



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 04:17 PM EDT

PDB ID : 6QV1 / pdb_00006qv1
Title : Structure of ATPgS-bound outward-facing TM287/288 in complex with nanobody Nb_TM1
Authors : Hutter, C.A.J.; Huerlimann, L.M.; Zimmermann, I.; Egloff, P.; Seeger, M.A.
Deposited on : 2019-03-01
Resolution : 3.48 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

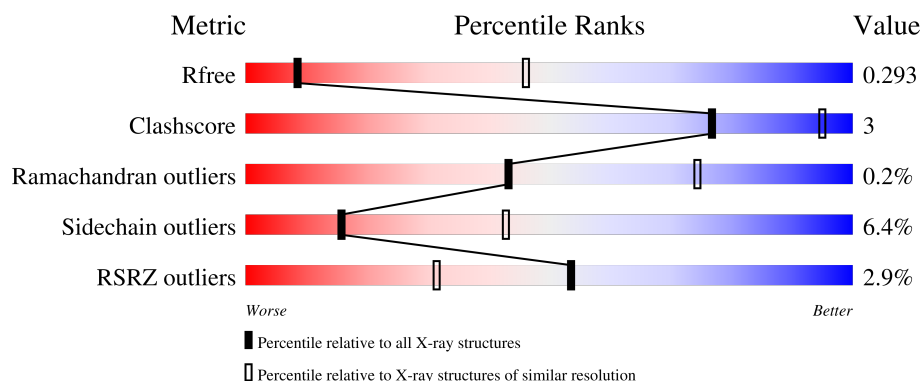
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.48 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1083 (3.52-3.44)
Clashscore	190562	1139 (3.52-3.44)
Ramachandran outliers	187476	1111 (3.52-3.44)
Sidechain outliers	187428	1112 (3.52-3.44)
RSRZ outliers	180081	1082 (3.52-3.44)

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

Mol	Chain	Length	Quality of chain
1	A	587	3% 82% 14% ••
1	C	587	4% 82% 14% •
2	B	599	% 82% 13% •
2	D	599	4% 81% 14% ••
3	E	118	4% 80% 18% •

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Mol	Chain	Length	Quality of chain
3	F	118	2% 84% 14%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19916 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
1	A	569	Total	C	N	O	S	0	0	0
			4468	2881	769	799	19			
1	C	569	Total	C	N	O	S	0	0	0
			4468	2881	769	799	19			

There are 24 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
A	41	ALA	ASP	engineered mutation	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
C	41	ALA	ASP	engineered mutation	UNP Q9WYC3

- Molecule 2 is a protein called Uncharacterized ABC transporter ATP-binding protein TM_0288.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	573	Total	C	N	O	S	0	0	0
			4560	2949	769	828	14			
2	D	573	Total	C	N	O	S	0	0	0
			4560	2949	769	828	14			

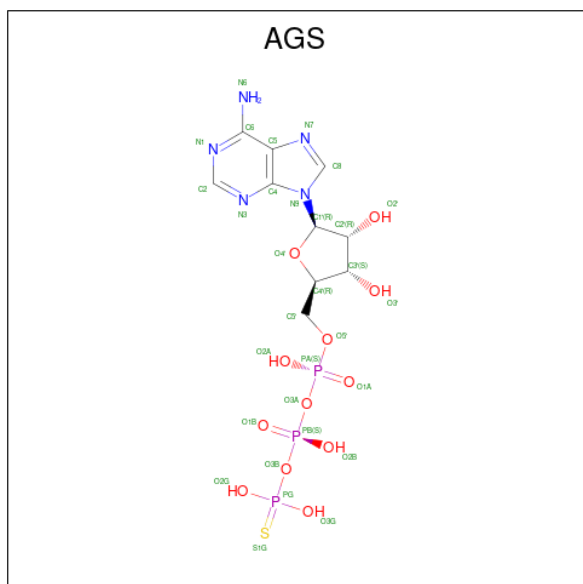
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	65	ALA	ASP	engineered mutation	UNP Q9WYC4
B	517	ALA	GLU	engineered mutation	UNP Q9WYC4
B	599	ALA	-	expression tag	UNP Q9WYC4
D	65	ALA	ASP	engineered mutation	UNP Q9WYC4
D	517	ALA	GLU	engineered mutation	UNP Q9WYC4
D	599	ALA	-	expression tag	UNP Q9WYC4

- Molecule 3 is a protein called Nb_TM1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	115	Total	C	N	O	S	0	0	0
			866	543	153	166	4			
3	F	115	Total	C	N	O	S	0	0	0
			866	543	153	166	4			

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



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

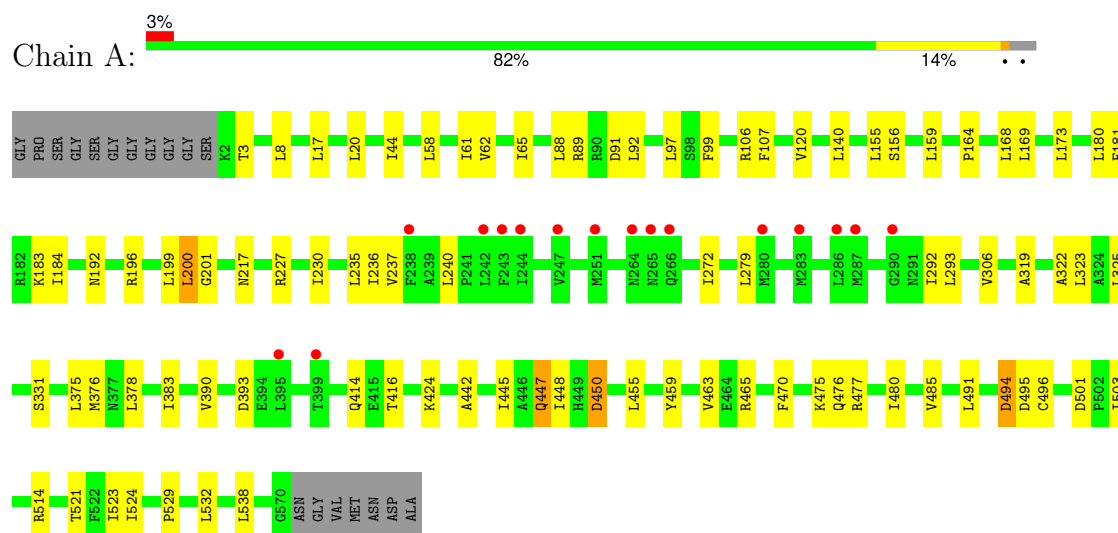
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

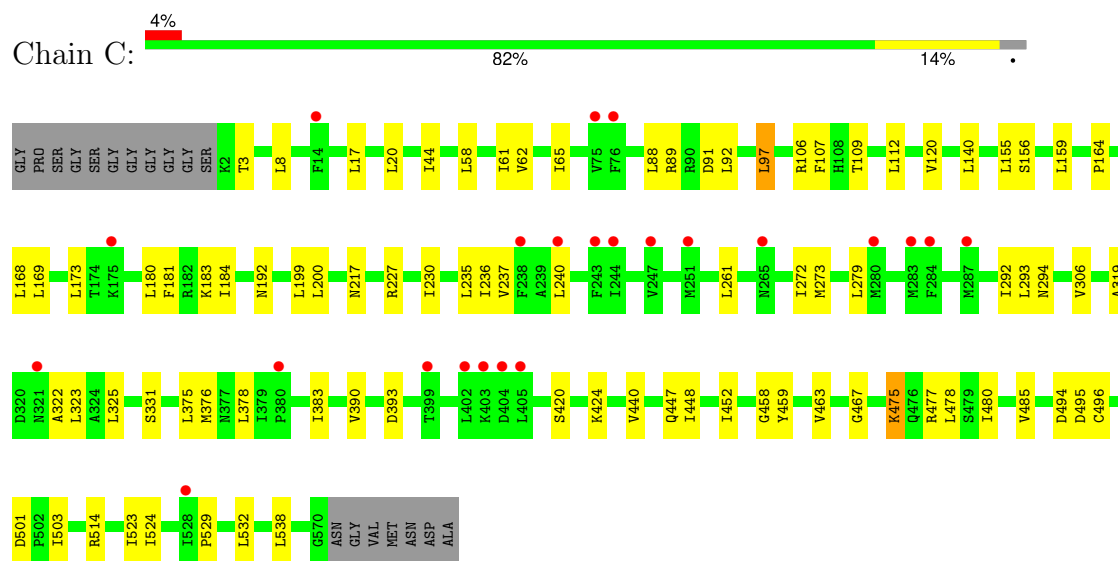
3 Residue-property plots [i](#)

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.

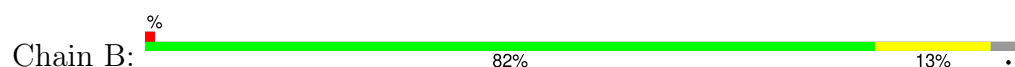
- Molecule 1: ABC transporter, ATP-binding protein

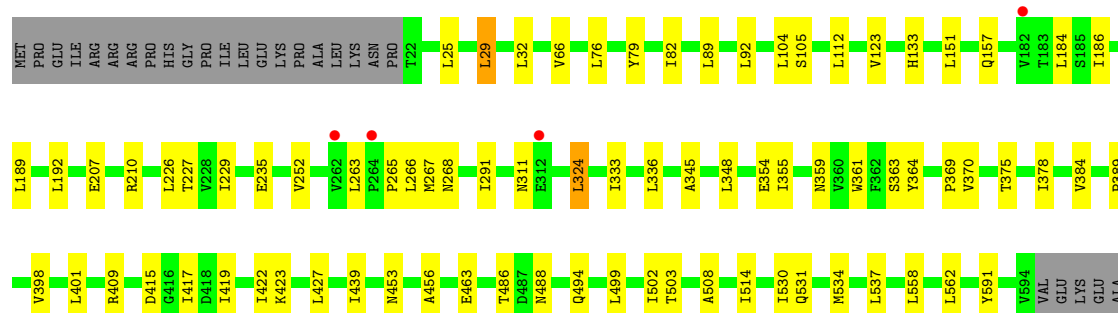


- Molecule 1: ABC transporter, ATP-binding protein

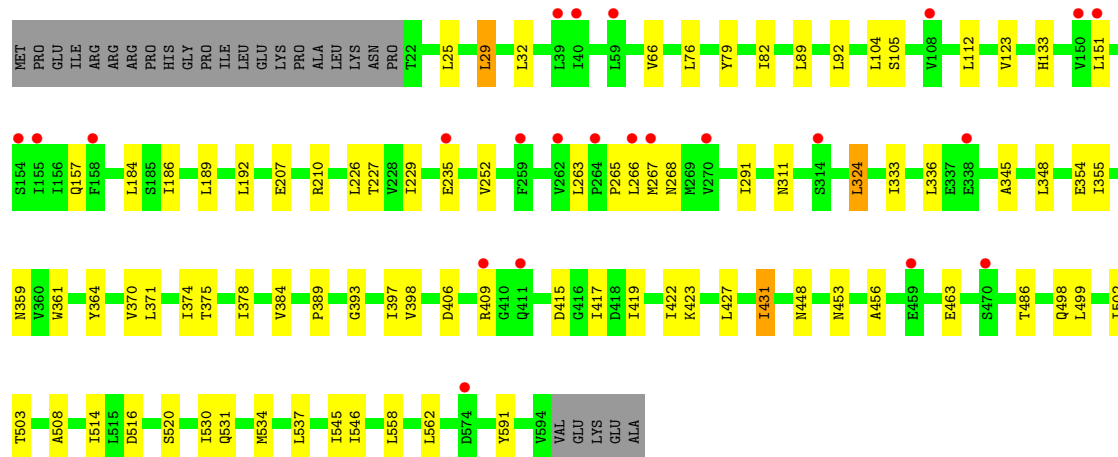
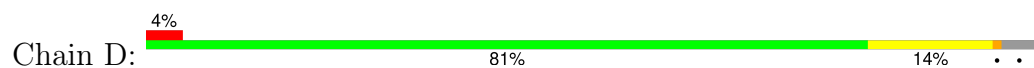


- Molecule 2: Uncharacterized ABC transporter ATP-binding protein TM_0288

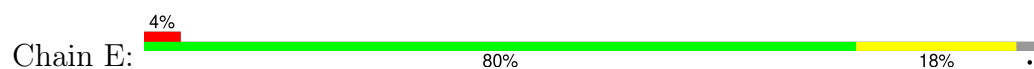




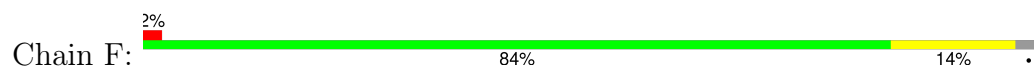
• Molecule 2: Uncharacterized ABC transporter ATP-binding protein TM_0288



• Molecule 3: Nb_TM1



• Molecule 3: Nb_TM1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.75Å 199.26Å 113.16Å 90.00° 91.26° 90.00°	Depositor
Resolution (Å)	34.64 – 3.48 34.64 – 3.48	Depositor EDS
% Data completeness (in resolution range)	58.2 (34.64-3.48) 58.2 (34.64-3.48)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 3.48Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.267 , 0.303 0.286 , 0.293	Depositor DCC
R_{free} test set	1514 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	118.5	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.19 , 385.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.149 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	19916	wwPDB-VP
Average B, all atoms (Å ²)	189.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.77	0/4543	1.35	8/6144 (0.1%)
1	C	0.77	0/4543	1.35	7/6144 (0.1%)
2	B	0.76	0/4638	1.35	2/6271 (0.0%)
2	D	0.76	0/4638	1.36	6/6271 (0.1%)
3	E	0.75	0/883	1.08	0/1195
3	F	0.75	0/883	1.08	0/1195
All	All	0.76	0/20128	1.33	23/27220 (0.1%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	186	ILE	CA-C-N	6.99	125.92	120.33
2	D	186	ILE	C-N-CA	6.99	125.92	120.33
2	B	186	ILE	CA-C-N	6.96	125.90	120.33
2	B	186	ILE	C-N-CA	6.96	125.90	120.33
1	A	450	ASP	CA-CB-CG	6.84	119.44	112.60
1	C	107	PHE	N-CA-C	-6.21	100.40	110.20
1	C	467	GLY	CA-C-N	5.87	128.96	120.38
1	C	467	GLY	C-N-CA	5.87	128.96	120.38
1	A	107	PHE	N-CA-C	-5.68	100.41	109.96
1	A	106	ARG	N-CA-C	-5.61	104.80	111.03
1	C	106	ARG	N-CA-C	-5.58	104.83	111.03
1	A	164	PRO	N-CA-C	5.56	117.48	110.70
1	C	495	ASP	CA-C-N	5.48	127.94	120.54
1	C	495	ASP	C-N-CA	5.48	127.94	120.54
2	D	431	ILE	CA-C-N	5.41	125.91	122.18
2	D	431	ILE	C-N-CA	5.41	125.91	122.18
1	A	475	LYS	CA-C-N	5.40	127.52	120.28
1	A	475	LYS	C-N-CA	5.40	127.52	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	164	PRO	N-CA-C	5.20	117.04	110.70
2	D	397	ILE	CA-C-N	5.11	127.00	120.56
2	D	397	ILE	C-N-CA	5.11	127.00	120.56
1	A	494	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	99	PHE	CA-CB-CG	5.02	118.82	113.80

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	4468	0	4669	29	0
1	C	4468	0	4669	30	0
2	B	4560	0	4748	26	0
2	D	4560	0	4748	28	0
3	E	866	0	858	8	0
3	F	866	0	858	6	0
4	A	31	0	12	0	0
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	19916	0	20598	119	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 (119) 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:A:424:LYS:HB2	1:A:459:TYR:HB3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:424:LYS:HB2	1:C:459:TYR:HB3	1.82	0.60
1:C:199:LEU:HB3	2:D:133:HIS:HD2	1.67	0.60
2:B:267:MET:HE3	2:B:311:ASN:HD22	1.65	0.60
2:D:267:MET:HE3	2:D:311:ASN:HD22	1.66	0.59
1:A:501:ASP:HB3	2:B:389:PRO:HA	1.84	0.58
2:D:359:ASN:H	2:D:375:THR:HB	1.70	0.57
2:B:453:ASN:HB2	2:B:508:ALA:HA	1.87	0.57
2:B:345:ALA:HB1	2:B:423:LYS:HB3	1.86	0.57
1:C:529:PRO:HA	1:C:532:LEU:HD12	1.86	0.57
2:B:359:ASN:H	2:B:375:THR:HB	1.70	0.56
1:A:529:PRO:HA	1:A:532:LEU:HD12	1.86	0.56
2:D:345:ALA:HB1	2:D:423:LYS:HB3	1.87	0.55
2:B:453:ASN:HD22	2:B:456:ALA:HB2	1.72	0.55
1:C:319:ALA:HB3	1:C:322:ALA:HB2	1.89	0.54
1:A:448:ILE:HB	1:A:477:ARG:HB3	1.90	0.54
1:A:319:ALA:HB3	1:A:322:ALA:HB2	1.89	0.53
1:C:376:MET:HG3	1:C:524:ILE:HD11	1.90	0.53
2:B:401:LEU:HD23	2:B:514:ILE:HD11	1.91	0.52
2:D:384:VAL:HG22	2:D:558:LEU:HB3	1.91	0.52
1:A:376:MET:HG3	1:A:524:ILE:HD11	1.90	0.52
1:A:494:ASP:HA	1:A:524:ILE:HB	1.90	0.52
1:C:89:ARG:HG3	1:C:120:VAL:HG11	1.92	0.52
1:A:89:ARG:HG3	1:A:120:VAL:HG11	1.92	0.51
2:B:384:VAL:HG22	2:B:558:LEU:HB3	1.91	0.51
2:D:499:LEU:HA	2:D:502:ILE:HD12	1.92	0.51
3:E:53:SER:HA	3:E:71:ARG:HH12	1.75	0.51
3:E:5:VAL:HA	3:E:107:GLN:HE22	1.76	0.50
1:A:331:SER:HB2	1:A:393:ASP:HA	1.93	0.50
3:F:5:VAL:HA	3:F:107:GLN:HE22	1.76	0.50
1:A:463:VAL:HG22	1:A:470:PHE:HE2	1.77	0.50
2:D:371:LEU:HD22	2:D:374:ILE:HG13	1.93	0.50
3:E:32:PHE:HB3	3:E:99:LEU:HG	1.93	0.50
2:B:363:SER:HB2	2:B:369:PRO:HA	1.92	0.50
3:F:53:SER:HA	3:F:71:ARG:HH12	1.77	0.50
1:C:331:SER:HB2	1:C:393:ASP:HA	1.92	0.50
1:A:156:SER:HA	1:A:159:LEU:HD12	1.93	0.49
2:B:333:ILE:HA	2:B:336:LEU:HD12	1.95	0.49
1:C:109:THR:HA	1:C:112:LEU:HD12	1.93	0.49
3:F:32:PHE:HB3	3:F:99:LEU:HG	1.93	0.49
2:D:361:TRP:HB2	2:D:409:ARG:HG3	1.95	0.49
2:D:333:ILE:HA	2:D:336:LEU:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:361:TRP:HB2	2:B:409:ARG:HG3	1.95	0.48
1:C:155:LEU:HD11	1:C:261:LEU:HD11	1.94	0.48
1:C:494:ASP:HA	1:C:524:ILE:HB	1.95	0.48
2:D:79:TYR:HA	2:D:82:ILE:HD12	1.96	0.47
2:B:417:ILE:HB	2:B:422:ILE:HD11	1.97	0.47
1:C:452:ILE:O	1:C:458:GLY:HA2	2.14	0.47
3:E:22:CYS:HB3	3:E:78:VAL:HG13	1.97	0.47
2:B:79:TYR:HA	2:B:82:ILE:HD12	1.96	0.47
2:D:417:ILE:HB	2:D:422:ILE:HD11	1.97	0.47
1:A:199:LEU:HB3	2:B:133:HIS:HD2	1.79	0.47
1:C:199:LEU:HB3	2:D:133:HIS:CD2	2.48	0.47
2:D:265:PRO:HA	2:D:268:ASN:HD22	1.80	0.47
2:B:265:PRO:HA	2:B:268:ASN:HD22	1.80	0.46
1:C:501:ASP:HB3	2:D:389:PRO:HA	1.97	0.46
1:A:375:LEU:HA	1:A:378:LEU:HD12	1.98	0.46
1:C:375:LEU:HA	1:C:378:LEU:HD12	1.98	0.46
1:A:477:ARG:HA	1:A:480:ILE:HD12	1.98	0.46
1:A:442:ALA:HA	1:A:445:ILE:HD12	1.98	0.46
2:D:105:SER:HA	2:D:151:LEU:HD22	1.98	0.46
3:F:90:THR:HG23	3:F:112:THR:HA	1.98	0.46
2:B:530:ILE:HG22	2:B:534:MET:HB2	1.99	0.45
2:D:530:ILE:HG22	2:D:534:MET:HB2	1.98	0.45
1:C:448:ILE:HB	1:C:477:ARG:HB3	1.99	0.45
2:D:453:ASN:HB2	2:D:508:ALA:HA	1.98	0.45
2:D:398:VAL:HG13	2:D:514:ILE:HD13	1.99	0.45
2:D:355:ILE:HB	2:D:378:ILE:HB	1.99	0.45
2:D:516:ASP:HA	2:D:546:ILE:HB	1.98	0.45
1:A:416:THR:HG21	1:A:476:GLN:HA	1.99	0.45
2:B:105:SER:HA	2:B:151:LEU:HD22	1.99	0.45
1:A:62:VAL:HA	1:A:65:ILE:HD12	1.99	0.44
3:E:90:THR:HG23	3:E:112:THR:HA	1.98	0.44
1:C:62:VAL:HA	1:C:65:ILE:HD12	2.00	0.44
2:B:355:ILE:HB	2:B:378:ILE:HB	1.99	0.44
1:C:58:LEU:HA	1:C:61:ILE:HD12	2.00	0.44
2:B:499:LEU:HA	2:B:502:ILE:HD12	2.00	0.44
1:A:201:GLY:HA3	2:B:439:ILE:HG21	1.99	0.44
1:C:92:LEU:HD11	1:C:306:VAL:HG13	2.00	0.44
1:C:227:ARG:HA	1:C:230:ILE:HG12	2.00	0.44
1:A:58:LEU:HA	1:A:61:ILE:HD12	2.00	0.43
1:A:180:LEU:HA	1:A:183:LYS:HD2	2.00	0.43
2:B:364:TYR:HD2	2:B:370:VAL:HG21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:LEU:HA	1:C:183:LYS:HD2	2.00	0.43
1:A:414:GLN:HB3	2:B:494:GLN:HG3	1.99	0.43
3:E:40:ALA:HB3	3:E:43:LYS:HB2	2.00	0.43
1:C:181:PHE:HZ	1:C:236:ILE:HD11	1.83	0.43
2:D:453:ASN:HD22	2:D:456:ALA:HB2	1.83	0.43
3:F:40:ALA:HB3	3:F:43:LYS:HB2	2.01	0.43
1:A:92:LEU:HD11	1:A:306:VAL:HG13	1.99	0.43
3:E:60:ALA:HB3	3:E:63:VAL:HG22	2.01	0.43
1:A:227:ARG:HA	1:A:230:ILE:HG12	2.00	0.43
3:E:7:SER:HB2	3:E:21:SER:HB3	2.01	0.43
2:D:207:GLU:HB3	2:D:252:VAL:HG21	2.01	0.42
1:C:156:SER:HA	1:C:159:LEU:HD12	2.00	0.42
1:C:477:ARG:HA	1:C:480:ILE:HD12	2.01	0.42
1:A:181:PHE:HZ	1:A:236:ILE:HD11	1.83	0.42
2:B:207:GLU:HB3	2:B:252:VAL:HG21	2.01	0.42
2:D:29:LEU:HA	2:D:32:LEU:HD12	2.02	0.42
2:D:364:TYR:HD2	2:D:370:VAL:HG21	1.85	0.42
1:A:200:LEU:HD11	1:A:465:ARG:NH2	2.36	0.41
2:B:226:LEU:HA	2:B:229:ILE:HD12	2.02	0.41
1:C:181:PHE:HA	1:C:184:ILE:HD12	2.02	0.41
1:A:237:VAL:HA	1:A:240:LEU:HD12	2.03	0.41
1:C:237:VAL:HA	1:C:240:LEU:HD12	2.03	0.41
3:F:60:ALA:HB3	3:F:63:VAL:HG22	2.01	0.41
2:B:29:LEU:HA	2:B:32:LEU:HD12	2.02	0.41
2:D:226:LEU:HA	2:D:229:ILE:HD12	2.03	0.41
1:A:378:LEU:HB3	1:A:390:VAL:HG21	2.03	0.41
1:C:475:LYS:HA	1:C:478:LEU:HD12	2.02	0.41
2:D:25:LEU:HD13	2:D:324:LEU:HD11	2.03	0.41
1:C:420:SER:HA	1:C:463:VAL:O	2.21	0.41
1:A:181:PHE:HA	1:A:184:ILE:HD12	2.02	0.40
2:B:25:LEU:HD13	2:B:324:LEU:HD11	2.03	0.40
1:C:97:LEU:HA	2:D:226:LEU:HD11	2.03	0.40
2:D:498:GLN:HE22	2:D:520:SER:H	1.69	0.40
1:C:236:ILE:HD13	1:C:294:ASN:HD21	1.86	0.40
1:A:491:LEU:HD23	1:A:521:THR:HG23	2.03	0.40
1:C:378:LEU:HB3	1:C:390:VAL:HG21	2.04	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	567/587 (97%)	542 (96%)	24 (4%)	1 (0%)	43	74
1	C	567/587 (97%)	542 (96%)	25 (4%)	0	100	100
2	B	571/599 (95%)	543 (95%)	26 (5%)	2 (0%)	30	62
2	D	571/599 (95%)	541 (95%)	27 (5%)	3 (0%)	24	58
3	E	113/118 (96%)	100 (88%)	13 (12%)	0	100	100
3	F	113/118 (96%)	101 (89%)	12 (11%)	0	100	100
All	All	2502/2608 (96%)	2369 (95%)	127 (5%)	6 (0%)	43	74

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	531	GLN
2	D	393	GLY
2	D	531	GLN
1	A	447	GLN
2	B	291	ILE
2	D	291	ILE

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	494/503 (98%)	459 (93%)	35 (7%)	13	39
1	C	494/503 (98%)	461 (93%)	33 (7%)	15	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	508/531 (96%)	477 (94%)	31 (6%)	17	44
2	D	508/531 (96%)	475 (94%)	33 (6%)	15	42
3	E	92/94 (98%)	87 (95%)	5 (5%)	20	47
3	F	92/94 (98%)	88 (96%)	4 (4%)	26	52
All	All	2188/2256 (97%)	2047 (94%)	141 (6%)	16	43

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	8	LEU
1	A	17	LEU
1	A	20	LEU
1	A	44	ILE
1	A	88	LEU
1	A	91	ASP
1	A	97	LEU
1	A	140	LEU
1	A	155	LEU
1	A	168	LEU
1	A	169	LEU
1	A	173	LEU
1	A	192	ASN
1	A	196	ARG
1	A	200	LEU
1	A	217	ASN
1	A	235	LEU
1	A	272	ILE
1	A	279	LEU
1	A	292	ILE
1	A	293	LEU
1	A	323	LEU
1	A	325	LEU
1	A	383	ILE
1	A	447	GLN
1	A	450	ASP
1	A	455	LEU
1	A	485	VAL
1	A	495	ASP
1	A	496	CYS
1	A	503	ILE

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Mol	Chain	Res	Type
1	A	514	ARG
1	A	523	ILE
1	A	538	LEU
2	B	29	LEU
2	B	66	VAL
2	B	76	LEU
2	B	89	LEU
2	B	92	LEU
2	B	104	LEU
2	B	112	LEU
2	B	123	VAL
2	B	157	GLN
2	B	184	LEU
2	B	189	LEU
2	B	192	LEU
2	B	210	ARG
2	B	227	THR
2	B	235	GLU
2	B	263	LEU
2	B	266	LEU
2	B	324	LEU
2	B	348	LEU
2	B	354	GLU
2	B	398	VAL
2	B	415	ASP
2	B	419	ILE
2	B	427	LEU
2	B	463	GLU
2	B	486	THR
2	B	488	ASN
2	B	503	THR
2	B	537	LEU
2	B	562	LEU
2	B	591	TYR
1	C	3	THR
1	C	8	LEU
1	C	17	LEU
1	C	20	LEU
1	C	44	ILE
1	C	88	LEU
1	C	91	ASP
1	C	97	LEU

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Mol	Chain	Res	Type
1	C	140	LEU
1	C	168	LEU
1	C	169	LEU
1	C	173	LEU
1	C	192	ASN
1	C	200	LEU
1	C	217	ASN
1	C	235	LEU
1	C	272	ILE
1	C	273	MET
1	C	279	LEU
1	C	292	ILE
1	C	293	LEU
1	C	323	LEU
1	C	325	LEU
1	C	383	ILE
1	C	440	VAL
1	C	447	GLN
1	C	475	LYS
1	C	485	VAL
1	C	496	CYS
1	C	503	ILE
1	C	514	ARG
1	C	523	ILE
1	C	538	LEU
2	D	29	LEU
2	D	66	VAL
2	D	76	LEU
2	D	89	LEU
2	D	92	LEU
2	D	104	LEU
2	D	112	LEU
2	D	123	VAL
2	D	157	GLN
2	D	184	LEU
2	D	189	LEU
2	D	192	LEU
2	D	210	ARG
2	D	227	THR
2	D	235	GLU
2	D	263	LEU
2	D	266	LEU

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Mol	Chain	Res	Type
2	D	324	LEU
2	D	348	LEU
2	D	354	GLU
2	D	406	ASP
2	D	415	ASP
2	D	419	ILE
2	D	427	LEU
2	D	431	ILE
2	D	448	ASN
2	D	463	GLU
2	D	486	THR
2	D	503	THR
2	D	537	LEU
2	D	545	ILE
2	D	562	LEU
2	D	591	TYR
3	E	18	LEU
3	E	26	VAL
3	E	29	ILE
3	E	57	ILE
3	E	102	LEU
3	F	18	LEU
3	F	26	VAL
3	F	57	ILE
3	F	102	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	152	ASN
1	A	178	ASN
1	A	185	GLN
1	A	215	ASN
1	A	217	ASN
1	A	248	ASN
1	A	277	ASN
1	A	291	ASN
1	A	336	ASN
1	A	344	ASN
1	A	474	GLN
1	A	526	GLN

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Mol	Chain	Res	Type
2	B	35	HIS
2	B	146	ASN
2	B	148	ASN
2	B	208	ASN
2	B	216	ASN
2	B	268	ASN
2	B	271	ASN
2	B	311	ASN
2	B	316	GLN
2	B	448	ASN
2	B	453	ASN
2	B	476	HIS
2	B	509	ASN
2	B	551	ASN
1	C	83	ASN
1	C	152	ASN
1	C	178	ASN
1	C	185	GLN
1	C	215	ASN
1	C	217	ASN
1	C	277	ASN
1	C	291	ASN
1	C	336	ASN
1	C	426	ASN
2	D	35	HIS
2	D	142	ASN
2	D	146	ASN
2	D	148	ASN
2	D	208	ASN
2	D	216	ASN
2	D	268	ASN
2	D	311	ASN
2	D	316	GLN
2	D	436	GLN
2	D	453	ASN
2	D	476	HIS
2	D	488	ASN
2	D	509	ASN
2	D	551	ASN
3	E	107	GLN
3	F	76	ASN
3	F	107	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 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	A	600	5	32,33,33	0.28	0	45,52,52	0.36	0
4	AGS	B	600	5	32,33,33	0.28	0	45,52,52	0.36	0
4	AGS	D	600	5	32,33,33	0.30	0	45,52,52	0.35	0
4	AGS	C	600	5	32,33,33	0.27	0	45,52,52	0.36	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AGS	A	600	5	-	2/21/38/38	0/3/3/3
4	AGS	B	600	5	-	1/21/38/38	0/3/3/3
4	AGS	D	600	5	-	5/21/38/38	0/3/3/3
4	AGS	C	600	5	-	2/21/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

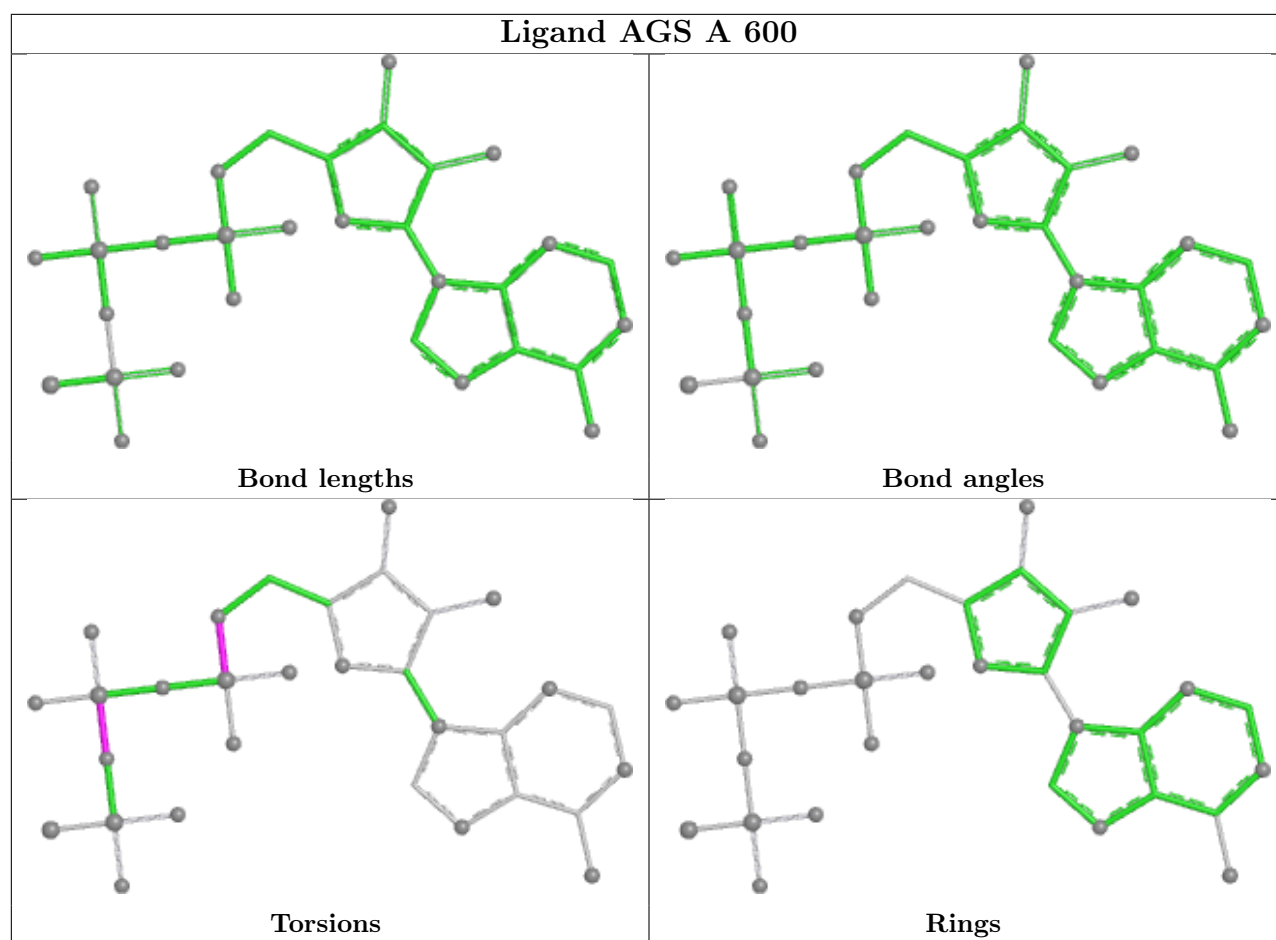
All (10) torsion outliers are listed below:

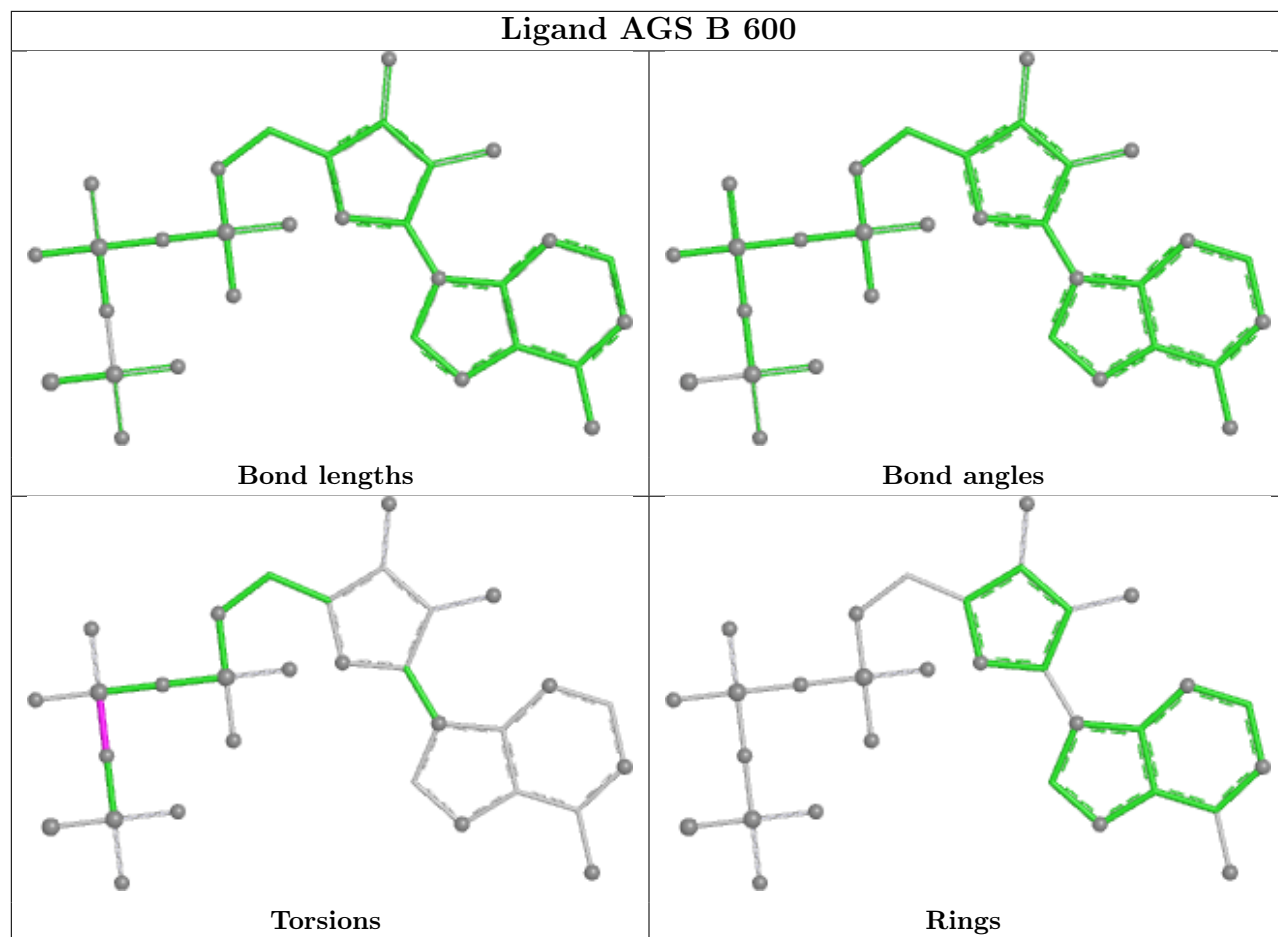
Mol	Chain	Res	Type	Atoms
4	D	600	AGS	PB-O3B-PG-O2G
4	A	600	AGS	C5'-O5'-PA-O1A
4	C	600	AGS	C5'-O5'-PA-O1A
4	D	600	AGS	C5'-O5'-PA-O1A
4	A	600	AGS	PG-O3B-PB-O2B
4	B	600	AGS	PG-O3B-PB-O2B
4	C	600	AGS	PG-O3B-PB-O2B
4	D	600	AGS	PG-O3B-PB-O1B
4	D	600	AGS	O4'-C4'-C5'-O5'
4	D	600	AGS	C3'-C4'-C5'-O5'

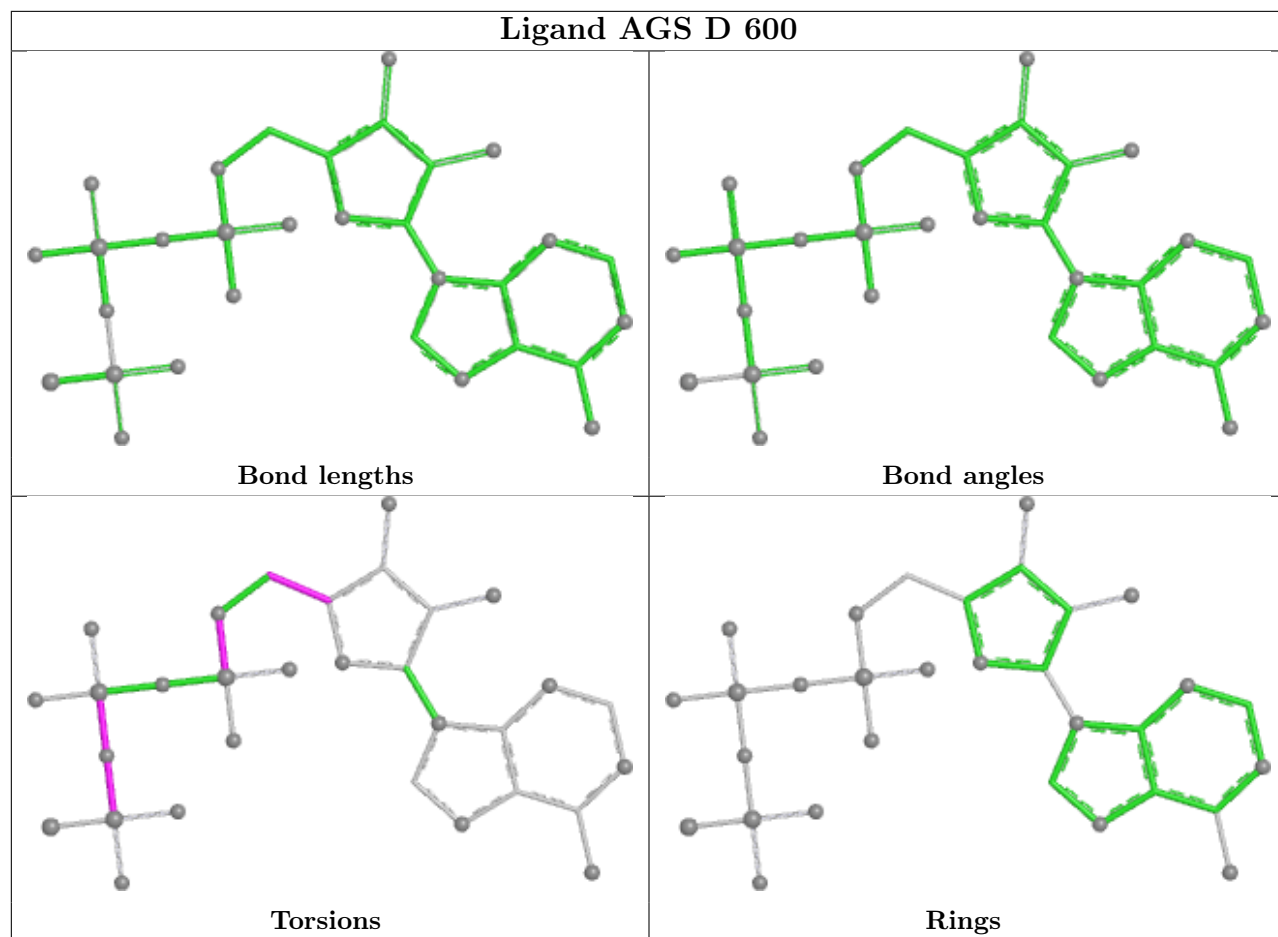
There are no ring outliers.

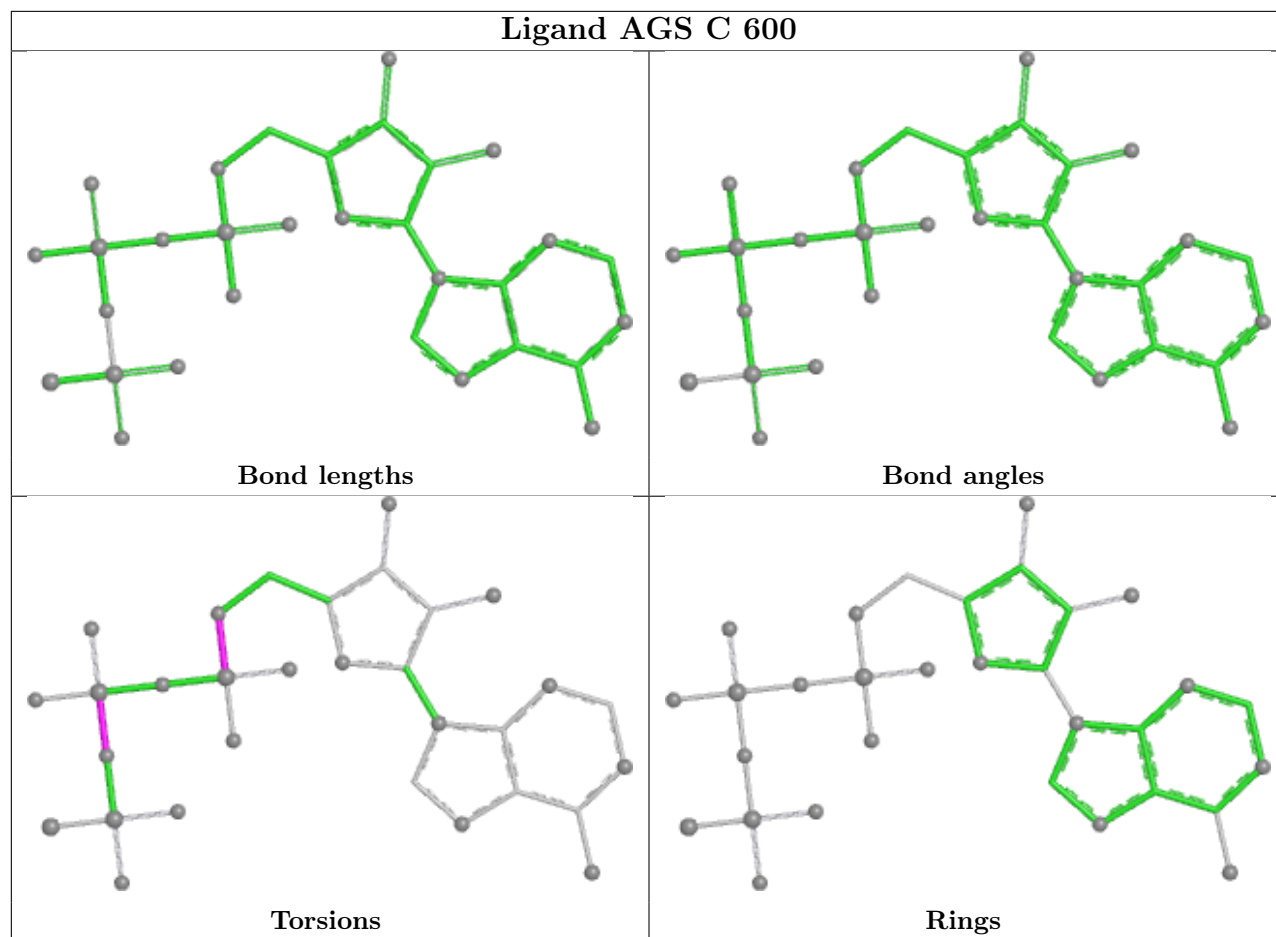
No monomer is involved in short contacts.

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 ⓘ

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	569/587 (96%)	-0.61	16 (2%) 55 32	73, 177, 277, 287	0
1	C	569/587 (96%)	-0.32	23 (4%) 42 24	99, 206, 269, 277	0
2	B	573/599 (95%)	-0.60	4 (0%) 84 63	76, 151, 276, 280	0
2	D	573/599 (95%)	-0.31	23 (4%) 42 24	103, 188, 267, 276	0
3	E	115/118 (97%)	-0.33	5 (4%) 40 22	154, 195, 215, 225	0
3	F	115/118 (97%)	-0.35	2 (1%) 69 44	181, 230, 248, 257	0
All	All	2514/2608 (96%)	-0.45	73 (2%) 53 31	73, 188, 271, 287	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	283	MET	7.7
1	C	247	VAL	7.3
2	D	574	ASP	7.2
1	A	264	ASN	6.9
1	C	280	MET	6.2
1	C	403	LYS	5.9
1	C	251	MET	5.8
2	D	262	VAL	5.4
2	D	40	ILE	5.3
1	C	75	VAL	5.1
2	D	266	LEU	4.9
1	C	243	PHE	4.8
2	D	150	VAL	4.7
1	C	399	THR	4.6
1	A	265	ASN	4.6
1	C	284	PHE	4.5
1	A	399	THR	4.3
1	A	247	VAL	4.3
1	A	238	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
2	D	264	PRO	4.0
3	E	75	LYS	3.9
2	D	314	SER	3.8
1	A	286	LEU	3.7
1	C	265	ASN	3.7
1	C	244	ILE	3.7
1	A	244	ILE	3.6
1	A	280	MET	3.5
3	F	72	ASP	3.5
1	A	243	PHE	3.4
2	D	39	LEU	3.4
3	E	72	ASP	3.4
1	C	14	PHE	3.3
1	A	251	MET	3.3
1	C	287	MET	3.3
1	C	402	LEU	3.2
1	A	266	GLN	3.2
1	C	240	LEU	3.2
1	A	283	MET	3.2
2	D	409	ARG	3.2
2	D	154	SER	3.1
2	D	267	MET	3.1
1	A	290	GLY	3.0
3	E	45	ARG	3.0
1	C	404	ASP	3.0
1	C	321	ASN	2.9
2	D	151	LEU	2.9
1	C	405	LEU	2.7
2	D	235	GLU	2.7
1	A	242	LEU	2.7
2	D	158	PHE	2.7
2	D	259	PHE	2.6
1	C	238	PHE	2.6
3	F	29	ILE	2.5
2	D	411	GLN	2.5
3	E	73	ASP	2.4
2	D	155	ILE	2.4
2	B	262	VAL	2.4
1	C	76	PHE	2.3
2	D	470	SER	2.3
2	B	312	GLU	2.3
2	B	264	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	287	MET	2.2
1	A	395	LEU	2.2
1	C	175	LYS	2.2
3	E	77	THR	2.2
1	C	528	ILE	2.2
2	D	459	GLU	2.1
2	D	108	VAL	2.1
1	C	380	PRO	2.1
2	D	270	VAL	2.1
2	D	338	GLU	2.0
2	B	182	VAL	2.0
2	D	59	LEU	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 oligosaccharides in this entry.

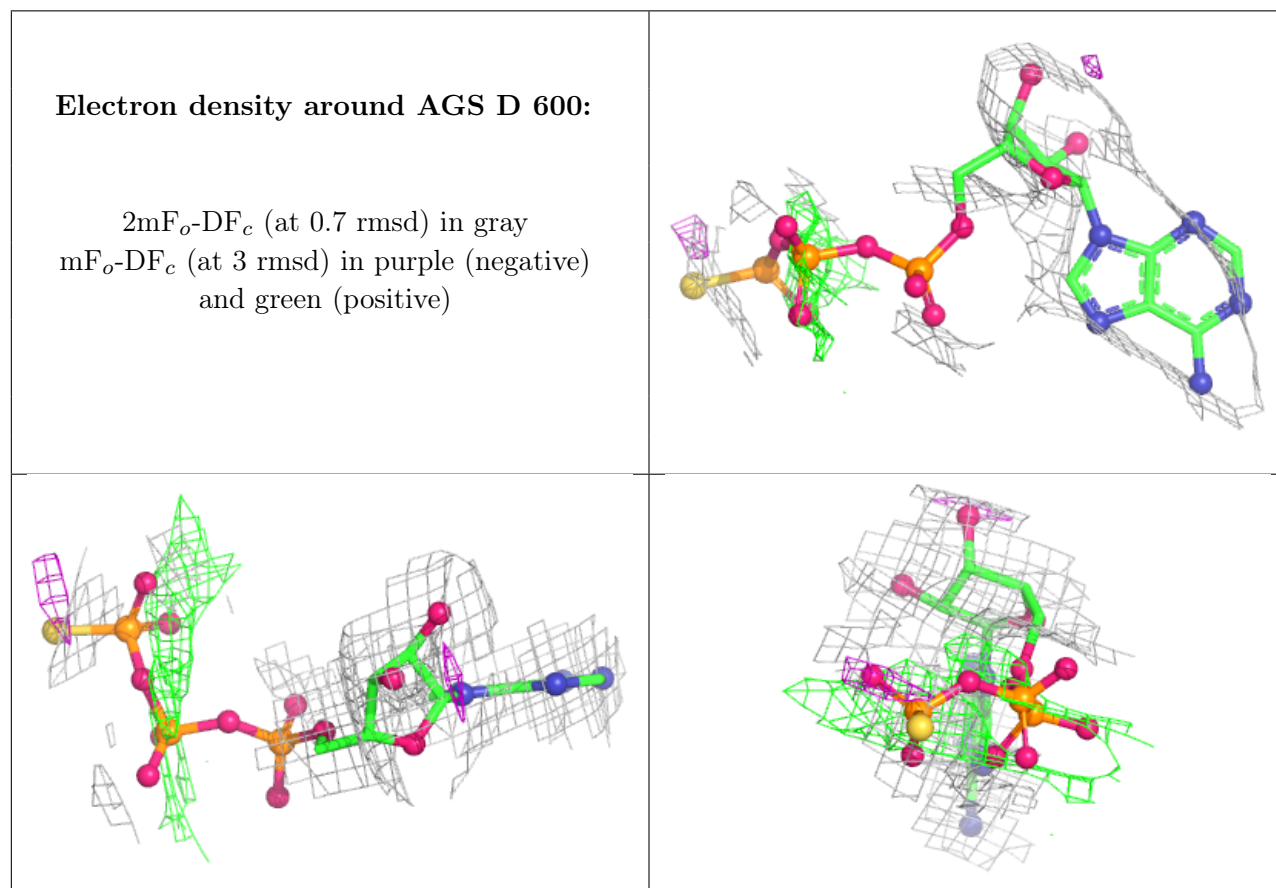
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MG	C	601	1/1	0.96	0.07	143,143,143,143	0
4	AGS	D	600	31/31	0.98	0.07	157,163,169,169	0
4	AGS	C	600	31/31	0.99	0.07	150,155,163,164	0
4	AGS	A	600	31/31	0.99	0.04	120,124,126,127	0
4	AGS	B	600	31/31	0.99	0.04	94,97,100,102	0
5	MG	B	601	1/1	1.00	0.04	76,76,76,76	0
5	MG	A	601	1/1	1.00	0.08	87,87,87,87	0
5	MG	D	601	1/1	1.00	0.08	121,121,121,121	0

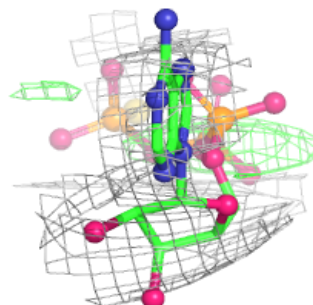
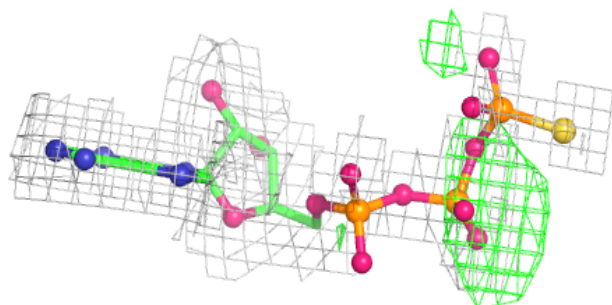
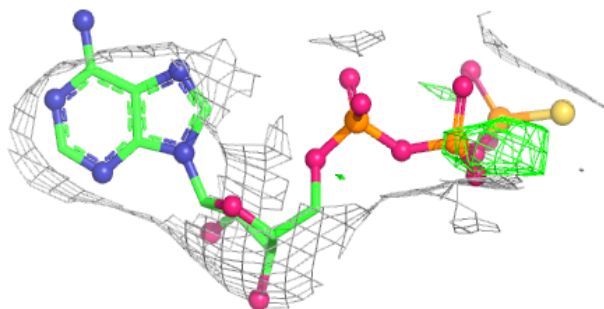
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

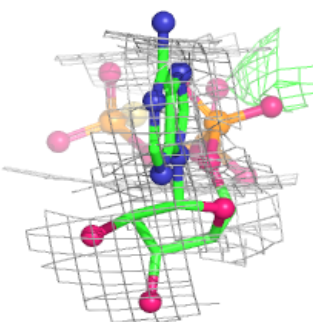
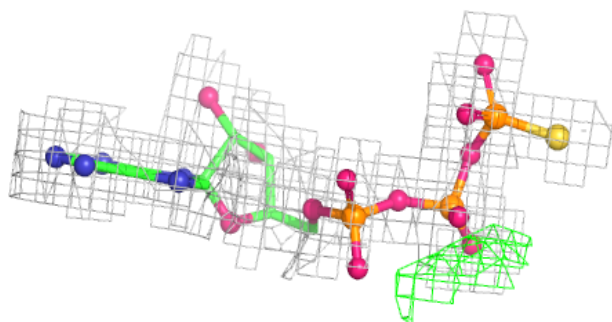
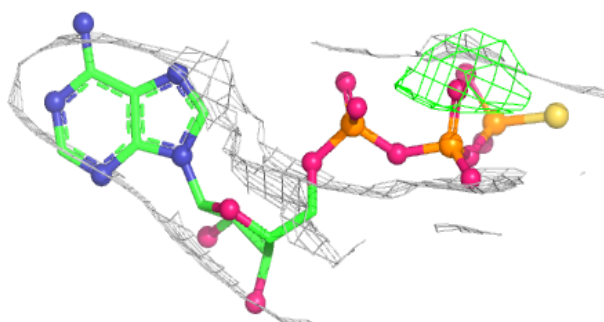


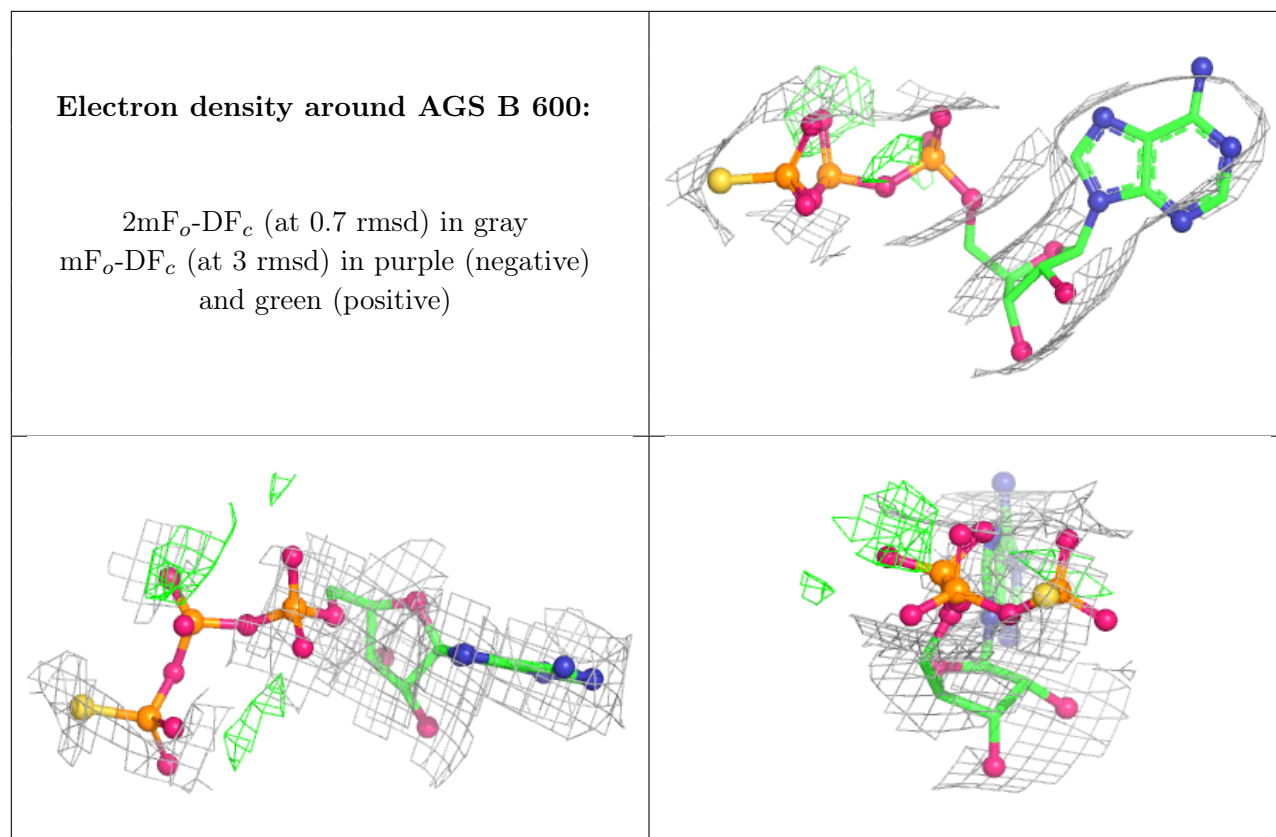
Electron density around AGS C 600:

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

**Electron density around AGS A 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.