



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:11 AM UTC

PDB ID : 6QV2 / pdb_00006qv2
Title : Structure of ATPgS-bound outward-facing TM287/288 in complex with nanobody Nb_TM#2
Authors : Hutter, C.A.J.; Huerlimann, L.M.; Zimmermann, I.; Egloff, P.; Seeger, M.A.
Deposited on : 2019-03-01
Resolution : 4.23 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

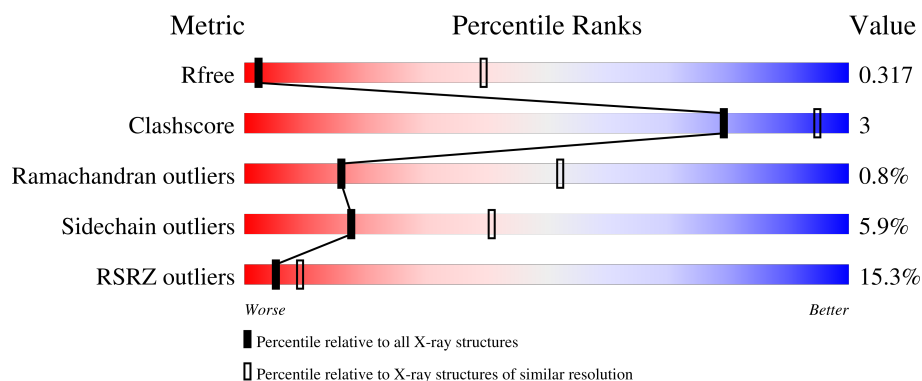
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.23 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	1042 (4.60-3.88)
Clashscore	190562	1043 (4.58-3.90)
Ramachandran outliers	187476	1031 (4.62-3.86)
Sidechain outliers	187428	1016 (4.62-3.86)
RSRZ outliers	180081	1039 (4.60-3.88)

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	17% 85% 11% ..
1	C	587	18% 86% 11% ..
2	B	599	10% 82% 12% 5%
2	D	599	12% 82% 12% 5%
3	E	132	19% 77% 18% ..

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Mol	Chain	Length	Quality of chain
3	F	132	20% 80% 16% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20086 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	568	Total	C	N	O	S	0	0	0
			4464	2879	768	798	19			
1	C	568	Total	C	N	O	S	0	0	0
			4464	2879	768	798	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	570	Total	C	N	O	S	0	0	0
			4541	2936	766	825	14			
2	D	570	Total	C	N	O	S	0	0	0
			4541	2936	766	825	14			

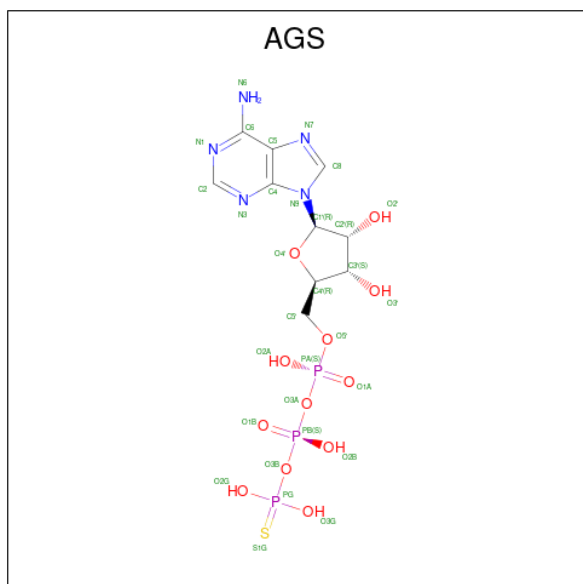
There are 6 discrepancies between the modelled and reference sequences:

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_TM No.2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	129	Total	C	N	O	S	0	0	0
			974	611	164	193	6			
3	F	129	Total	C	N	O	S	0	0	0
			974	611	164	193	6			

- 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		

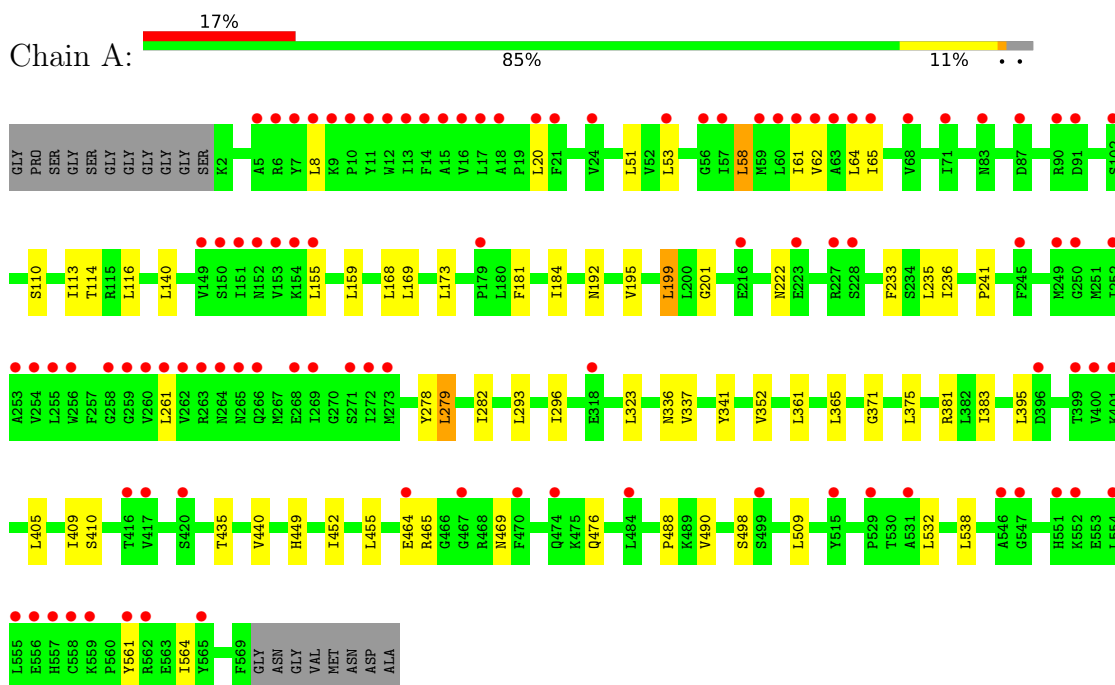
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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		

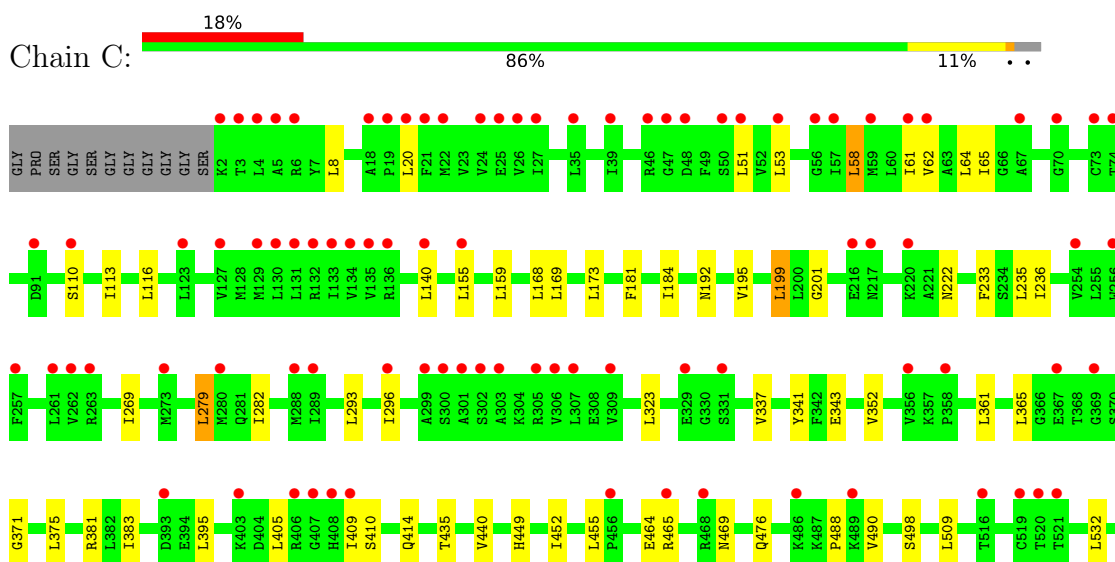
3 Residue-property plots [i](#)

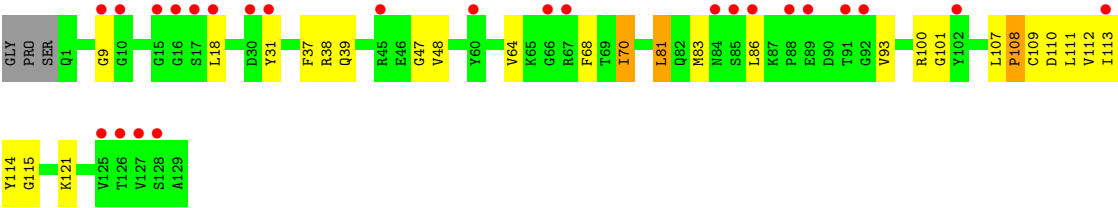
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

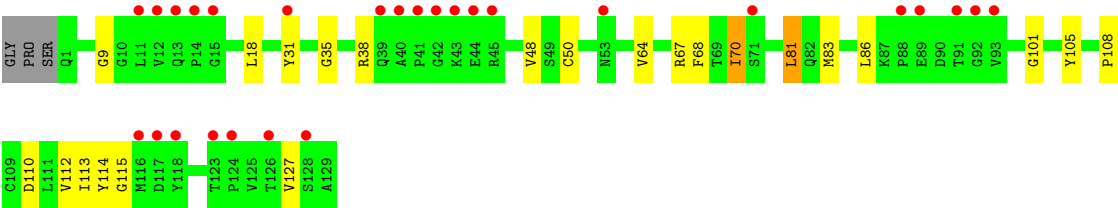
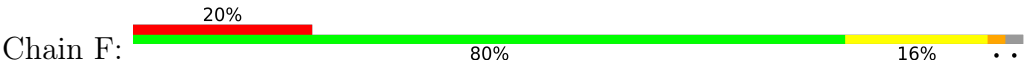


- Molecule 1: ABC transporter, ATP-binding protein





● Molecule 3: Nb_TM No.2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	88.60Å 113.07Å 126.89Å 83.18° 73.00° 67.37°	Depositor
Resolution (Å)	32.59 – 4.23 32.59 – 4.23	Depositor EDS
% Data completeness (in resolution range)	57.9 (32.59-4.23) 58.4 (32.59-4.23)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.82 (at 4.29Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.306 , 0.330 0.340 , 0.317	Depositor DCC
R_{free} test set	919 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	129.8	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.46 , 999.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.018 for -h,-h+k,-l	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	20086	wwPDB-VP
Average B, all atoms (Å ²)	167.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.07% 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	0.74	0/4539	1.29	0/6139
1	C	0.75	0/4539	1.29	0/6139
2	B	0.75	0/4619	1.35	5/6245 (0.1%)
2	D	0.75	0/4619	1.34	2/6245 (0.0%)
3	E	0.73	0/995	1.10	2/1345 (0.1%)
3	F	0.76	0/995	1.13	0/1345
All	All	0.75	0/20306	1.30	9/27458 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	186	ILE	CA-C-N	6.33	125.39	120.33
2	D	186	ILE	C-N-CA	6.33	125.39	120.33
2	B	186	ILE	CA-C-N	6.23	125.32	120.33
2	B	186	ILE	C-N-CA	6.23	125.32	120.33
3	E	108	PRO	CA-C-N	5.80	132.14	121.70
3	E	108	PRO	C-N-CA	5.80	132.14	121.70
2	B	124	PRO	CA-C-N	5.34	127.77	120.46
2	B	124	PRO	C-N-CA	5.34	127.77	120.46
2	B	317	PHE	N-CA-C	-5.13	107.15	113.41

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4464	0	4666	21	0
1	C	4464	0	4666	22	0
2	B	4541	0	4724	31	0
2	D	4541	0	4724	31	0
3	E	974	0	934	9	0
3	F	974	0	934	9	0
4	A	31	0	12	0	0
4	B	31	0	12	2	0
4	C	31	0	12	0	0
4	D	31	0	12	2	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	20086	0	20696	108	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 (108) 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)
3:F:38:ARG:HG2	3:F:48:VAL:HG22	1.79	0.64
2:D:216:ASN:HA	2:D:219:ILE:HD12	1.87	0.56
2:B:32:LEU:HB3	2:B:39:LEU:HD11	1.89	0.55
2:D:32:LEU:HB3	2:D:39:LEU:HD11	1.89	0.55
2:B:216:ASN:HA	2:B:219:ILE:HD12	1.89	0.55
3:E:9:GLY:HA2	3:E:18:LEU:HD22	1.89	0.55
2:B:198:SER:HB2	2:B:321:GLN:HG3	1.88	0.54
3:E:38:ARG:HH22	3:E:83:MET:HE3	1.71	0.54
2:B:117:PHE:HA	2:B:120:LEU:HD12	1.89	0.54
1:C:465:ARG:HG3	2:D:221:GLU:HG3	1.89	0.54
2:B:176:ASN:HD21	2:B:291:ILE:HD13	1.73	0.54
1:C:199:LEU:HB3	2:D:133:HIS:HD2	1.73	0.53
3:F:9:GLY:HA2	3:F:18:LEU:HD22	1.91	0.53
1:A:465:ARG:HG3	2:B:221:GLU:HG3	1.91	0.52
2:B:333:ILE:HA	2:B:336:LEU:HD12	1.91	0.52
3:E:38:ARG:HG2	3:E:48:VAL:HG22	1.92	0.52
1:A:476:GLN:HE22	1:A:498:SER:H	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:226:LEU:HA	2:B:229:ILE:HD12	1.91	0.52
1:C:561:TYR:HA	1:C:564:ILE:HD12	1.92	0.52
3:E:37:PHE:HA	3:E:47:GLY:HA2	1.92	0.51
1:C:201:GLY:HA3	2:D:439:ILE:HG21	1.92	0.51
1:C:476:GLN:HE22	1:C:498:SER:H	1.58	0.51
1:A:561:TYR:HA	1:A:564:ILE:HD12	1.93	0.51
2:D:226:LEU:HA	2:D:229:ILE:HD12	1.91	0.51
2:D:150:VAL:HG23	2:D:320:ILE:HG22	1.93	0.51
1:A:201:GLY:HA3	2:B:439:ILE:HG21	1.92	0.50
2:D:113:ARG:HG3	2:D:144:VAL:HG11	1.93	0.50
3:F:35:GLY:HA3	3:F:50:CYS:HA	1.93	0.50
1:A:233:PHE:HA	1:A:236:ILE:HD12	1.94	0.50
2:D:365:ASP:HB3	4:D:600:AGS:H2	1.93	0.50
3:E:100:ARG:HB2	3:E:111:LEU:HD23	1.92	0.50
1:A:199:LEU:HD21	2:B:136:ILE:HD13	1.94	0.50
1:C:233:PHE:HA	1:C:236:ILE:HD12	1.94	0.50
2:B:365:ASP:HB3	4:B:600:AGS:H2	1.93	0.50
3:F:70:ILE:HG23	3:F:81:LEU:HD23	1.95	0.49
1:C:181:PHE:HA	1:C:184:ILE:HD12	1.94	0.49
1:A:181:PHE:HA	1:A:184:ILE:HD12	1.94	0.49
3:F:64:VAL:HG13	3:F:67:ARG:HH11	1.78	0.48
3:E:70:ILE:HG23	3:E:81:LEU:HD23	1.96	0.48
1:A:222:ASN:HD21	2:B:113:ARG:HB3	1.77	0.48
1:A:464:GLU:HB2	1:A:469:ASN:HB3	1.95	0.48
1:A:279:LEU:HA	1:A:282:ILE:HD12	1.96	0.48
2:B:355:ILE:HD12	2:B:401:LEU:HD11	1.96	0.48
1:C:279:LEU:HA	1:C:282:ILE:HD12	1.95	0.48
2:D:79:TYR:HA	2:D:82:ILE:HD12	1.95	0.48
2:D:293:VAL:HA	2:D:296:ILE:HD12	1.96	0.48
1:C:464:GLU:HB2	1:C:469:ASN:HB3	1.95	0.47
2:D:355:ILE:HD12	2:D:401:LEU:HD11	1.96	0.47
1:C:337:VAL:HB	1:C:352:VAL:HB	1.96	0.47
1:A:337:VAL:HB	1:A:352:VAL:HB	1.96	0.47
1:C:199:LEU:HD21	2:D:136:ILE:HD13	1.98	0.46
2:D:409:ARG:HD2	3:F:105:TYR:HB2	1.98	0.46
2:D:105:SER:HA	2:D:151:LEU:HD22	1.99	0.45
2:B:67:VAL:HG13	2:B:70:PRO:HG2	1.98	0.45
2:B:441:PHE:H	2:B:448:ASN:HD21	1.64	0.45
1:C:410:SER:HB2	1:C:488:PRO:HG3	1.98	0.45
1:A:195:VAL:HG21	2:B:140:VAL:HG21	1.98	0.45
1:A:62:VAL:HA	1:A:65:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:80:MET:HA	2:D:83:LEU:HD12	1.98	0.45
2:B:327:ALA:HA	2:B:330:ILE:HD12	1.99	0.45
2:B:440:LEU:HD22	2:B:489:GLY:HA3	1.98	0.45
1:A:410:SER:HB2	1:A:488:PRO:HG3	1.98	0.45
3:E:39:GLN:HB2	3:E:93:VAL:O	2.17	0.45
1:A:409:ILE:HG12	1:A:490:VAL:HB	1.98	0.45
1:A:449:HIS:HA	1:A:452:ILE:HD12	1.99	0.45
1:C:293:LEU:HA	1:C:296:ILE:HD12	1.99	0.44
1:C:409:ILE:HG12	1:C:490:VAL:HB	1.98	0.44
1:C:449:HIS:HA	1:C:452:ILE:HD12	1.99	0.44
2:D:270:VAL:HA	2:D:273:LEU:HD12	1.98	0.44
2:B:419:ILE:HG23	2:B:420:ARG:HD3	2.00	0.44
1:C:62:VAL:HA	1:C:65:ILE:HD12	1.98	0.44
2:D:385:ALA:HB3	2:D:559:ILE:HG12	1.99	0.44
2:B:282:GLY:HA2	2:B:285:LEU:HD12	2.00	0.44
1:C:195:VAL:HG21	2:D:140:VAL:HG21	1.99	0.44
1:C:222:ASN:HD21	2:D:113:ARG:HB3	1.83	0.44
2:D:419:ILE:HG23	2:D:420:ARG:HD3	1.99	0.44
1:A:293:LEU:HA	1:A:296:ILE:HD12	1.99	0.44
2:B:270:VAL:HA	2:B:273:LEU:HD12	1.98	0.44
3:E:64:VAL:HB	3:E:68:PHE:CE2	2.53	0.44
2:B:67:VAL:HG11	2:B:76:LEU:HB2	2.00	0.43
2:B:25:LEU:HB2	2:B:324:LEU:HD21	1.99	0.42
2:B:409:ARG:HD3	3:E:107:LEU:HG	2.00	0.42
2:D:115:GLU:HB3	2:D:334:LEU:HD21	2.01	0.42
2:B:178:ILE:HA	2:B:181:LEU:HD12	2.01	0.42
1:A:452:ILE:HA	1:A:455:LEU:HD12	2.02	0.42
2:D:139:ARG:HA	2:D:143:ASP:HB2	2.00	0.42
2:B:63:THR:HG21	2:B:83:LEU:HD11	2.02	0.42
1:C:452:ILE:HA	1:C:455:LEU:HD12	2.02	0.42
1:C:110:SER:HA	1:C:113:ILE:HD12	2.02	0.42
2:D:178:ILE:HA	2:D:181:LEU:HD12	2.01	0.42
1:A:110:SER:HA	1:A:113:ILE:HD12	2.01	0.41
2:D:151:LEU:HA	2:D:155:ILE:HD12	2.03	0.41
2:D:134:GLY:HA2	2:D:137:ILE:HD12	2.03	0.41
1:C:58:LEU:HA	1:C:61:ILE:HD12	2.01	0.41
2:B:359:ASN:H	2:B:375:THR:HB	1.86	0.41
2:B:573:HIS:HA	2:B:576:LEU:HD12	2.03	0.41
1:A:58:LEU:HA	1:A:61:ILE:HD12	2.01	0.41
2:D:359:ASN:H	2:D:375:THR:HB	1.86	0.41
3:F:38:ARG:HH12	3:F:83:MET:HG2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:86:LEU:HD13	3:F:127:VAL:HG11	2.02	0.41
1:C:414:GLN:HB3	2:D:494:GLN:HG3	2.03	0.41
1:A:241:PRO:HB3	2:B:94:PHE:HB3	2.02	0.40
2:D:393:GLY:HA2	4:D:600:AGS:H5'1	2.03	0.40
2:D:69:VAL:HB	2:D:70:PRO:HD3	2.03	0.40
2:D:240:GLU:HA	2:D:243:ASP:HB2	2.03	0.40
2:B:240:GLU:HA	2:B:243:ASP:HB2	2.03	0.40
2:B:393:GLY:HA2	4:B:600:AGS:H5'1	2.04	0.40
3:F:68:PHE:HB3	3:F:81:LEU:HD21	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%)	544 (96%)	19 (3%)	3 (0%)	24	62
1	C	566/587 (96%)	542 (96%)	22 (4%)	2 (0%)	30	66
2	B	568/599 (95%)	541 (95%)	24 (4%)	3 (0%)	24	62
2	D	568/599 (95%)	540 (95%)	26 (5%)	2 (0%)	30	66
3	E	127/132 (96%)	93 (73%)	28 (22%)	6 (5%)	2	17
3	F	127/132 (96%)	94 (74%)	28 (22%)	5 (4%)	2	19
All	All	2522/2636 (96%)	2354 (93%)	147 (6%)	21 (1%)	16	52

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	108	PRO
3	F	108	PRO
3	E	101	GLY

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Mol	Chain	Res	Type
2	B	71	ARG
3	F	113	ILE
2	B	74	ASP
2	D	74	ASP
3	E	113	ILE
3	E	121	LYS
3	F	101	GLY
3	F	112	VAL
1	A	336	ASN
1	C	371	GLY
1	A	371	GLY
1	A	381	ARG
1	C	381	ARG
3	E	112	VAL
3	F	115	GLY
2	B	393	GLY
2	D	393	GLY
3	E	115	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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	494/503 (98%)	461 (93%)	33 (7%)	15	37
1	C	494/503 (98%)	462 (94%)	32 (6%)	15	38
2	B	506/531 (95%)	478 (94%)	28 (6%)	19	43
2	D	506/531 (95%)	480 (95%)	26 (5%)	21	44
3	E	102/104 (98%)	95 (93%)	7 (7%)	14	37
3	F	102/104 (98%)	97 (95%)	5 (5%)	22	45
All	All	2204/2276 (97%)	2073 (94%)	131 (6%)	18	41

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	20	LEU
1	A	51	LEU
1	A	53	LEU
1	A	58	LEU
1	A	64	LEU
1	A	114	THR
1	A	116	LEU
1	A	140	LEU
1	A	155	LEU
1	A	159	LEU
1	A	168	LEU
1	A	169	LEU
1	A	173	LEU
1	A	192	ASN
1	A	199	LEU
1	A	235	LEU
1	A	261	LEU
1	A	278	TYR
1	A	279	LEU
1	A	323	LEU
1	A	341	TYR
1	A	361	LEU
1	A	365	LEU
1	A	375	LEU
1	A	383	ILE
1	A	395	LEU
1	A	405	LEU
1	A	435	THR
1	A	440	VAL
1	A	509	LEU
1	A	532	LEU
1	A	538	LEU
2	B	76	LEU
2	B	92	LEU
2	B	96	LEU
2	B	107	ASP
2	B	116	LEU
2	B	145	ASP
2	B	172	MET
2	B	205	PHE
2	B	207	GLU
2	B	243	ASP

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Mol	Chain	Res	Type
2	B	246	ASN
2	B	266	LEU
2	B	277	LEU
2	B	291	ILE
2	B	295	THR
2	B	312	GLU
2	B	324	LEU
2	B	334	LEU
2	B	335	ASP
2	B	342	ASP
2	B	365	ASP
2	B	406	ASP
2	B	486	THR
2	B	514	ILE
2	B	550	LEU
2	B	558	LEU
2	B	562	LEU
2	B	587	PHE
1	C	8	LEU
1	C	20	LEU
1	C	51	LEU
1	C	53	LEU
1	C	58	LEU
1	C	64	LEU
1	C	116	LEU
1	C	140	LEU
1	C	155	LEU
1	C	159	LEU
1	C	168	LEU
1	C	169	LEU
1	C	173	LEU
1	C	192	ASN
1	C	199	LEU
1	C	235	LEU
1	C	269	ILE
1	C	279	LEU
1	C	323	LEU
1	C	341	TYR
1	C	343	GLU
1	C	361	LEU
1	C	365	LEU
1	C	375	LEU

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Mol	Chain	Res	Type
1	C	383	ILE
1	C	395	LEU
1	C	405	LEU
1	C	435	THR
1	C	440	VAL
1	C	509	LEU
1	C	532	LEU
1	C	538	LEU
2	D	75	LEU
2	D	92	LEU
2	D	96	LEU
2	D	107	ASP
2	D	116	LEU
2	D	123	VAL
2	D	172	MET
2	D	205	PHE
2	D	207	GLU
2	D	243	ASP
2	D	246	ASN
2	D	266	LEU
2	D	277	LEU
2	D	292	THR
2	D	312	GLU
2	D	332	GLU
2	D	338	GLU
2	D	342	ASP
2	D	365	ASP
2	D	406	ASP
2	D	451	TYR
2	D	486	THR
2	D	514	ILE
2	D	553	ILE
2	D	562	LEU
2	D	587	PHE
3	E	31	TYR
3	E	70	ILE
3	E	81	LEU
3	E	86	LEU
3	E	109	CYS
3	E	110	ASP
3	E	114	TYR
3	F	31	TYR

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Mol	Chain	Res	Type
3	F	70	ILE
3	F	81	LEU
3	F	110	ASP
3	F	114	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	105	ASN
1	A	185	GLN
1	A	215	ASN
1	A	266	GLN
1	A	291	ASN
1	A	344	ASN
1	A	447	GLN
1	A	476	GLN
2	B	121	GLN
2	B	146	ASN
2	B	176	ASN
2	B	195	GLN
2	B	216	ASN
2	B	246	ASN
2	B	271	ASN
2	B	272	ASN
2	B	359	ASN
2	B	448	ASN
2	B	488	ASN
2	B	509	ASN
2	B	521	ASN
2	B	551	ASN
1	C	105	ASN
1	C	185	GLN
1	C	222	ASN
1	C	266	GLN
1	C	291	ASN
1	C	336	ASN
1	C	474	GLN
1	C	476	GLN
2	D	148	ASN
2	D	195	GLN
2	D	246	ASN

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Mol	Chain	Res	Type
2	D	271	ASN
2	D	359	ASN
2	D	448	ASN
2	D	453	ASN
2	D	509	ASN
2	D	521	ASN
3	E	53	ASN
3	E	77	ASN
3	F	53	ASN
3	F	82	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 oligosaccharides 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	32,33,33	0.32	0	45,52,52	0.38	0
4	AGS	D	600	5	32,33,33	0.31	0	45,52,52	0.38	0
4	AGS	C	600	5	32,33,33	0.30	0	45,52,52	0.32	0
4	AGS	A	600	5	32,33,33	0.31	0	45,52,52	0.34	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	B	600	5	-	5/21/38/38	0/3/3/3
4	AGS	D	600	5	-	5/21/38/38	0/3/3/3
4	AGS	C	600	5	-	0/21/38/38	0/3/3/3
4	AGS	A	600	5	-	3/21/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	600	AGS	C5'-O5'-PA-O1A
4	B	600	AGS	C5'-O5'-PA-O3A
4	D	600	AGS	C5'-O5'-PA-O1A
4	D	600	AGS	C5'-O5'-PA-O3A
4	B	600	AGS	C5'-O5'-PA-O2A
4	D	600	AGS	C5'-O5'-PA-O2A
4	B	600	AGS	PA-O3A-PB-O1B
4	D	600	AGS	PA-O3A-PB-O1B
4	A	600	AGS	PB-O3B-PG-O3G
4	A	600	AGS	PG-O3B-PB-O1B
4	A	600	AGS	PG-O3B-PB-O2B
4	B	600	AGS	PA-O3A-PB-O2B
4	D	600	AGS	PA-O3A-PB-O2B

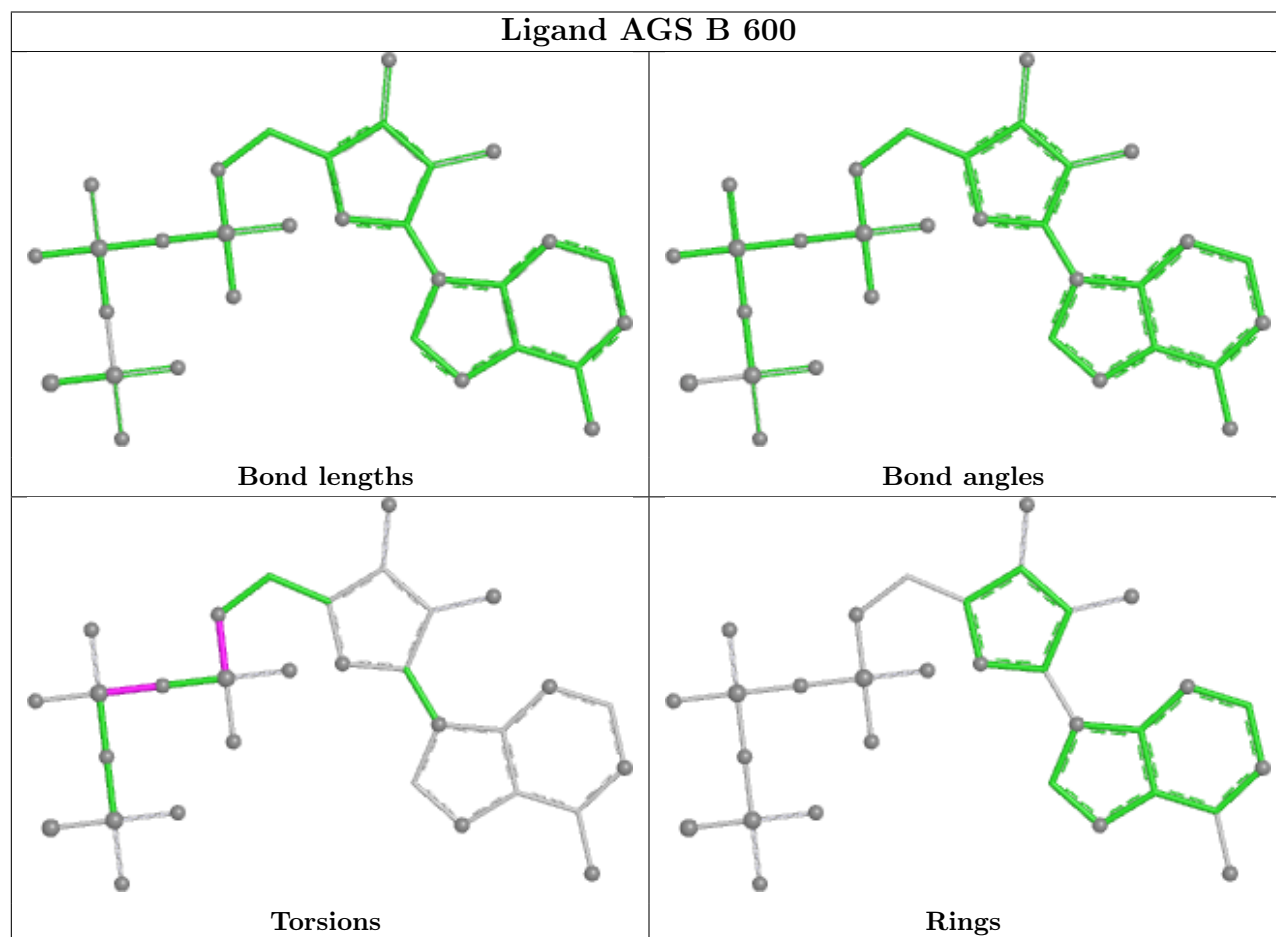
There are no ring outliers.

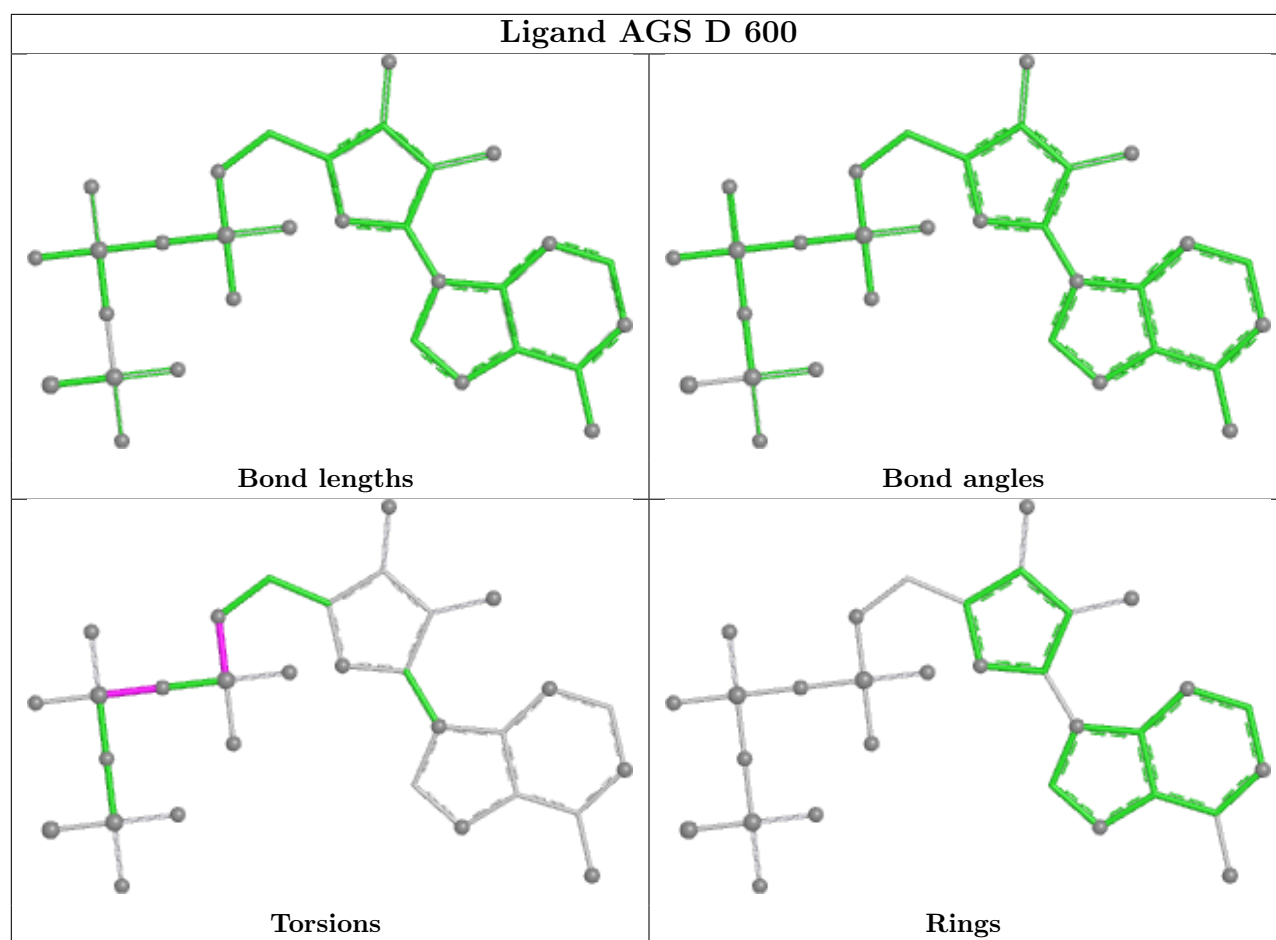
2 monomers are involved in 4 short contacts:

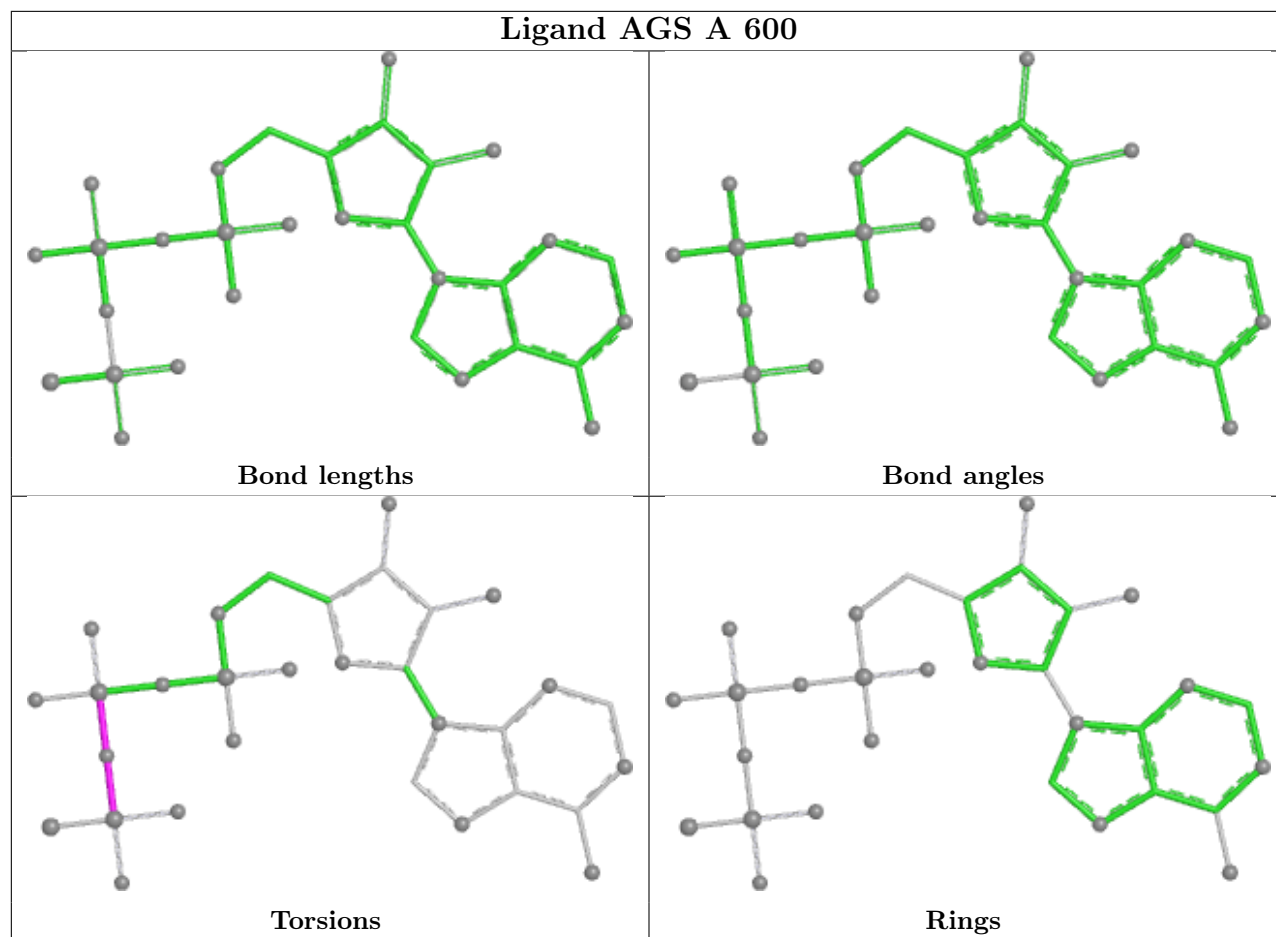
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	600	AGS	2	0
4	D	600	AGS	2	0

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.







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	568/587 (96%)	1.06	98 (17%) 4 7	36, 173, 288, 300	0
1	C	568/587 (96%)	1.05	106 (18%) 3 7	23, 229, 269, 283	0
2	B	570/599 (95%)	0.43	62 (10%) 10 14	3, 94, 191, 232	0
2	D	570/599 (95%)	0.64	70 (12%) 8 12	19, 193, 267, 289	0
3	E	129/132 (97%)	1.31	25 (19%) 3 7	94, 178, 298, 300	0
3	F	129/132 (97%)	1.27	27 (20%) 2 6	80, 133, 277, 300	0
All	All	2534/2636 (96%)	0.85	388 (15%) 5 9	3, 180, 276, 300	0

All (388) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	57	PRO	14.2
3	F	42	GLY	13.9
1	A	15	ALA	13.6
1	C	2	LYS	13.6
1	A	153	VAL	13.2
2	D	540	GLY	12.6
2	B	288	LYS	12.6
2	B	555	ASN	11.6
1	A	558	CYS	11.5
1	A	87	ASP	11.4
1	A	264	ASN	11.4
1	A	265	ASN	11.3
1	A	10	PRO	11.1
2	B	291	ILE	11.0
1	A	57	ILE	10.2
2	D	236	GLU	10.0
3	F	43	LYS	9.8
1	C	519	CYS	9.6
2	D	85	THR	9.3

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Mol	Chain	Res	Type	RSRZ
3	F	39	GLN	9.2
1	C	3	THR	9.1
1	A	253	ALA	9.1
3	E	128	SER	8.9
1	A	249	MET	8.8
2	B	56	SER	8.7
2	D	365	ASP	8.7
1	C	557	HIS	8.7
1	C	134	VAL	8.3
1	C	135	VAL	8.3
1	C	130	LEU	8.3
1	C	555	LEU	8.2
1	A	268	GLU	8.0
1	A	11	TYR	8.0
1	A	266	GLN	7.9
1	C	393	ASP	7.9
2	D	432	GLY	7.8
1	A	149	VAL	7.7
1	C	50	SER	7.6
1	C	5	ALA	7.5
1	A	555	LEU	7.5
1	C	547	GLY	7.5
1	A	61	ILE	7.5
1	A	250	GLY	7.3
2	D	78	ARG	7.2
1	A	551	HIS	7.2
3	E	85	SER	7.0
2	D	81	LEU	6.9
2	D	82	ILE	6.9
1	C	46	ARG	6.9
1	C	48	ASP	6.8
1	C	136	ARG	6.7
1	A	8	LEU	6.7
1	A	546	ALA	6.6
1	A	554	LEU	6.5
1	C	567	SER	6.5
1	A	64	LEU	6.5
1	A	252	ILE	6.5
2	D	380	PRO	6.5
1	A	90	ARG	6.4
1	C	296	ILE	6.4
2	B	508	ALA	6.4

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Mol	Chain	Res	Type	RSRZ
1	C	300	SER	6.4
1	A	562	ARG	6.4
1	A	60	LEU	6.3
1	C	554	LEU	6.3
1	C	403	LYS	6.3
2	B	72	ARG	6.3
3	E	88	PRO	6.3
2	D	72	ARG	6.2
2	B	71	ARG	6.2
1	C	261	LEU	6.2
1	A	18	ALA	6.1
1	C	329	GLU	6.1
1	A	20	LEU	6.0
1	A	259	GLY	5.9
1	A	152	ASN	5.9
1	A	83	ASN	5.9
3	E	66	GLY	5.9
1	C	407	GLY	5.7
2	D	381	GLY	5.7
3	F	117	ASP	5.7
1	C	302	SER	5.7
1	C	47	GLY	5.7
1	A	417	VAL	5.6
1	A	13	ILE	5.5
3	E	16	GLY	5.5
2	B	572	LYS	5.5
1	C	563	GLU	5.5
1	A	14	PHE	5.4
1	A	6	ARG	5.4
1	C	566	GLU	5.4
1	C	562	ARG	5.4
3	F	41	PRO	5.4
2	D	77	PRO	5.4
3	F	91	THR	5.3
1	C	305	ARG	5.3
1	C	301	ALA	5.3
1	C	22	MET	5.2
3	F	14	PRO	5.2
3	F	40	ALA	5.2
1	A	515	TYR	5.2
1	C	565	TYR	5.2
1	C	73	CYS	5.2

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Mol	Chain	Res	Type	RSRZ
1	C	558	CYS	5.2
1	C	155	LEU	5.2
3	F	88	PRO	5.2
3	F	13	GLN	5.1
2	B	26	ARG	5.1
3	E	127	VAL	5.1
1	C	546	ALA	5.1
2	D	79	TYR	5.1
1	A	260	VAL	5.1
1	C	521	THR	5.0
3	F	15	GLY	5.0
1	A	91	ASP	5.0
2	B	61	GLY	5.0
2	D	216	ASN	5.0
1	A	16	VAL	5.0
1	C	486	LYS	5.0
1	C	4	LEU	4.9
1	A	561	TYR	4.9
3	F	123	THR	4.9
1	C	132	ARG	4.9
1	C	74	THR	4.9
3	E	86	LEU	4.9
2	B	22	THR	4.8
2	B	541	LYS	4.8
3	F	126	THR	4.8
3	F	44	GLU	4.8
3	E	17	SER	4.8
1	A	318	GLU	4.7
2	D	233	THR	4.7
1	A	272	ILE	4.7
1	C	289	ILE	4.6
2	D	67	VAL	4.6
3	F	11	LEU	4.6
2	D	74	ASP	4.6
1	C	59	MET	4.6
1	A	499	SER	4.6
2	D	473	PHE	4.5
1	C	556	GLU	4.5
2	D	511	LYS	4.5
1	C	19	PRO	4.5
2	B	556	ALA	4.5
1	C	21	PHE	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	154	LYS	4.4
1	A	150	SER	4.4
3	F	89	GLU	4.4
1	C	299	ALA	4.3
2	B	281	PHE	4.3
2	B	571	GLY	4.3
2	B	347	GLU	4.3
1	C	256	TRP	4.3
2	B	554	LYS	4.2
1	A	62	VAL	4.2
2	D	484	VAL	4.2
1	C	307	LEU	4.2
2	D	469	HIS	4.2
1	A	254	VAL	4.2
1	C	24	VAL	4.2
2	D	217	GLY	4.2
1	C	57	ILE	4.2
2	B	378	ILE	4.2
2	D	367	LYS	4.2
1	A	399	THR	4.1
1	C	131	LEU	4.1
2	D	483	THR	4.1
1	A	271	SER	4.1
2	B	290	ILE	4.1
1	C	35	LEU	4.1
3	E	126	THR	4.1
1	A	396	ASP	4.1
2	D	541	LYS	4.1
1	A	258	GLY	4.1
1	A	547	GLY	4.1
1	A	17	LEU	4.0
1	C	303	ALA	4.0
1	A	5	ALA	4.0
1	A	269	ILE	4.0
1	C	409	ILE	4.0
2	B	29	LEU	3.9
1	A	56	GLY	3.9
2	B	58	TYR	3.9
2	B	59	LEU	3.9
2	B	185	SER	3.9
1	C	257	PHE	3.9
3	E	31	TYR	3.9

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Mol	Chain	Res	Type	RSRZ
2	D	538	MET	3.8
1	C	456	PRO	3.8
2	D	472	HIS	3.8
2	B	453	ASN	3.8
2	B	478	PRO	3.8
2	D	474	ILE	3.8
1	C	123	LEU	3.8
2	D	86	ILE	3.7
3	E	15	GLY	3.6
1	C	26	VAL	3.6
1	A	63	ALA	3.6
1	C	53	LEU	3.6
2	D	75	LEU	3.6
1	A	400	VAL	3.5
1	C	358	PRO	3.5
3	F	92	GLY	3.5
1	C	133	ILE	3.5
1	C	25	GLU	3.5
1	A	467	GLY	3.5
3	E	125	VAL	3.5
2	D	89	LEU	3.5
1	C	254	VAL	3.4
2	B	559	ILE	3.4
2	D	395	THR	3.4
1	A	151	ILE	3.4
2	D	23	ALA	3.4
2	D	68	PHE	3.4
1	C	288	MET	3.4
2	B	377	HIS	3.4
2	D	588	THR	3.4
1	A	556	GLU	3.4
2	D	398	VAL	3.4
1	A	552	LYS	3.4
1	C	20	LEU	3.3
1	C	216	GLU	3.3
2	B	73	PHE	3.3
1	A	12	TRP	3.3
3	E	18	LEU	3.3
3	E	89	GLU	3.3
1	A	464	GLU	3.3
1	C	129	MET	3.2
1	C	306	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	510	PRO	3.2
1	A	9	LYS	3.2
1	C	561	TYR	3.2
1	A	21	PHE	3.2
1	A	273	MET	3.2
3	E	60	TYR	3.2
2	D	73	PHE	3.2
1	A	401	LYS	3.2
1	C	51	LEU	3.2
2	D	43	PHE	3.2
1	A	155	LEU	3.1
2	D	487	ASP	3.1
1	A	263	ARG	3.1
2	D	353	GLY	3.1
1	C	406	ARG	3.1
1	C	27	ILE	3.1
2	D	571	GLY	3.1
1	C	6	ARG	3.1
1	A	416	THR	3.1
3	F	128	SER	3.1
1	C	18	ALA	3.1
2	D	377	HIS	3.1
3	F	93	VAL	3.1
1	C	220	LYS	3.1
2	B	367	LYS	3.1
1	A	65	ILE	3.1
2	D	80	MET	3.1
3	E	113	ILE	3.1
2	D	130	ARG	3.0
2	D	399	ASN	3.0
1	A	245	PHE	3.0
1	C	110	SER	3.0
1	C	70	GLY	3.0
2	D	70	PRO	3.0
2	D	350	GLU	3.0
2	B	28	LEU	3.0
2	B	573	HIS	3.0
2	D	159	PHE	3.0
1	C	560	PRO	2.9
1	A	261	LEU	2.9
1	C	217	ASN	2.9
2	D	364	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	420	SER	2.9
3	E	67	ARG	2.9
3	E	91	THR	2.9
1	A	557	HIS	2.9
2	B	289	ASP	2.9
1	A	24	VAL	2.9
2	B	293	VAL	2.8
1	C	262	VAL	2.8
2	B	558	LEU	2.8
2	B	418	ASP	2.8
1	C	280	MET	2.8
3	E	45	ARG	2.8
3	F	31	TYR	2.8
2	D	525	LYS	2.8
1	C	489	LYS	2.8
3	E	102	TYR	2.8
2	B	30	GLY	2.8
1	A	7	TYR	2.7
1	C	568	GLN	2.7
1	C	61	ILE	2.7
2	D	366	LYS	2.7
3	F	12	VAL	2.7
1	A	565	TYR	2.7
2	D	491	ASP	2.7
2	D	214	GLN	2.7
2	D	476	HIS	2.6
3	F	45	ARG	2.6
1	C	516	THR	2.6
2	D	71	ARG	2.6
1	A	255	LEU	2.6
2	B	557	ASP	2.6
2	B	509	ASN	2.6
1	C	39	ILE	2.6
1	C	140	LEU	2.6
1	A	470	PHE	2.6
1	A	102	SER	2.6
2	D	83	LEU	2.6
3	F	116	MET	2.6
3	F	71	SER	2.5
3	E	9	GLY	2.5
1	C	356	VAL	2.5
2	B	60	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	216	GLU	2.5
3	F	53	ASN	2.5
2	B	550	LEU	2.5
1	A	256	TRP	2.5
1	C	367	GLU	2.5
3	F	124	PRO	2.5
1	A	474	GLN	2.5
1	C	569	PHE	2.4
1	A	529	PRO	2.4
2	D	66	VAL	2.4
1	C	369	GLY	2.4
2	D	305	GLN	2.4
2	B	269	MET	2.4
3	E	30	ASP	2.4
2	D	368	LYS	2.4
2	D	76	LEU	2.4
1	C	309	VAL	2.4
3	F	118	TYR	2.4
1	C	62	VAL	2.4
2	B	31	TYR	2.4
1	A	179	PRO	2.4
2	B	85	THR	2.4
1	C	465	ARG	2.4
1	C	56	GLY	2.3
3	E	10	GLY	2.3
1	C	331	SER	2.3
1	C	408	HIS	2.3
1	A	223	GLU	2.3
2	B	53	GLY	2.3
2	D	64	ILE	2.3
2	B	429	SER	2.3
2	D	45	PHE	2.3
1	A	262	VAL	2.3
2	D	352	ARG	2.3
1	A	484	LEU	2.3
2	B	87	TYR	2.3
1	C	263	ARG	2.3
2	B	80	MET	2.3
1	A	68	VAL	2.3
1	A	227	ARG	2.3
1	C	273	MET	2.3
2	B	285	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	356	GLU	2.2
1	A	559	LYS	2.2
2	B	282	GLY	2.2
2	B	366	LYS	2.2
2	B	574	ASP	2.2
2	B	292	THR	2.2
1	C	67	ALA	2.1
2	D	514	ILE	2.1
2	D	442	SER	2.1
1	C	542	GLU	2.1
2	B	88	ALA	2.1
2	D	512	ILE	2.1
1	A	228	SER	2.1
2	B	52	LEU	2.1
1	C	91	ASP	2.1
2	D	539	GLU	2.1
2	D	351	VAL	2.1
1	A	59	MET	2.1
1	C	520	THR	2.1
2	D	44	VAL	2.1
1	C	468	ARG	2.0
1	A	71	ILE	2.0
3	E	92	GLY	2.0
2	B	63	THR	2.0
1	A	53	LEU	2.0
2	B	433	ILE	2.0
2	B	97	GLN	2.0
2	B	33	ARG	2.0
2	D	583	TYR	2.0
1	A	531	ALA	2.0
2	B	107	ASP	2.0
1	C	127	VAL	2.0
3	E	84	ASN	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](#)

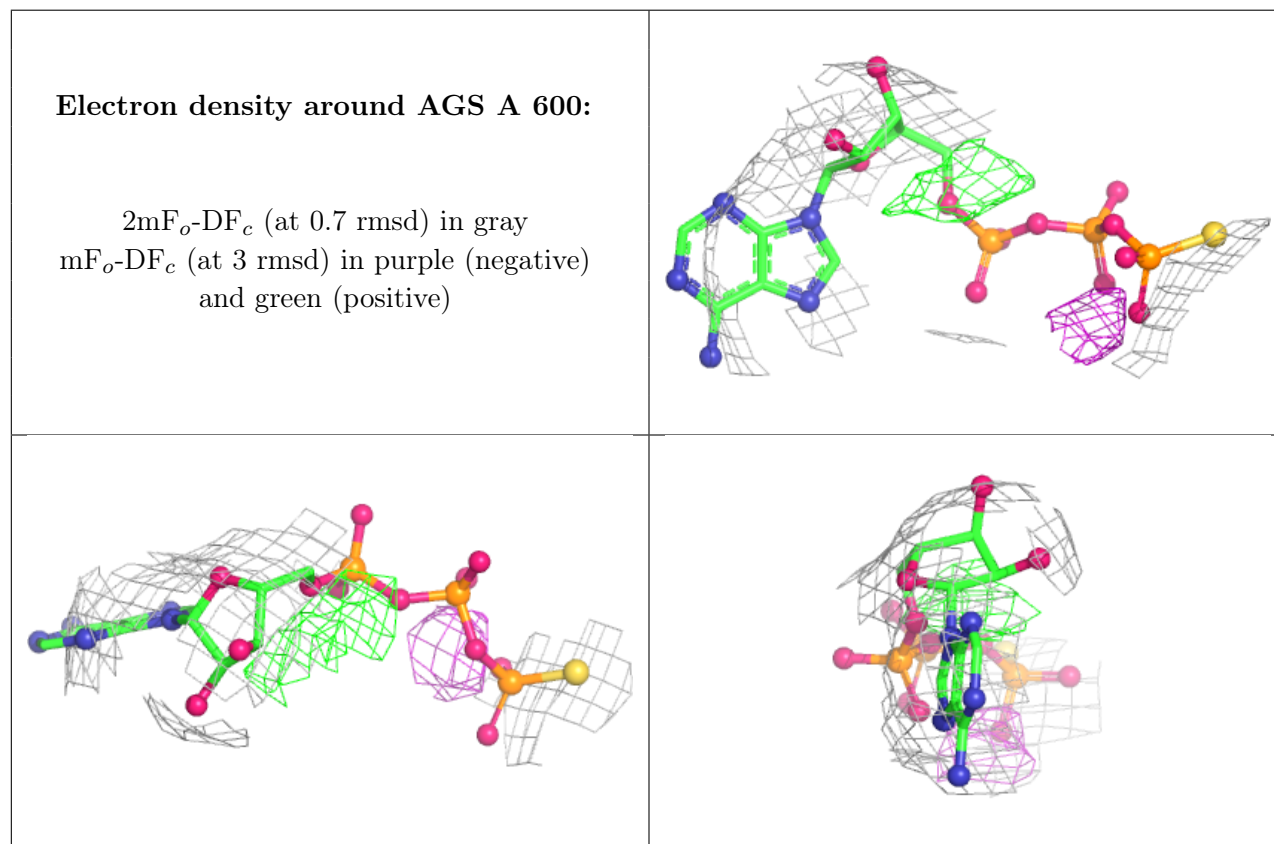
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

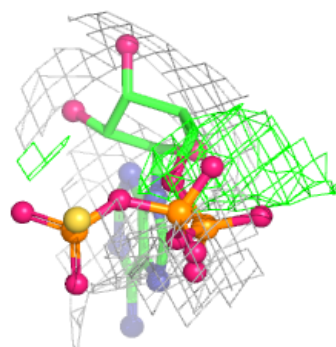
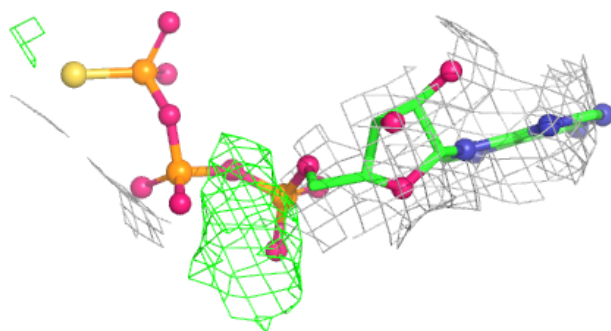
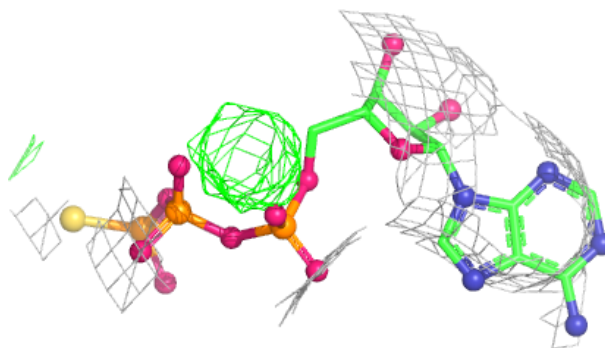
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MG	D	601	1/1	0.84	0.12	176,176,176,176	0
4	AGS	A	600	31/31	0.91	0.12	99,135,179,183	0
5	MG	C	601	1/1	0.93	0.08	217,217,217,217	0
5	MG	A	601	1/1	0.95	0.16	116,116,116,116	0
4	AGS	C	600	31/31	0.95	0.10	187,206,221,225	0
4	AGS	D	600	31/31	0.95	0.09	162,196,218,226	0
4	AGS	B	600	31/31	0.97	0.08	4,26,78,82	0
5	MG	B	601	1/1	1.00	0.04	70,70,70,70	0

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

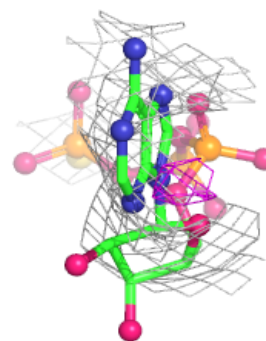
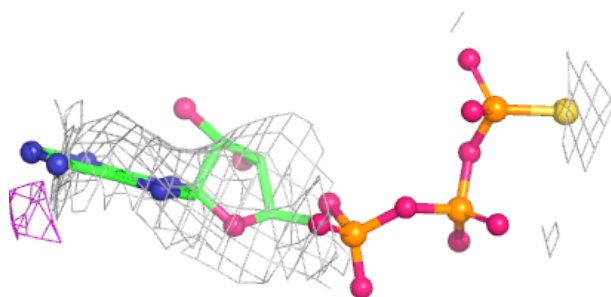
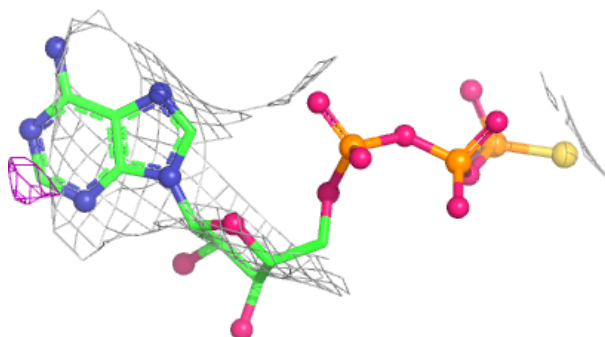


Electron density around AGS D 600:

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

**Electron density around AGS 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.