



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 03:16 PM BST

PDB ID : 6QUZ  
Title : Structure of ATPgS-bound outward-facing TM287/288 in complex with sy-body Sb\_TM35  
Authors : Hutter, C.A.J.; Huerlimann, L.M.; Zimmermann, I.; Egloff, P.; Seeger, M.A.  
Deposited on : 2019-03-01  
Resolution : 3.21 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](mailto: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.

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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 : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

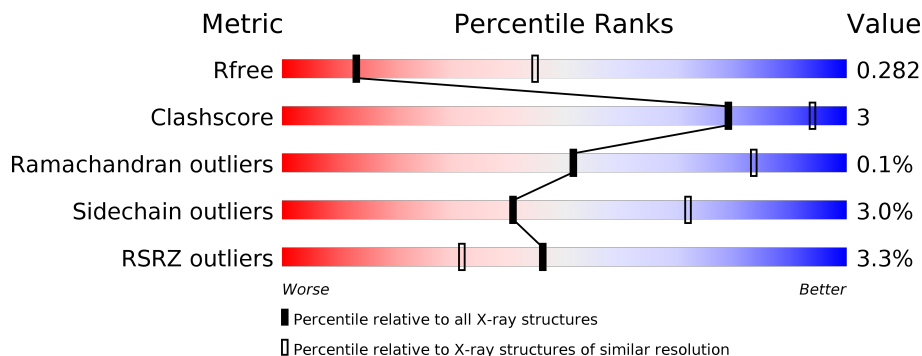
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.21 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	1335 (3.24-3.20)
Clashscore	141614	1460 (3.24-3.20)
Ramachandran outliers	138981	1437 (3.24-3.20)
Sidechain outliers	138945	1436 (3.24-3.20)
RSRZ outliers	127900	1291 (3.24-3.20)

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  $\geq 3$ , 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	587	 85% 12% •
1	C	587	 86% 10% •
2	B	599	 86% 9% 5%
2	D	599	 86% 9% ••
3	E	128	 86% 9% •••
3	F	128	 91% 6% •

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 20098 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 ABC transporter, ATP-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	568	4467	2880	768	800	19	0	0	0
1	C	569	4473	2883	769	802	19	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	GLY	-	expression tag	UNP Q9WYC3
A	-8	PRO	-	expression tag	UNP Q9WYC3
A	-7	SER	-	expression tag	UNP Q9WYC3
A	-6	GLY	-	expression tag	UNP Q9WYC3
A	-5	SER	-	expression tag	UNP Q9WYC3
A	-4	GLY	-	expression tag	UNP Q9WYC3
A	-3	GLY	-	expression tag	UNP Q9WYC3
A	-2	GLY	-	expression tag	UNP Q9WYC3
A	-1	GLY	-	expression tag	UNP Q9WYC3
A	0	GLY	-	expression tag	UNP Q9WYC3
A	1	SER	-	expression tag	UNP Q9WYC3
C	-9	GLY	-	expression tag	UNP Q9WYC3
C	-8	PRO	-	expression tag	UNP Q9WYC3
C	-7	SER	-	expression tag	UNP Q9WYC3
C	-6	GLY	-	expression tag	UNP Q9WYC3
C	-5	SER	-	expression tag	UNP Q9WYC3
C	-4	GLY	-	expression tag	UNP Q9WYC3
C	-3	GLY	-	expression tag	UNP Q9WYC3
C	-2	GLY	-	expression tag	UNP Q9WYC3
C	-1	GLY	-	expression tag	UNP Q9WYC3
C	0	GLY	-	expression tag	UNP Q9WYC3
C	1	SER	-	expression tag	UNP Q9WYC3

- Molecule 2 is a protein called Uncharacterized ABC transporter ATP-binding protein TM\_0288.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	570	Total 4544	C 2937	N 766	O 827	S 14	0	0	0
2	D	574	Total 4576	C 2958	N 772	O 832	S 14	0	0	0

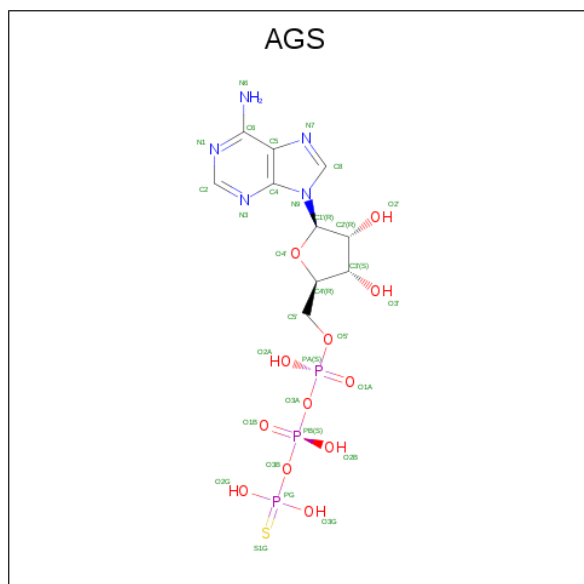
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	517	ALA	GLU	engineered mutation	UNP Q9WYC4
B	599	ALA	-	expression tag	UNP Q9WYC4
D	517	ALA	GLU	engineered mutation	UNP Q9WYC4
D	599	ALA	-	expression tag	UNP Q9WYC4

- Molecule 3 is a protein called Sb\_TM35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	124	Total 955	C 603	N 163	O 186	S 3	0	0	0
3	F	124	Total 955	C 603	N 163	O 186	S 3	0	0	0

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
4	A	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	B	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	C	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	D	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

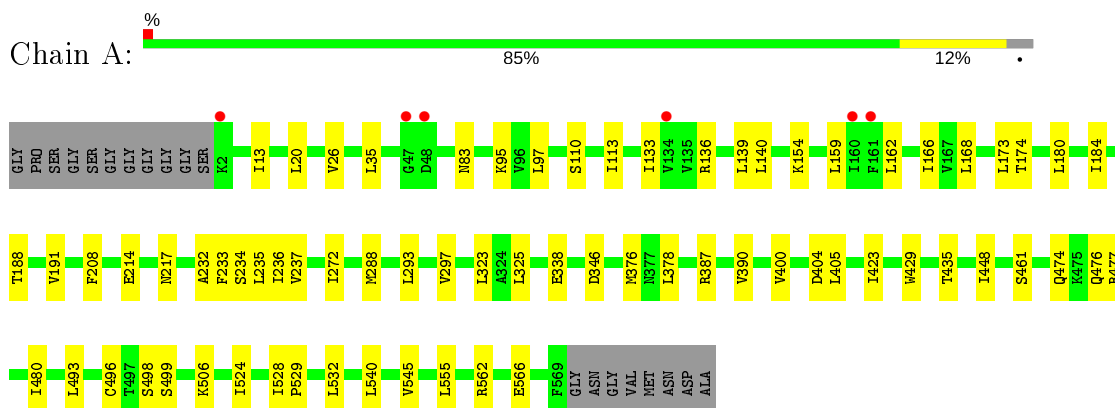
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

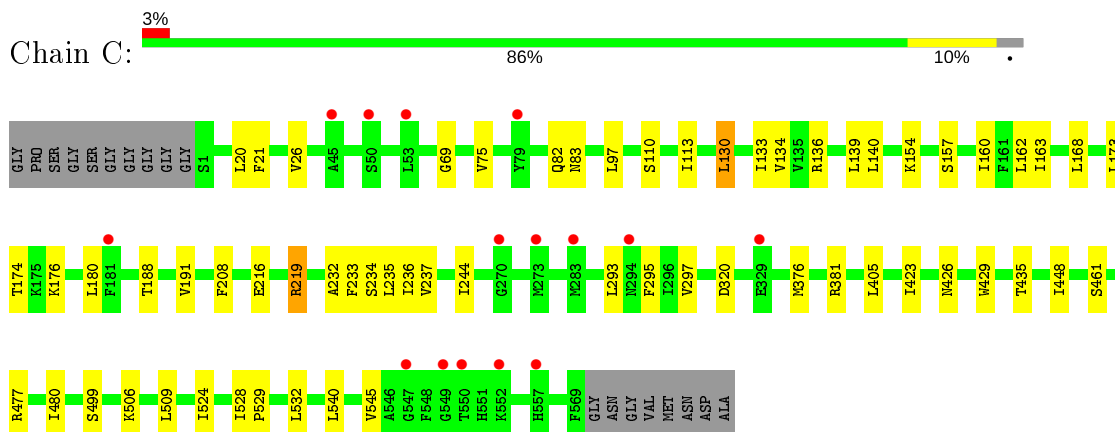
### 3 Residue-property plots [i](#)

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

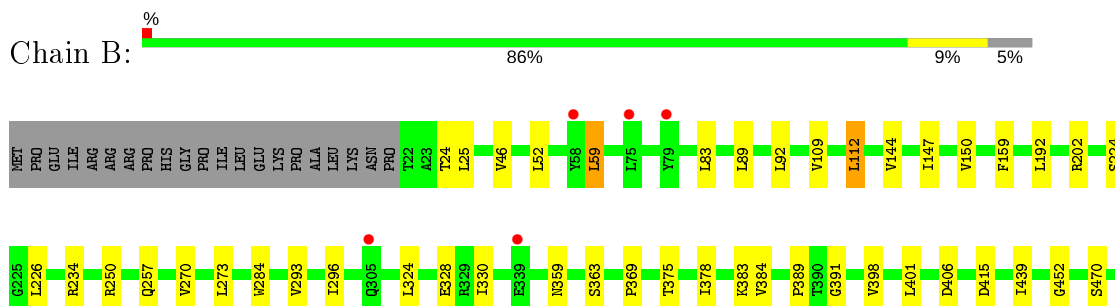
- Molecule 1: ABC transporter, ATP-binding protein



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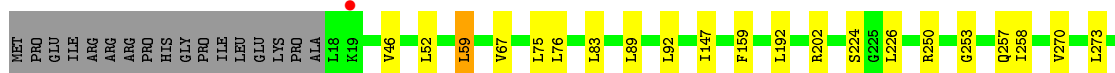
- Molecule 2: Uncharacterized ABC transporter ATP-binding protein TM\_0288





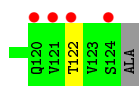
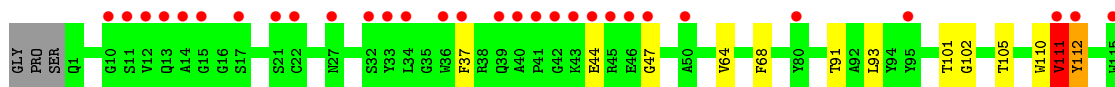
- Molecule 2: Uncharacterized ABC transporter ATP-binding protein TM\_0288

Chain D: 86% 9% . .



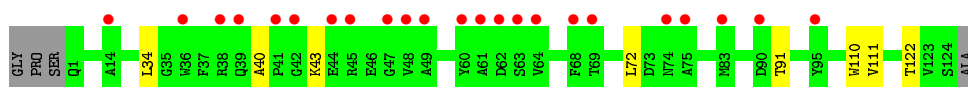
- Molecule 3: Sb\_TM35

Chain E: 27% 86% 9% . . .



- Molecule 3: Sb\_TM35

Chain F: 18% 91% 6% .



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	165.34Å 77.11Å 207.01Å 90.00° 112.49° 90.00°	Depositor
Resolution (Å)	48.84 – 3.21 49.14 – 3.20	Depositor EDS
% Data completeness (in resolution range)	79.8 (48.84-3.21) 79.8 (49.14-3.20)	Depositor EDS
$R_{merge}$	0.25	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.62 (at 3.19Å)	Xtrriage
Refinement program	BUSTER 2.10.3	Depositor
R, $R_{free}$	0.243 , 0.263 0.259 , 0.282	Depositor DCC
$R_{free}$ test set	3232 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.5	Xtrriage
Anisotropy	0.043	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 25.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	20098	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.58% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

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	0/4542	0.59	0/6143
1	C	0.41	0/4548	0.59	0/6151
2	B	0.40	0/4622	0.58	0/6249
2	D	0.40	0/4655	0.58	0/6294
3	E	0.37	0/981	0.54	0/1337
3	F	0.36	0/981	0.52	0/1337
All	All	0.40	0/20329	0.58	0/27511

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	4467	0	4665	30	0
1	C	4473	0	4673	27	0
2	B	4544	0	4724	28	0
2	D	4576	0	4761	30	0
3	E	955	0	895	8	0
3	F	955	0	895	5	0
4	A	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	31	0	12	0	0
4	C	31	0	12	0	0
4	D	31	0	12	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	20098	0	20661	115	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 (115) 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)
2:D:284:TRP:HH2	3:F:110:TRP:HA	1.49	0.76
2:B:46:VAL:HG11	2:B:159:PHE:HB3	1.72	0.71
2:D:46:VAL:HG11	2:D:159:PHE:HB3	1.72	0.71
3:E:102:GLY:H	3:E:111:VAL:HG11	1.55	0.71
1:A:562:ARG:O	1:A:566:GLU:HG2	1.90	0.70
2:B:359:ASN:H	2:B:375:THR:HB	1.63	0.62
2:D:359:ASN:H	2:D:375:THR:HB	1.63	0.61
1:A:208:PHE:HB3	2:B:452:GLY:HA2	1.84	0.59
1:A:555:LEU:HD22	1:A:562:ARG:HD2	1.83	0.59
2:B:112:LEU:HD23	2:B:330:ILE:HG21	1.84	0.59
2:B:384:VAL:HG22	2:B:558:LEU:HB3	1.84	0.59
2:D:384:VAL:HG22	2:D:558:LEU:HB3	1.85	0.58
3:F:91:THR:HG23	3:F:122:THR:HA	1.87	0.57
1:A:83:ASN:HD21	2:B:250:ARG:HH21	1.52	0.55
3:E:91:THR:HG23	3:E:122:THR:HA	1.88	0.55
1:C:130:LEU:O	1:C:134:VAL:HB	2.06	0.55
1:A:97:LEU:HA	2:B:226:LEU:HD11	1.88	0.54
2:D:284:TRP:CH2	3:F:110:TRP:HA	2.37	0.54
1:A:234:SER:HA	1:A:237:VAL:HG22	1.90	0.53
1:C:133:ILE:HG22	1:C:136:ARG:HD3	1.90	0.53
1:C:234:SER:HA	1:C:237:VAL:HG22	1.91	0.53
2:D:445:VAL:HG13	2:D:500:LEU:HD21	1.90	0.53
1:C:97:LEU:HA	2:D:226:LEU:HD11	1.90	0.52
2:D:293:VAL:HA	2:D:296:ILE:HD12	1.91	0.51
2:B:293:VAL:HA	2:B:296:ILE:HD12	1.92	0.51
3:E:37:PHE:HD1	3:E:47:GLY:HA2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:284:TRP:HE1	3:E:110:TRP:HB3	1.75	0.51
1:C:176:LYS:HB3	1:C:235:LEU:HD21	1.93	0.51
1:A:174:THR:HA	1:A:297:VAL:HG11	1.93	0.50
3:E:101:THR:HA	3:E:111:VAL:HG21	1.93	0.50
1:C:174:THR:HA	1:C:297:VAL:HG11	1.94	0.50
1:C:83:ASN:HD21	2:D:250:ARG:HH21	1.58	0.50
2:D:355:ILE:HG13	2:D:378:ILE:HB	1.93	0.50
1:C:477:ARG:HA	1:C:480:ILE:HD12	1.94	0.49
2:D:516:ASP:HA	2:D:546:ILE:HB	1.93	0.49
1:A:477:ARG:HA	1:A:480:ILE:HD12	1.95	0.49
2:B:516:ASP:HA	2:B:546:ILE:HB	1.93	0.49
1:A:493:LEU:HB3	1:A:496:CYS:HB2	1.95	0.48
1:C:233:PHE:HA	1:C:236:ILE:HD12	1.96	0.48
1:C:180:LEU:HB3	1:C:232:ALA:HB2	1.96	0.48
2:D:202:ARG:HB2	2:D:321:GLN:HE21	1.79	0.48
1:A:133:ILE:HG22	1:A:136:ARG:HD3	1.96	0.48
2:B:486:THR:HG22	2:B:487:ASP:H	1.80	0.47
3:E:105:THR:HG21	3:E:111:VAL:HG22	1.94	0.47
2:B:470:SER:HA	2:B:473:PHE:CE2	2.50	0.47
3:F:40:ALA:HB3	3:F:43:LYS:HB2	1.97	0.47
1:A:180:LEU:HB3	1:A:232:ALA:HB2	1.96	0.47
1:A:338:GLU:HB3	1:A:387:ARG:HB2	1.97	0.47
1:C:110:SER:HA	1:C:113:ILE:HD12	1.97	0.47
1:C:423:ILE:HD12	1:C:461:SER:HB2	1.97	0.47
1:A:423:ILE:HD12	1:A:461:SER:HB2	1.98	0.46
1:A:429:TRP:CE3	2:B:234:ARG:HG3	2.50	0.46
2:D:467:LEU:HD22	2:D:537:LEU:HD12	1.97	0.46
1:C:540:LEU:HD23	1:C:545:VAL:HA	1.98	0.46
1:A:540:LEU:HD23	1:A:545:VAL:HA	1.98	0.46
1:C:157:SER:HA	1:C:160:ILE:HD12	1.98	0.46
1:A:110:SER:HA	1:A:113:ILE:HD12	1.97	0.46
1:A:325:LEU:HD22	1:A:400:VAL:HG11	1.97	0.46
2:B:24:THR:HG21	2:B:328:GLU:HG2	1.98	0.46
2:D:354:GLU:HB3	2:D:415:ASP:HA	1.98	0.45
1:C:529:PRO:HA	1:C:532:LEU:HD12	1.99	0.45
2:D:348:LEU:HD11	2:D:415:ASP:HB2	1.99	0.45
1:C:82:GLN:NE2	2:D:253:GLY:HA3	2.32	0.44
2:D:398:VAL:HG13	2:D:514:ILE:HD13	2.00	0.44
2:B:363:SER:HB2	2:B:369:PRO:HA	2.00	0.44
1:A:529:PRO:HA	1:A:532:LEU:HD12	1.99	0.44
1:C:216:GLU:HA	1:C:219:ARG:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:398:VAL:HG13	2:B:514:ILE:HD13	2.00	0.44
1:A:233:PHE:HA	1:A:236:ILE:HD12	2.00	0.43
1:A:448:ILE:HB	1:A:477:ARG:HB3	2.00	0.43
2:B:270:VAL:HA	2:B:273:LEU:HD12	2.00	0.43
1:C:448:ILE:HB	1:C:477:ARG:HB3	2.00	0.43
2:B:52:LEU:HD11	2:B:89:LEU:HD23	2.00	0.43
1:C:26:VAL:HG21	1:C:136:ARG:HG3	2.00	0.43
1:A:474:GLN:NE2	2:B:391:GLY:HA3	2.33	0.43
1:C:21:PHE:HD2	1:C:69:GLY:HA2	1.83	0.43
2:D:52:LEU:HD11	2:D:89:LEU:HD23	2.00	0.42
2:D:202:ARG:HH22	2:D:324:LEU:HD22	1.84	0.42
1:C:208:PHE:HB3	2:D:452:GLY:HA2	2.00	0.42
2:B:378:ILE:HG12	2:B:384:VAL:HG21	2.01	0.42
2:D:270:VAL:HA	2:D:273:LEU:HD12	2.00	0.42
2:D:378:ILE:HG12	2:D:384:VAL:HG21	2.01	0.42
2:D:470:SER:HA	2:D:473:PHE:CE2	2.55	0.42
1:A:162:LEU:O	1:A:166:ILE:HG12	2.20	0.42
1:A:376:MET:HG3	1:A:524:ILE:HD11	2.02	0.42
1:C:160:ILE:HA	1:C:163:ILE:HD12	2.00	0.42
2:B:389:PRO:HG3	2:B:582:PHE:HZ	1.85	0.42
1:A:476:GLN:HE22	1:A:498:SER:H	1.66	0.42
3:E:111:VAL:HB	3:E:112:TYR:H	1.63	0.42
1:A:378:LEU:HB3	1:A:390:VAL:HG21	2.02	0.42
3:F:34:LEU:HD22	3:F:72:LEU:HB2	2.02	0.41
1:C:528:ILE:N	1:C:529:PRO:HD2	2.35	0.41
2:D:364:TYR:HD2	2:D:370:VAL:HG21	1.85	0.41
2:B:109:VAL:HG13	2:B:144:VAL:HG12	2.02	0.41
2:B:401:LEU:HD23	2:B:514:ILE:HD11	2.02	0.41
1:A:214:GLU:HA	1:A:217:ASN:HB2	2.02	0.41
1:C:376:MET:HG3	1:C:524:ILE:HD11	2.02	0.41
2:D:389:PRO:HG3	2:D:582:PHE:HZ	1.85	0.41
2:D:67:VAL:HG11	2:D:76:LEU:HB2	2.03	0.41
2:B:59:LEU:HB3	2:B:83:LEU:HD13	2.02	0.41
2:B:25:LEU:HB2	2:B:324:LEU:HD21	2.02	0.41
2:B:439:ILE:HG23	2:B:488:ASN:HD21	1.85	0.41
1:C:188:THR:HA	1:C:191:VAL:HG22	2.02	0.41
2:D:351:VAL:HG11	2:D:430:SER:HB3	2.03	0.41
1:A:188:THR:HA	1:A:191:VAL:HG22	2.03	0.41
2:B:202:ARG:HH22	2:B:324:LEU:HD22	1.85	0.41
1:A:184:ILE:HD11	1:A:232:ALA:HB3	2.03	0.41
1:C:426:ASN:O	1:C:429:TRP:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:64:VAL:HG11	3:E:68:PHE:HB2	2.03	0.40
1:A:528:ILE:N	1:A:529:PRO:HD2	2.35	0.40
2:B:147:ILE:O	2:B:150:VAL:HG12	2.21	0.40
2:D:401:LEU:HD23	2:D:514:ILE:HD11	2.04	0.40
1:C:75:VAL:HA	2:D:258:ILE:HG12	2.03	0.40
2:D:59:LEU:HB3	2:D:83:LEU:HD13	2.02	0.40
1:A:26:VAL:HG21	1:A:136:ARG:HG3	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	566/587 (96%)	550 (97%)	16 (3%)	0	100	100
1	C	567/587 (97%)	551 (97%)	16 (3%)	0	100	100
2	B	568/599 (95%)	551 (97%)	17 (3%)	0	100	100
2	D	572/599 (96%)	557 (97%)	15 (3%)	0	100	100
3	E	122/128 (95%)	108 (88%)	12 (10%)	2 (2%)	9	42
3	F	122/128 (95%)	113 (93%)	9 (7%)	0	100	100
All	All	2517/2628 (96%)	2430 (96%)	85 (3%)	2 (0%)	51	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	111	VAL
3	E	44	GLU

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	495/504 (98%)	474 (96%)	21 (4%)	30	64
1	C	496/504 (98%)	477 (96%)	19 (4%)	33	66
2	B	507/532 (95%)	497 (98%)	10 (2%)	55	79
2	D	511/532 (96%)	499 (98%)	12 (2%)	50	77
3	E	97/99 (98%)	94 (97%)	3 (3%)	40	71
3	F	97/99 (98%)	96 (99%)	1 (1%)	76	89
All	All	2203/2270 (97%)	2137 (97%)	66 (3%)	41	72

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ILE
1	A	20	LEU
1	A	35	LEU
1	A	95	LYS
1	A	139	LEU
1	A	140	LEU
1	A	154	LYS
1	A	159	LEU
1	A	168	LEU
1	A	173	LEU
1	A	235	LEU
1	A	272	ILE
1	A	288	MET
1	A	293	LEU
1	A	323	LEU
1	A	346	ASP
1	A	404	ASP
1	A	405	LEU
1	A	435	THR
1	A	499	SER
1	A	506	LYS
2	B	59	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	92	LEU
2	B	112	LEU
2	B	192	LEU
2	B	224	SER
2	B	257	GLN
2	B	383	LYS
2	B	406	ASP
2	B	415	ASP
2	B	500	LEU
1	C	20	LEU
1	C	130	LEU
1	C	139	LEU
1	C	140	LEU
1	C	154	LYS
1	C	162	LEU
1	C	168	LEU
1	C	173	LEU
1	C	219	ARG
1	C	244	ILE
1	C	293	LEU
1	C	295	PHE
1	C	320	ASP
1	C	381	ARG
1	C	405	LEU
1	C	435	THR
1	C	499	SER
1	C	506	LYS
1	C	509	LEU
2	D	59	LEU
2	D	75	LEU
2	D	92	LEU
2	D	147	ILE
2	D	192	LEU
2	D	224	SER
2	D	257	GLN
2	D	363	SER
2	D	467	LEU
2	D	486	THR
2	D	488	ASN
2	D	500	LEU
3	E	93	LEU
3	E	111	VAL

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Mol	Chain	Res	Type
3	E	112	TYR
3	F	111	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	215	ASN
1	A	474	GLN
2	B	142	ASN
1	C	83	ASN
2	D	133	HIS
2	D	142	ASN
2	D	321	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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
4	AGS	B	600	5	26,33,33	0.59	0	26,52,52	0.67	1 (3%)
4	AGS	A	600	5	26,33,33	0.61	0	26,52,52	0.71	1 (3%)
4	AGS	D	600	5	26,33,33	0.61	0	26,52,52	0.70	1 (3%)
4	AGS	C	600	5	26,33,33	0.59	0	26,52,52	0.68	1 (3%)

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
4	AGS	B	600	5	-	3/17/38/38	0/3/3/3
4	AGS	A	600	5	-	5/17/38/38	0/3/3/3
4	AGS	D	600	5	-	3/17/38/38	0/3/3/3
4	AGS	C	600	5	-	3/17/38/38	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	600	AGS	C5-C6-N6	2.30	123.84	120.35
4	C	600	AGS	C5-C6-N6	2.26	123.79	120.35
4	A	600	AGS	C5-C6-N6	2.25	123.77	120.35
4	B	600	AGS	C5-C6-N6	2.24	123.75	120.35

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	600	AGS	PB-O3B-PG-O3G
4	A	600	AGS	C5'-O5'-PA-O1A
4	D	600	AGS	PA-O3A-PB-O1B
4	B	600	AGS	PA-O3A-PB-O1B
4	C	600	AGS	PG-O3B-PB-O2B
4	D	600	AGS	PA-O3A-PB-O2B
4	B	600	AGS	PA-O3A-PB-O2B
4	A	600	AGS	PG-O3B-PB-O2B
4	A	600	AGS	PB-O3B-PG-O3G
4	B	600	AGS	PG-O3B-PB-O1B

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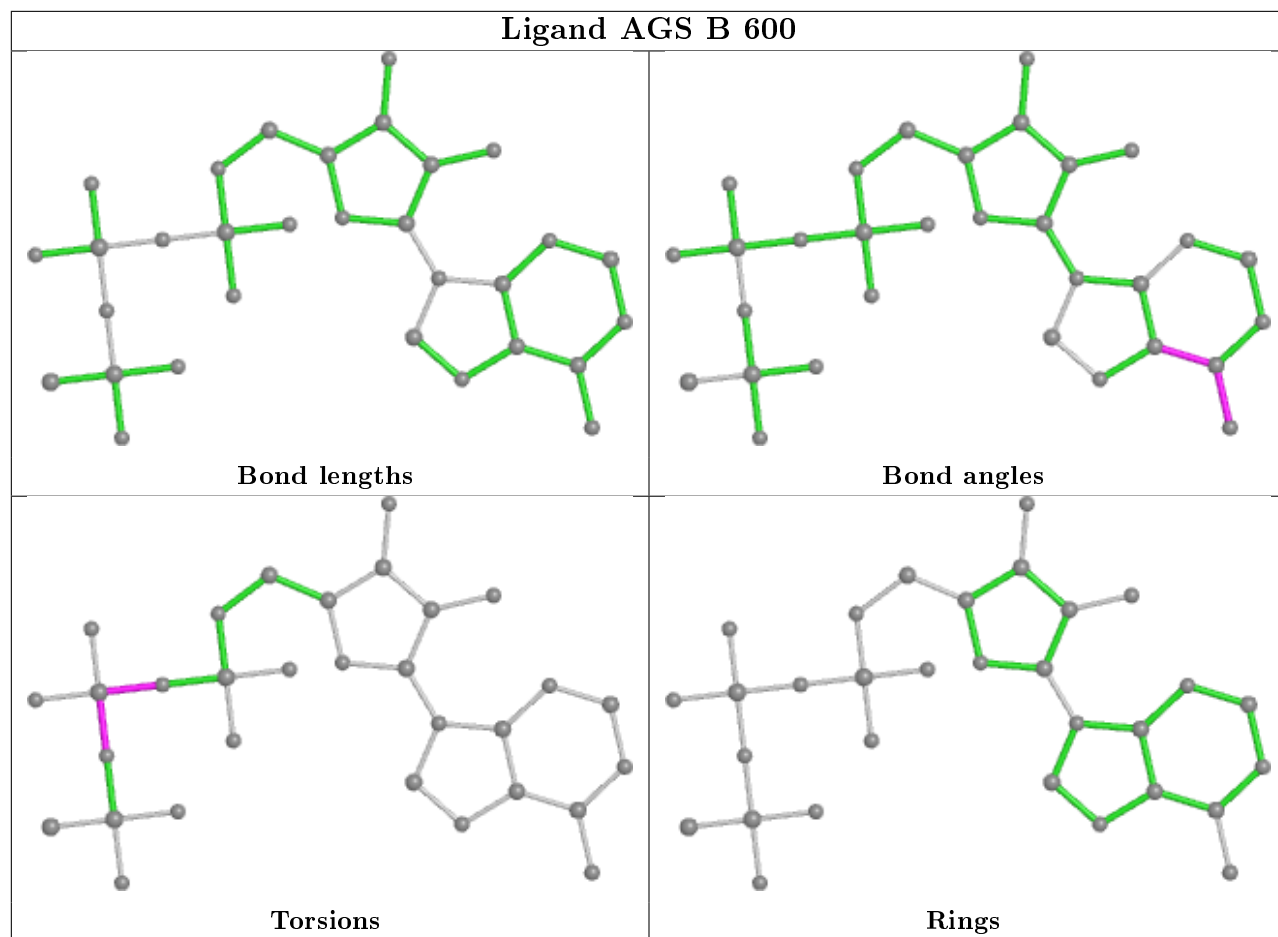
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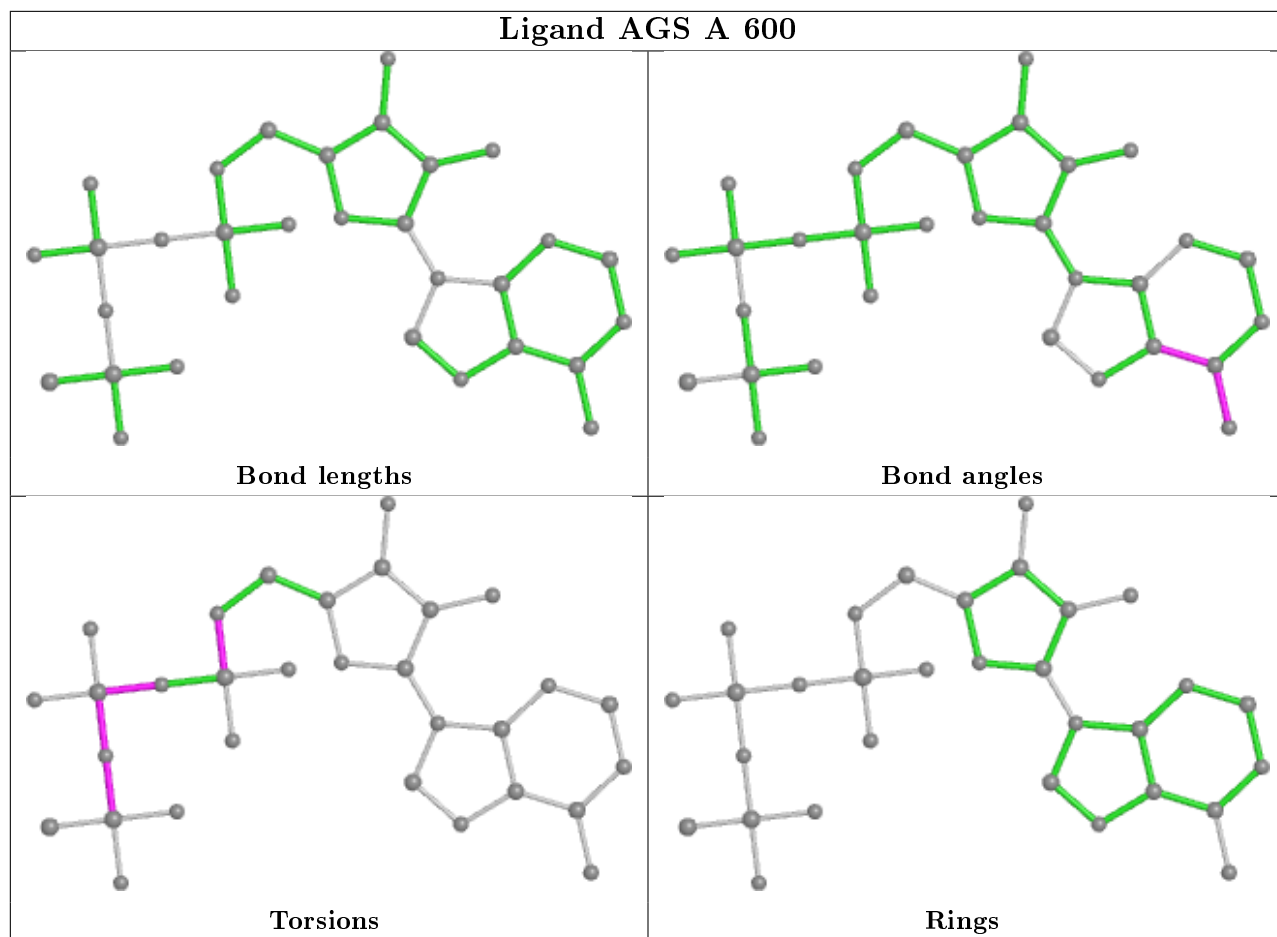
<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atoms</b>
4	A	600	AGS	PA-O3A-PB-O1B
4	A	600	AGS	PA-O3A-PB-O2B
4	D	600	AGS	C5'-O5'-PA-O1A
4	C	600	AGS	C5'-O5'-PA-O1A

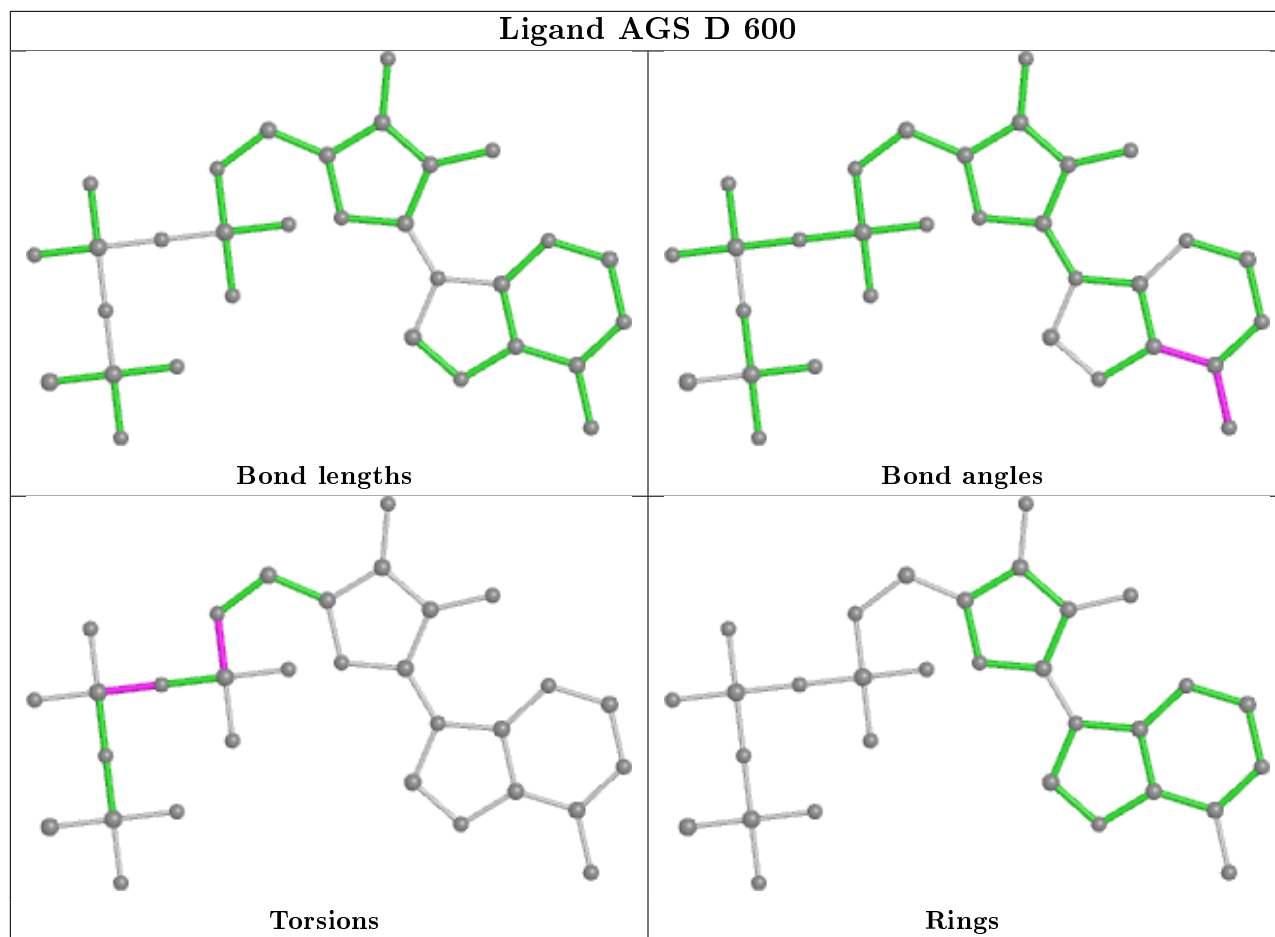
There are no ring outliers.

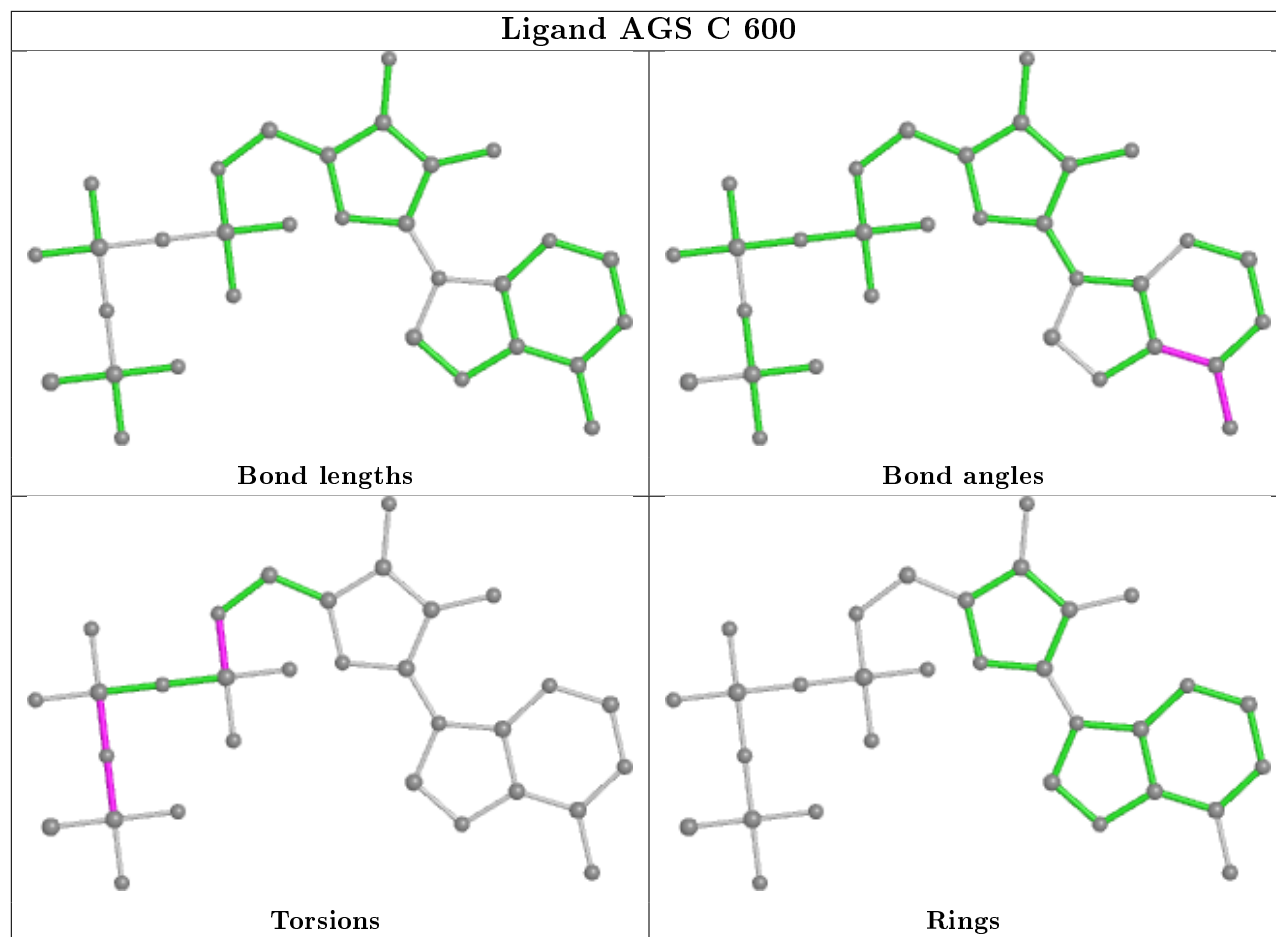
No monomer is involved in short contacts.

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.









## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	568/587 (96%)	-0.33	6 (1%) 80 70	19, 52, 106, 123	0
1	C	569/587 (96%)	-0.15	15 (2%) 56 42	35, 71, 121, 136	0
2	B	570/599 (95%)	-0.17	5 (0%) 84 76	22, 61, 98, 118	0
2	D	574/599 (95%)	-0.22	1 (0%) 95 94	35, 65, 95, 115	0
3	E	124/128 (96%)	1.44	34 (27%) 0 0	100, 136, 173, 188	0
3	F	124/128 (96%)	0.93	23 (18%) 1 0	92, 123, 141, 160	0
All	All	2529/2628 (96%)	-0.08	84 (3%) 46 32	19, 66, 130, 188	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	11	SER	6.5
3	F	60	TYR	6.2
3	E	36	TRP	5.6
3	E	41	PRO	5.5
3	F	39	GLN	5.4
3	E	124	SER	4.9
3	E	10	GLY	4.8
3	E	33	TYR	4.8
3	E	44	GLU	4.7
3	E	42	GLY	4.6
3	F	44	GLU	4.5
3	E	37	PHE	4.5
3	E	47	GLY	4.5
3	F	48	VAL	4.3
3	E	43	LYS	4.2
3	F	47	GLY	4.2
3	E	34	LEU	4.1
3	E	14	ALA	4.0
3	E	40	ALA	4.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	2	LYS	3.9
1	C	270	GLY	3.9
3	F	45	ARG	3.9
3	E	46	GLU	3.8
1	A	134	VAL	3.6
3	E	121	VAL	3.6
3	E	122	THR	3.4
3	E	15	GLY	3.4
3	F	64	VAL	3.4
3	E	13	GLN	3.4
1	C	552	LYS	3.3
3	F	62	ASP	3.2
3	F	49	ALA	3.1
3	E	115	TRP	3.1
3	E	80	TYR	3.1
3	E	39	GLN	3.0
3	E	45	ARG	3.0
3	F	42	GLY	3.0
3	E	12	VAL	2.9
1	C	294	ASN	2.9
3	E	17	SER	2.9
3	F	36	TRP	2.8
3	F	68	PHE	2.8
1	C	45	ALA	2.7
1	C	557	HIS	2.7
3	F	38	ARG	2.7
2	B	79	TYR	2.7
2	B	305	GLN	2.7
3	E	112	TYR	2.7
1	A	161	PHE	2.6
3	F	75	ALA	2.6
3	E	32	SER	2.6
1	C	329	GLU	2.5
1	A	160	ILE	2.5
3	E	27	ASN	2.4
3	E	111	VAL	2.4
1	C	273	MET	2.4
1	C	550	THR	2.4
3	F	74	ASN	2.4
2	B	58	TYR	2.3
2	D	19	LYS	2.3
2	B	75	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	549	GLY	2.3
3	E	21	SER	2.3
1	C	547	GLY	2.3
3	E	120	GLN	2.3
3	F	69	THR	2.3
3	F	90	ASP	2.3
3	F	41	PRO	2.3
3	F	63	SER	2.2
1	C	53	LEU	2.2
1	A	47	GLY	2.2
3	F	14	ALA	2.2
3	F	61	ALA	2.2
3	E	50	ALA	2.2
2	B	339	GLU	2.2
3	E	95	TYR	2.2
1	A	48	ASP	2.1
3	F	83	MET	2.1
1	C	50	SER	2.1
1	C	283	MET	2.1
1	C	181	PHE	2.1
1	C	79	TYR	2.1
3	E	22	CYS	2.0
3	F	95	TYR	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

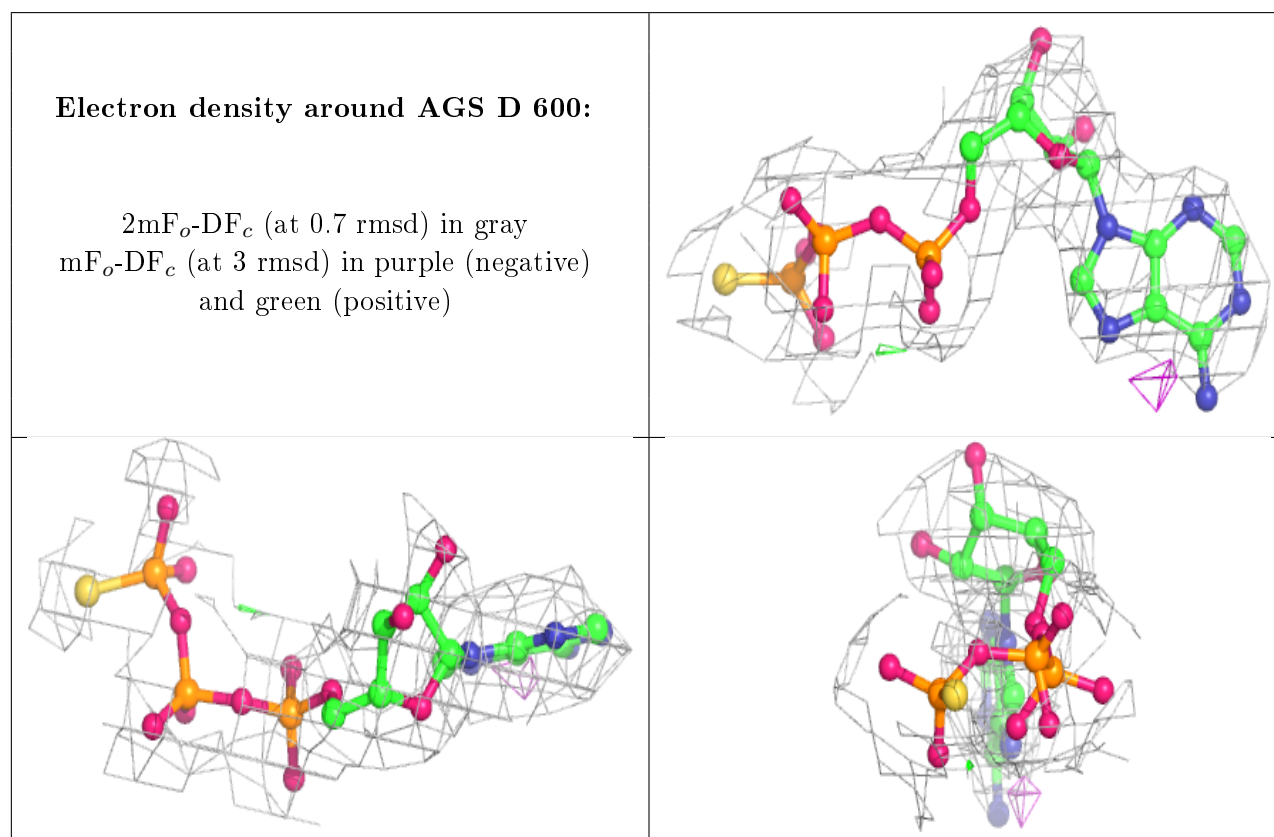
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

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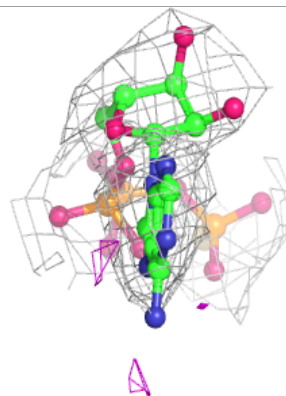
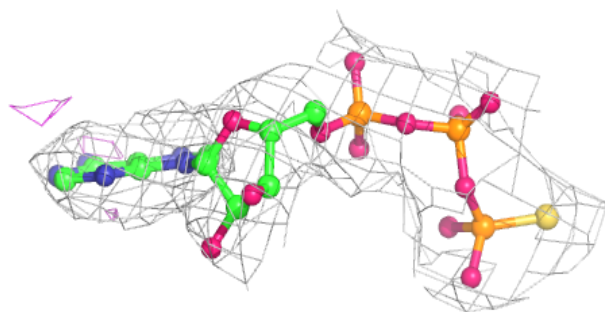
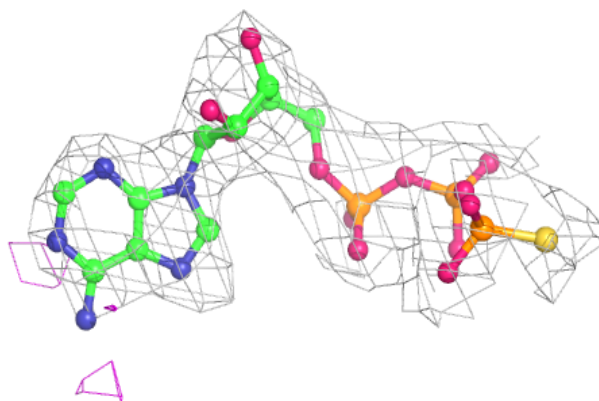
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	AGS	D	600	31/31	0.95	0.21	41,47,51,51	0
5	MG	D	601	1/1	0.95	0.18	16,16,16,16	0
4	AGS	B	600	31/31	0.96	0.18	41,46,52,54	0
4	AGS	C	600	31/31	0.96	0.17	62,65,66,66	0
5	MG	B	601	1/1	0.97	0.19	27,27,27,27	0
4	AGS	A	600	31/31	0.97	0.18	24,28,34,35	0
5	MG	A	601	1/1	0.98	0.26	16,16,16,16	0
5	MG	C	601	1/1	0.98	0.22	35,35,35,35	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.

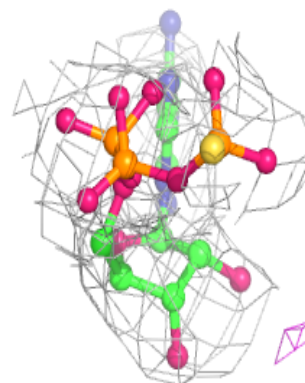
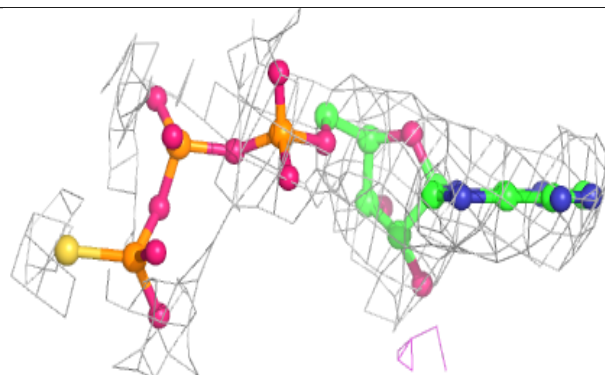
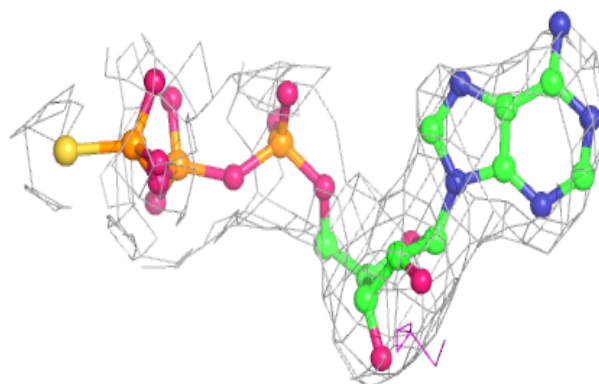


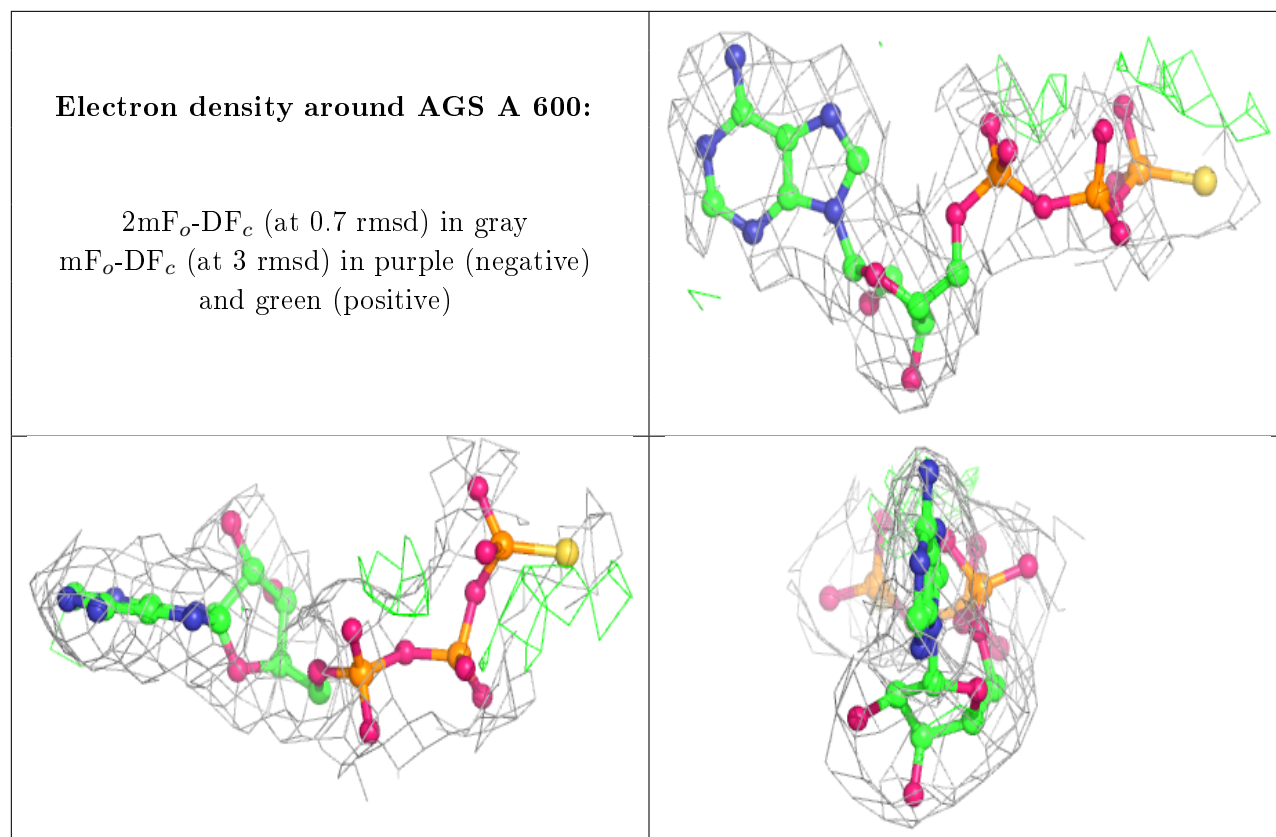
**Electron density around AGS B 600:**

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

**Electron density around AGS C 600:**

$2mF_o-DF_c$  (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.