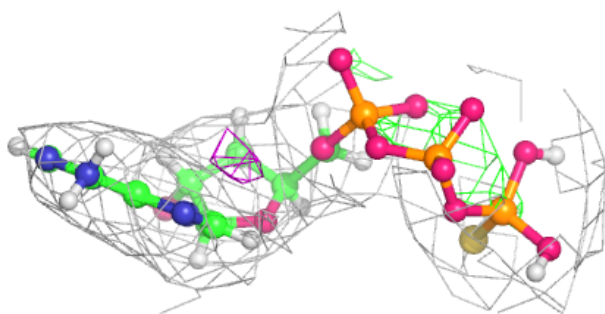
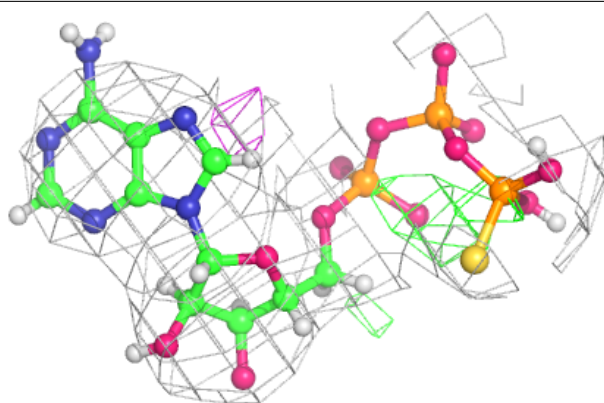
Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2 | AGS | D | 901 | 31/31 | 0.94 | 0.24 | 70,99,121,158 | 0 |
| 2 | AGS | C | 901 | 31/31 | 0.94 | 0.20 | 59,100,122,152 | 0 |
| 2 | AGS | A | 901 | 31/31 | 0.95 | 0.27 | 75,86,104,117 | 0 |
| 2 | AGS | D | 902 | 31/31 | 0.95 | 0.21 | 68,82,106,169 | 0 |
| 2 | AGS | F | 901 | 31/31 | 0.95 | 0.24 | 47,61,80,93 | 0 |
| 2 | AGS | F | 902 | 31/31 | 0.95 | 0.24 | 88,102,133,210 | 0 |
| 3 | MG | F | 904 | 1/1 | 0.96 | 0.27 | 76,76,76,76 | 0 |
| 2 | AGS | E | 902 | 31/31 | 0.96 | 0.20 | 75,89,127,165 | 0 |
| 3 | MG | F | 903 | 1/1 | 0.96 | 0.16 | 152,152,152,152 | 0 |
| 3 | MG | D | 904 | 1/1 | 0.96 | 0.31 | 99,99,99,99 | 0 |
| 2 | AGS | C | 902 | 31/31 | 0.96 | 0.26 | 59,76,122,189 | 0 |
| 3 | MG | A | 904 | 1/1 | 0.97 | 0.23 | 76,76,76,76 | 0 |
| 2 | AGS | B | 902 | 31/31 | 0.97 | 0.23 | 55,79,132,182 | 0 |
| 2 | AGS | A | 902 | 31/31 | 0.97 | 0.26 | 73,90,154,194 | 0 |
| 3 | MG | E | 903 | 1/1 | 0.97 | 0.14 | 81,81,81,81 | 0 |
| 3 | MG | C | 904 | 1/1 | 0.98 | 0.22 | 107,107,107,107 | 0 |
| 3 | MG | B | 903 | 1/1 | 0.98 | 0.17 | 119,119,119,119 | 0 |
| 3 | MG | C | 903 | 1/1 | 0.98 | 0.23 | 101,101,101,101 | 0 |
| 3 | MG | E | 904 | 1/1 | 0.98 | 0.26 | 96,96,96,96 | 0 |
| 3 | MG | B | 904 | 1/1 | 0.98 | 0.22 | 86,86,86,86 | 0 |

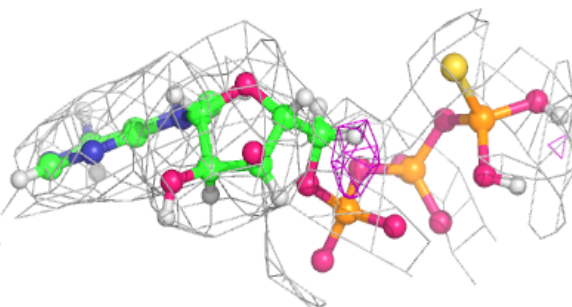
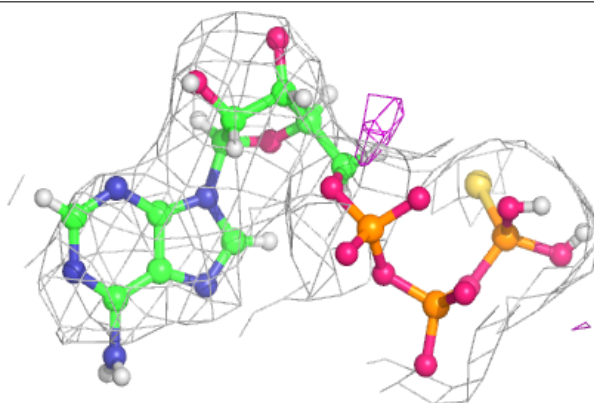
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around AGS E 901:

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

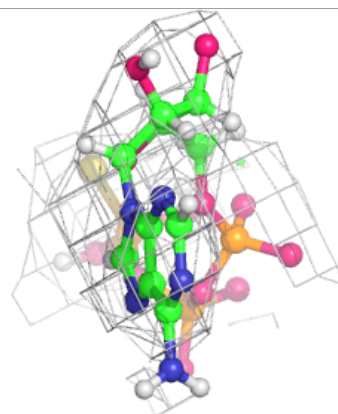
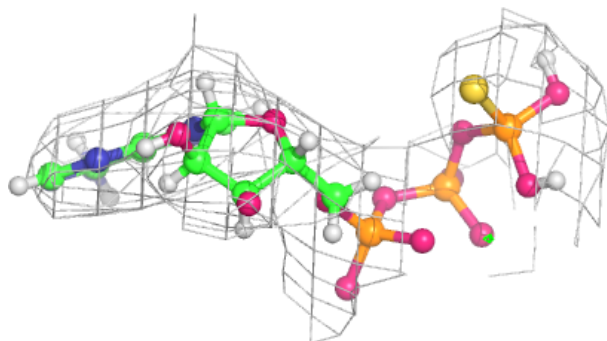
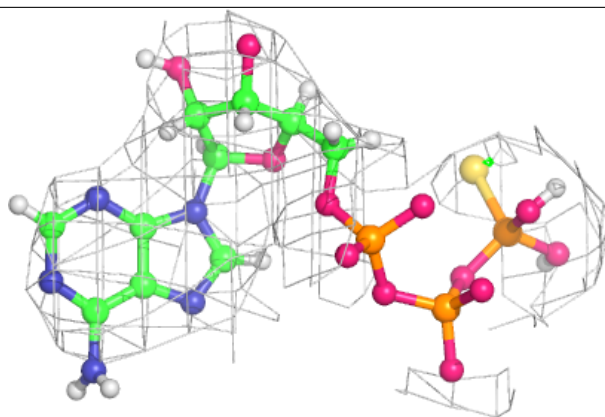
**Electron density around AGS B 901:**

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

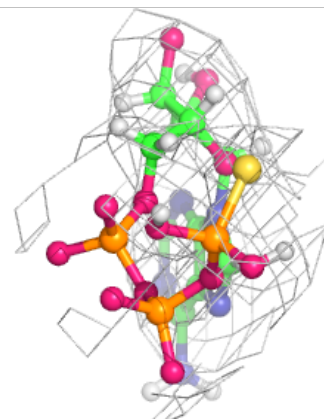
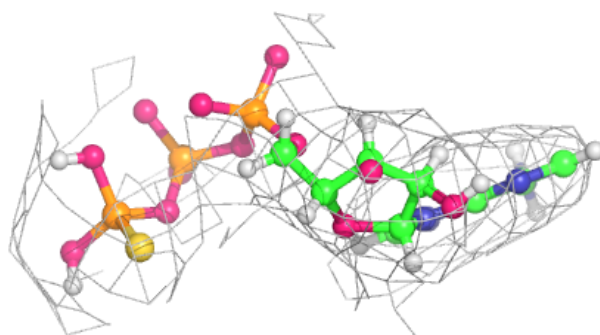
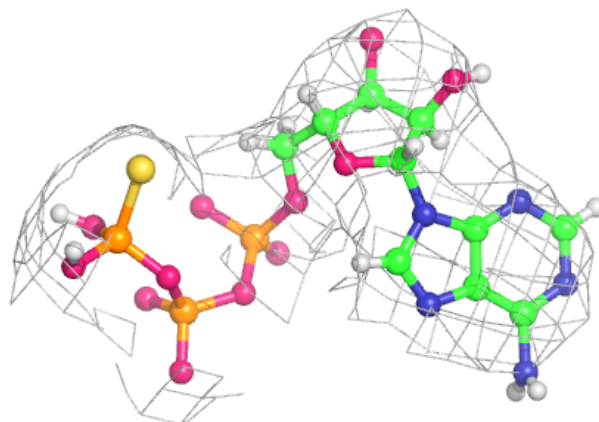


Electron density around AGS D 901:

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

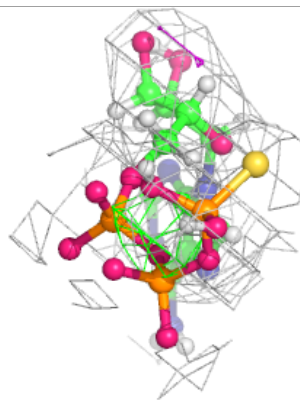
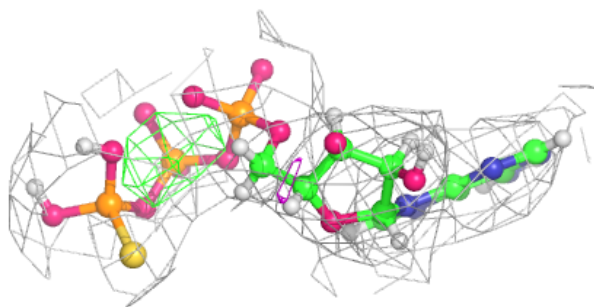
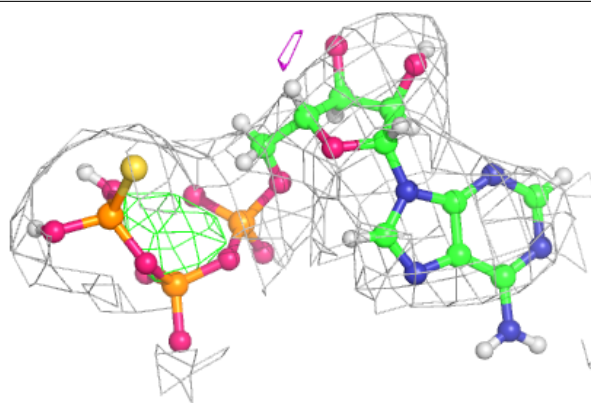
**Electron density around AGS C 901:**

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

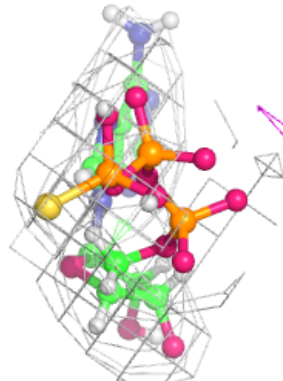
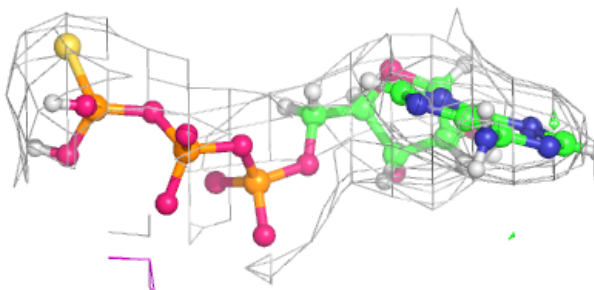
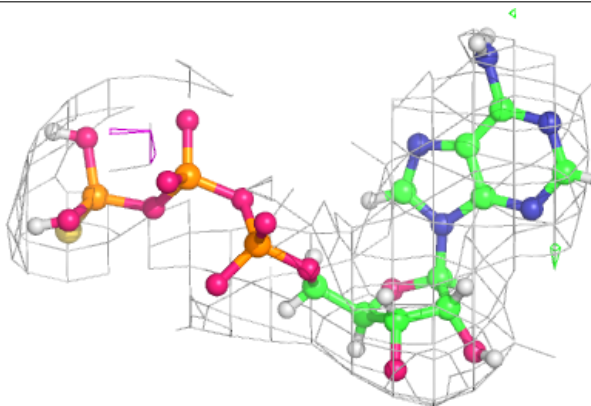


Electron density around AGS A 901:

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

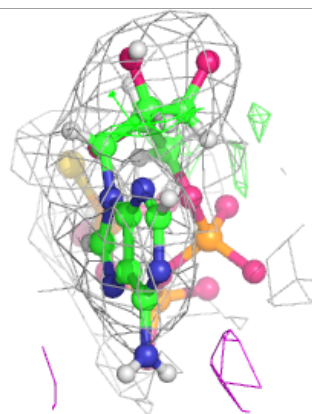
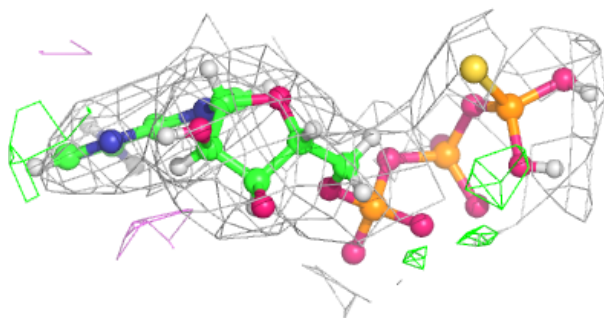
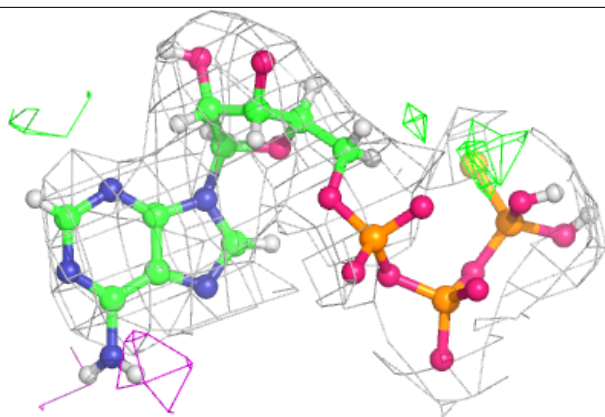
**Electron density around AGS D 902:**

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

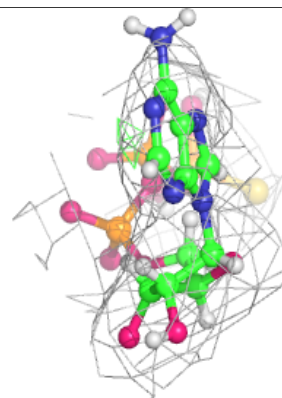
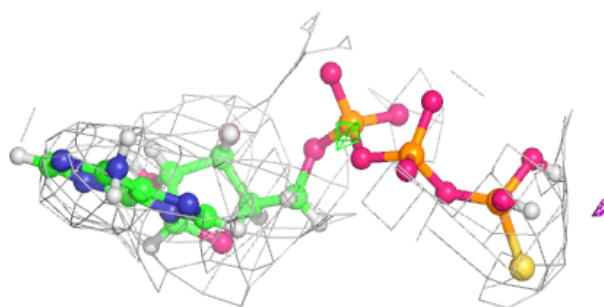
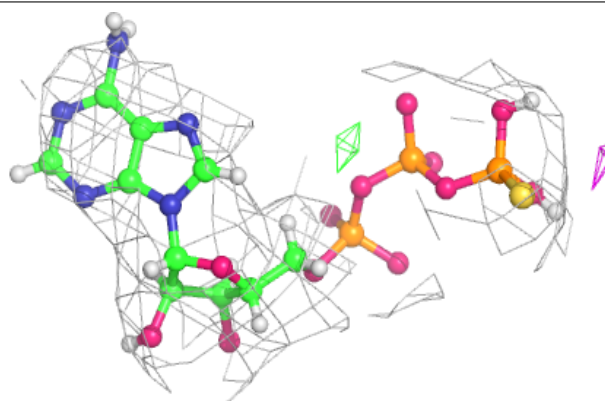


Electron density around AGS F 901:

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

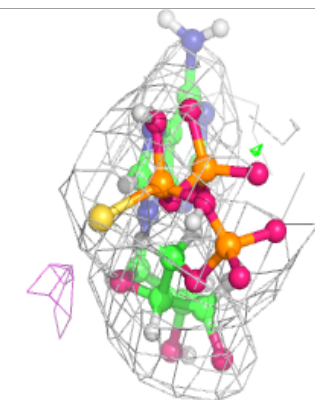
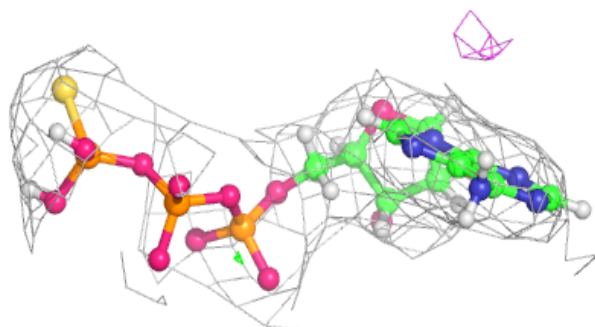
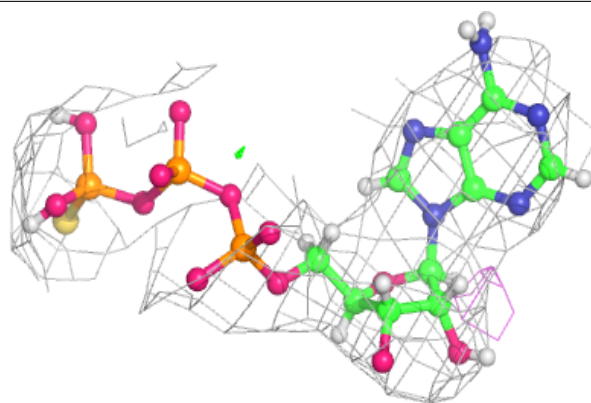
**Electron density around AGS F 902:**

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

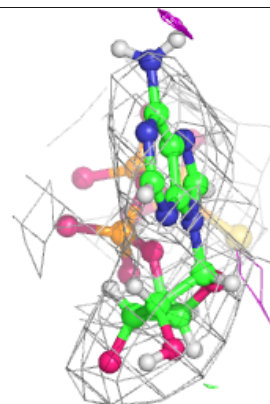
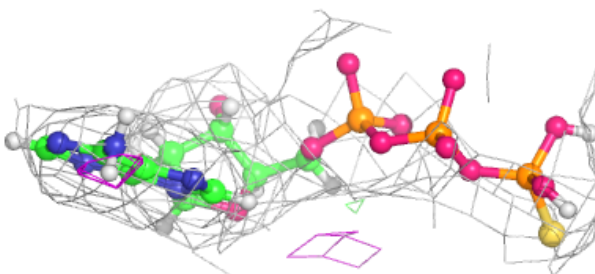
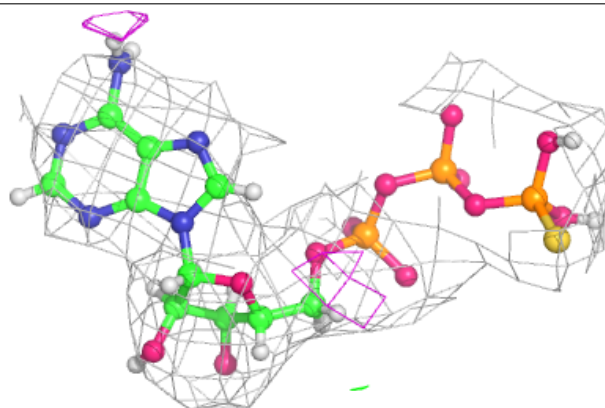


Electron density around AGS E 902:

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

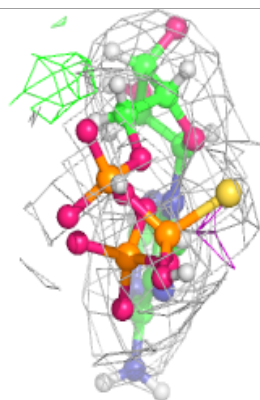
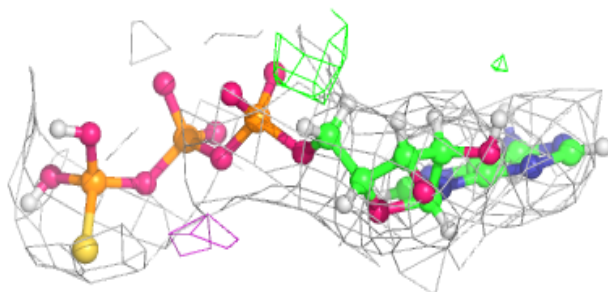
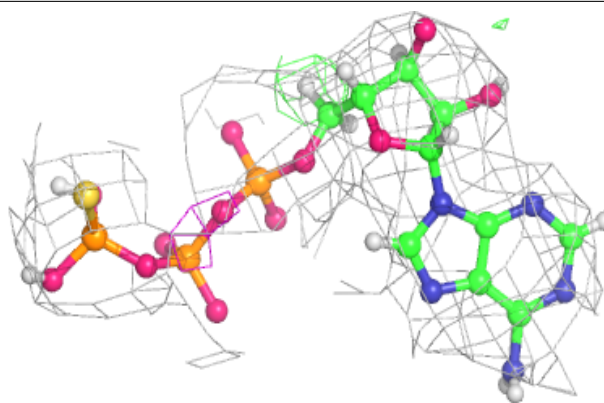
**Electron density around AGS C 902:**

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

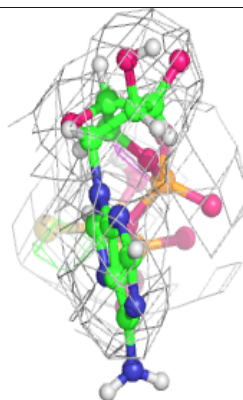
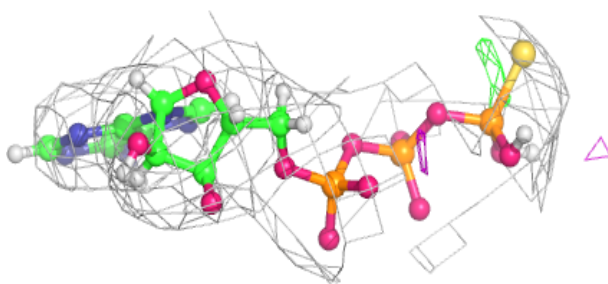
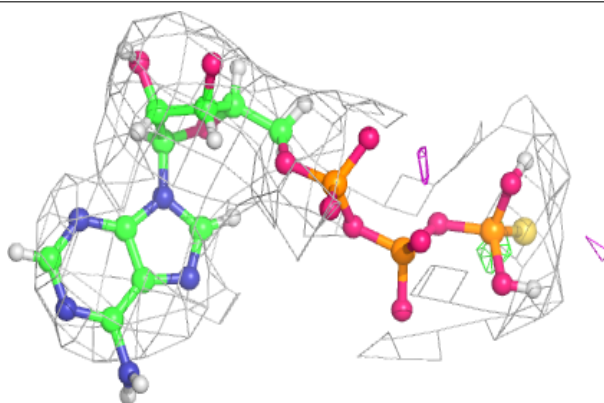


Electron density around AGS B 902:

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

**Electron density around AGS 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.