Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 06:00 pm BST

PDB ID	:	6QV1
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 following versions of software and data (see references ⓘ) were used in the production of this report:

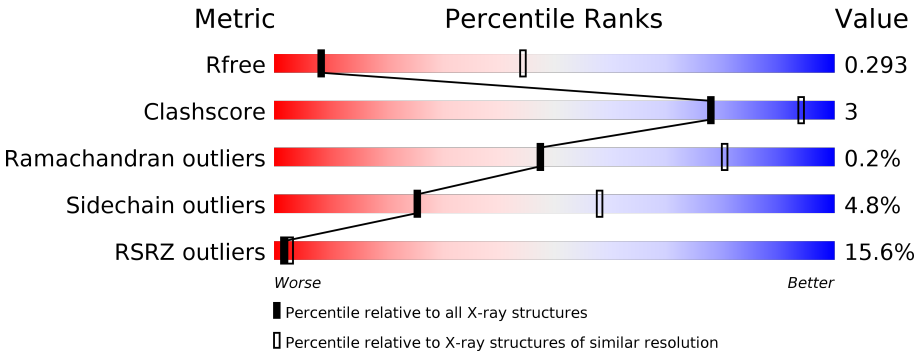
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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}	130704	1379 (3.56-3.40)
Clashscore	141614	1461 (3.56-3.40)
Ramachandran outliers	138981	1424 (3.56-3.40)
Sidechain outliers	138945	1425 (3.56-3.40)
RSRZ outliers	127900	1289 (3.56-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	12% 85% 12%
1	C	587	15% 86% 11%
2	B	599	8% 83% 12%
2	D	599	18% 82% 13%
3	E	118	28% 80% 18%
3	F	118	40% 83% 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			

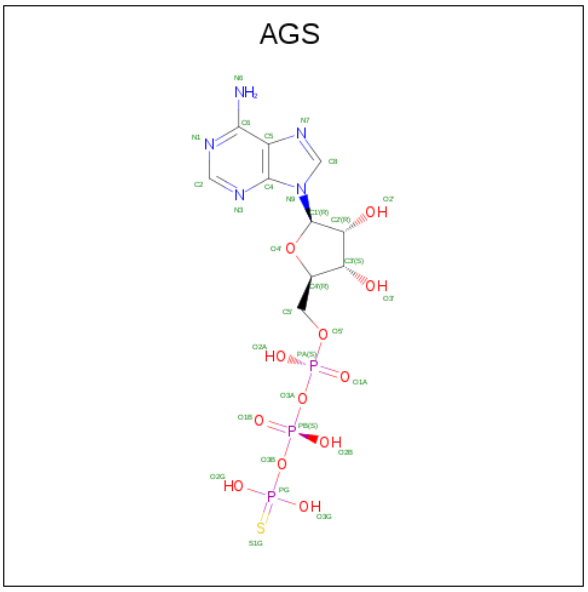
There are 6 discrepancies between the modelled and reference sequences:

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 (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



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 (three-letter code: MG) (formula: Mg).

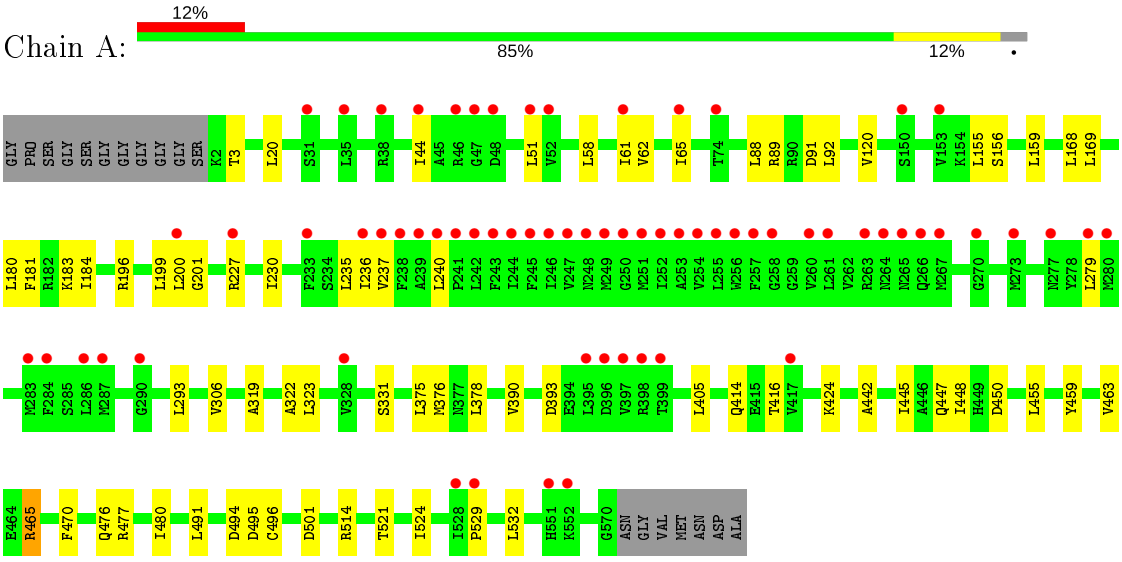
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (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.

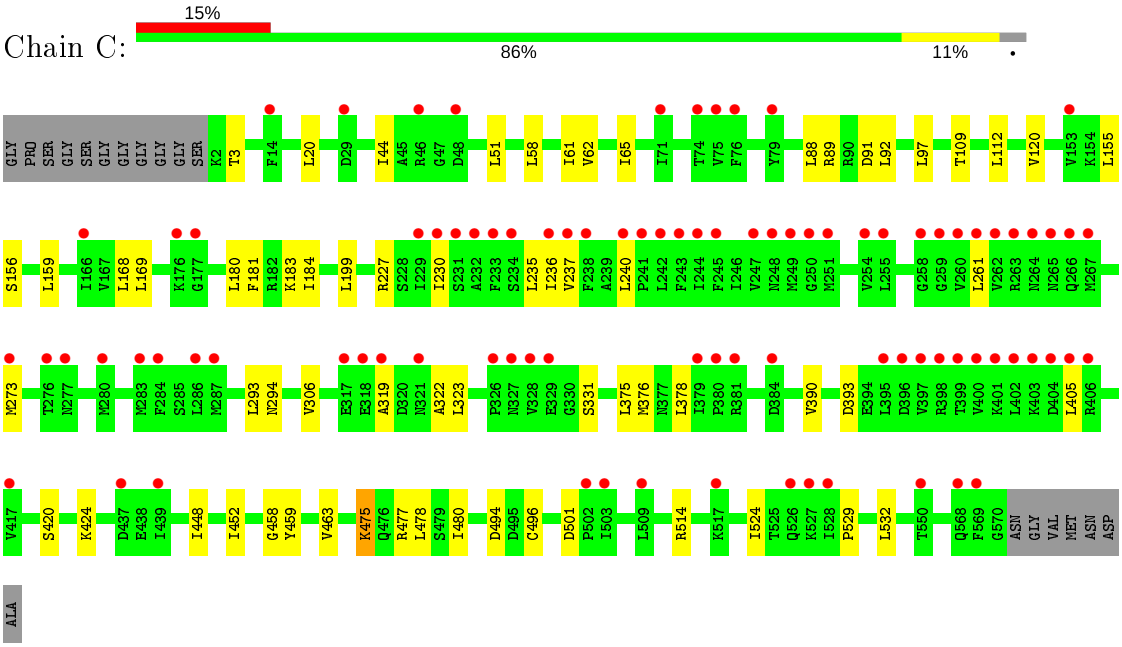
- Molecule 1: ABC transporter, ATP-binding protein

Chain A:



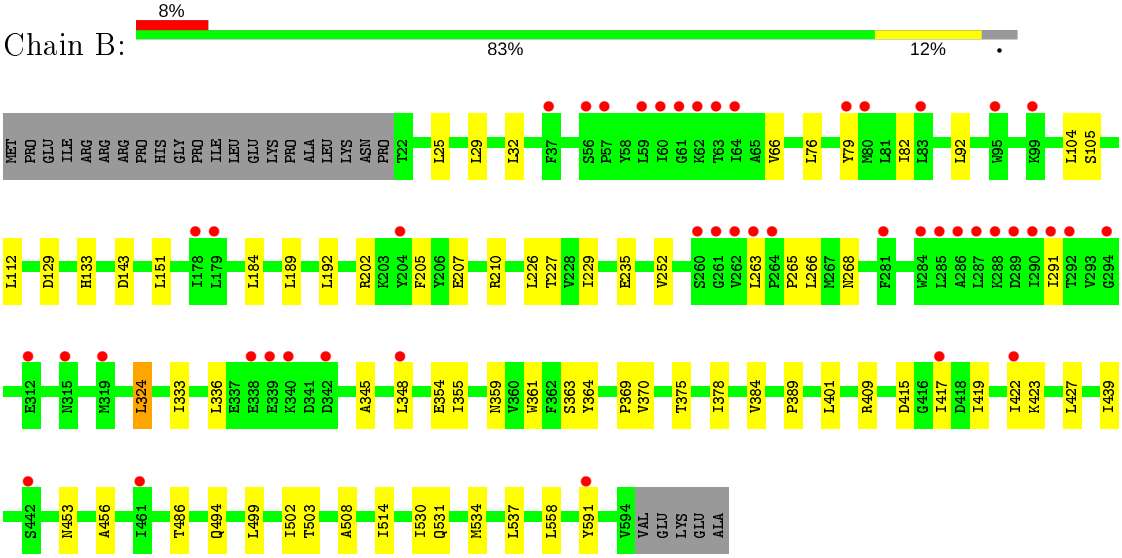
- Molecule 1: ABC transporter, ATP-binding protein

Chain C:



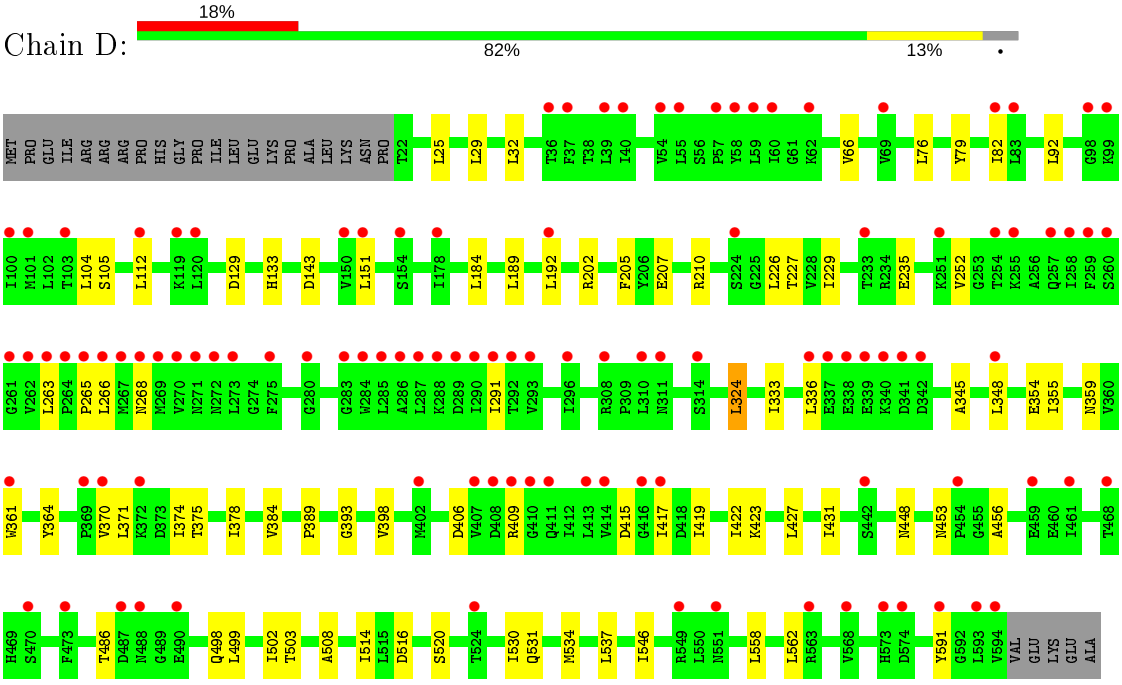
• Molecule 2: Uncharacterized ABC transporter ATP-binding protein TM_0288

Chain B:



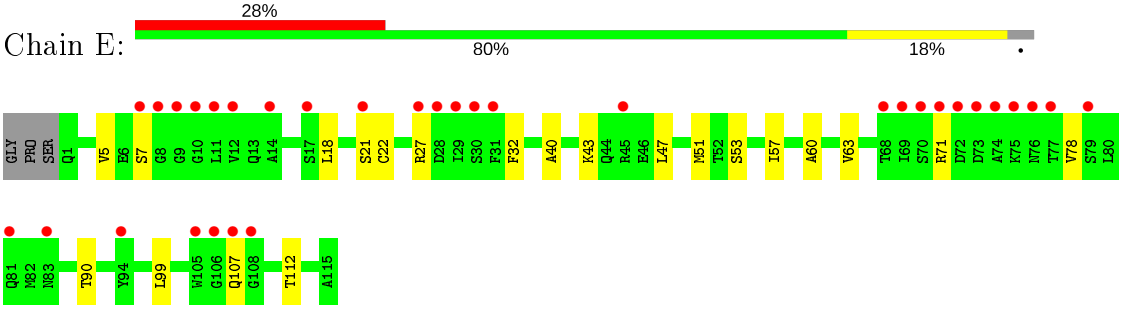
• Molecule 2: Uncharacterized ABC transporter ATP-binding protein TM_0288

Chain D:



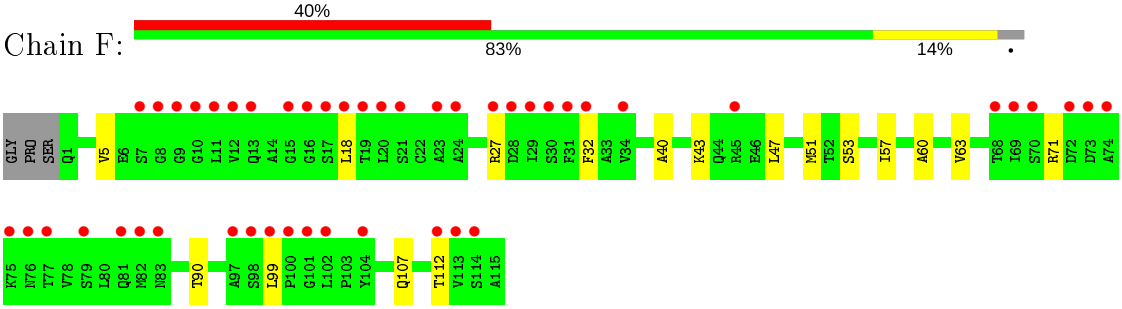
• Molecule 3: Nb_TM1

Chain E:



• Molecule 3: Nb_TM1

Chain F:



4 Data and refinement statistics (i)

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 48.48 – 3.48	Depositor EDS
% Data completeness (in resolution range)	58.2 (34.64-3.48) 58.2 (48.48-3.48)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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)	0.24 , 107.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.149 for h,-k,-l	Xtriage
F_o,F_c correlation	0.84	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0/4543	0.58	0/6144
1	C	0.41	0/4543	0.57	0/6144
2	B	0.40	0/4638	0.57	0/6271
2	D	0.41	0/4638	0.57	0/6271
3	E	0.39	0/883	0.57	0/1195
3	F	0.39	0/883	0.57	0/1195
All	All	0.41	0/20128	0.57	0/27220

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

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	25	0
2	D	4560	0	4748	27	0
3	E	866	0	858	8	0
3	F	866	0	858	6	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	19916	0	20598	117	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 (117) 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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:E:22:CYS:HB3	3:E:78:VAL:HG13	1.97	0.47
1:C:452:ILE:O	1:C:458:GLY:HA2	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:227:ARG:HA	1:C:230:ILE:HG12	2.00	0.44
1:C:92:LEU:HD11	1:C:306:VAL:HG13	2.00	0.44
1:A:180:LEU:HA	1:A:183:LYS:HD2	2.00	0.43
1:A:58:LEU:HA	1:A:61:ILE:HD12	2.00	0.43
2:B:364:TYR:HD2	2:B:370:VAL:HG21	1.83	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 (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	567/587 (97%)	542 (96%)	24 (4%)	1 (0%)	47 80
1	C	567/587 (97%)	542 (96%)	25 (4%)	0	100 100
2	B	571/599 (95%)	543 (95%)	26 (5%)	2 (0%)	34 70
2	D	571/599 (95%)	541 (95%)	27 (5%)	3 (0%)	29 66
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%)	47 80

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	531	GLN
2	D	393	GLY
2	D	531	GLN

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Mol	Chain	Res	Type
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%)	473 (96%)	21 (4%)	29	61
1	C	494/503 (98%)	478 (97%)	16 (3%)	39	68
2	B	508/531 (96%)	481 (95%)	27 (5%)	22	54
2	D	508/531 (96%)	477 (94%)	31 (6%)	18	50
3	E	92/94 (98%)	87 (95%)	5 (5%)	22	53
3	F	92/94 (98%)	87 (95%)	5 (5%)	22	53
All	All	2188/2256 (97%)	2083 (95%)	105 (5%)	25	58

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	20	LEU
1	A	44	ILE
1	A	51	LEU
1	A	88	LEU
1	A	91	ASP
1	A	155	LEU
1	A	168	LEU
1	A	169	LEU
1	A	196	ARG
1	A	235	LEU
1	A	279	LEU
1	A	293	LEU
1	A	323	LEU
1	A	405	LEU

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Mol	Chain	Res	Type
1	A	450	ASP
1	A	455	LEU
1	A	465	ARG
1	A	495	ASP
1	A	496	CYS
1	A	514	ARG
2	B	66	VAL
2	B	76	LEU
2	B	92	LEU
2	B	104	LEU
2	B	112	LEU
2	B	129	ASP
2	B	143	ASP
2	B	184	LEU
2	B	189	LEU
2	B	192	LEU
2	B	202	ARG
2	B	205	PHE
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	415	ASP
2	B	419	ILE
2	B	427	LEU
2	B	486	THR
2	B	503	THR
2	B	537	LEU
2	B	591	TYR
1	C	3	THR
1	C	20	LEU
1	C	44	ILE
1	C	51	LEU
1	C	88	LEU
1	C	91	ASP
1	C	168	LEU
1	C	169	LEU
1	C	235	LEU

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Mol	Chain	Res	Type
1	C	273	MET
1	C	293	LEU
1	C	323	LEU
1	C	405	LEU
1	C	475	LYS
1	C	496	CYS
1	C	514	ARG
2	D	66	VAL
2	D	76	LEU
2	D	92	LEU
2	D	104	LEU
2	D	112	LEU
2	D	129	ASP
2	D	143	ASP
2	D	184	LEU
2	D	189	LEU
2	D	192	LEU
2	D	202	ARG
2	D	205	PHE
2	D	210	ARG
2	D	227	THR
2	D	235	GLU
2	D	263	LEU
2	D	266	LEU
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	486	THR
2	D	503	THR
2	D	537	LEU
2	D	562	LEU
2	D	591	TYR
3	E	18	LEU
3	E	27	ARG
3	E	47	LEU
3	E	51	MET

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Mol	Chain	Res	Type
3	E	57	ILE
3	F	18	LEU
3	F	27	ARG
3	F	47	LEU
3	F	51	MET
3	F	57	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	ASN
1	A	215	ASN
1	A	248	ASN
2	B	268	ASN
2	B	271	ASN
2	B	311	ASN
2	B	448	ASN
2	B	453	ASN
1	C	152	ASN
1	C	215	ASN
1	C	248	ASN
2	D	133	HIS
2	D	268	ASN
2	D	271	ASN
2	D	311	ASN
2	D	436	GLN
2	D	453	ASN
2	D	476	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates 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	C	600	5	26,33,33	0.58	0	26,52,52	0.71	1 (3%)
4	AGS	B	600	5	26,33,33	0.58	0	26,52,52	0.70	1 (3%)
4	AGS	D	600	5	26,33,33	0.61	0	26,52,52	0.71	1 (3%)
4	AGS	A	600	5	26,33,33	0.59	0	26,52,52	0.70	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	C	600	5	-	2/17/38/38	0/3/3/3
4	AGS	B	600	5	-	1/17/38/38	0/3/3/3
4	AGS	D	600	5	-	5/17/38/38	0/3/3/3
4	AGS	A	600	5	-	2/17/38/38	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(^{o})	Ideal(^{o})
4	C	600	AGS	C5-C6-N6	2.25	123.77	120.35
4	A	600	AGS	C5-C6-N6	2.22	123.72	120.35
4	D	600	AGS	C5-C6-N6	2.21	123.71	120.35
4	B	600	AGS	C5-C6-N6	2.16	123.64	120.35

There are no chirality outliers.

All (10) torsion outliers are listed below:

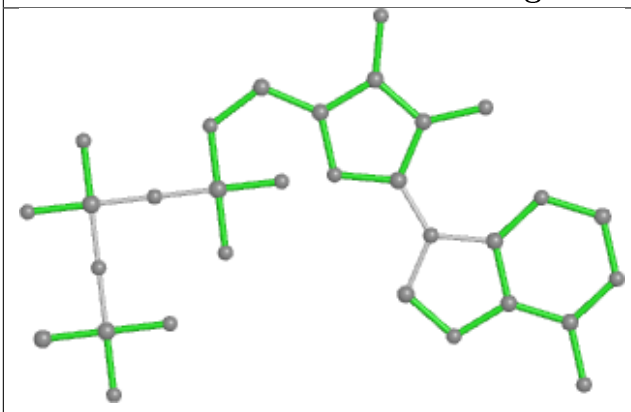
Mol	Chain	Res	Type	Atoms
4	D	600	AGS	PB-O3B-PG-O2G
4	C	600	AGS	PG-O3B-PB-O2B
4	B	600	AGS	PG-O3B-PB-O2B
4	D	600	AGS	PG-O3B-PB-O1B
4	A	600	AGS	PG-O3B-PB-O2B
4	D	600	AGS	C3'-C4'-C5'-O5'
4	D	600	AGS	O4'-C4'-C5'-O5'
4	C	600	AGS	C5'-O5'-PA-O1A
4	D	600	AGS	C5'-O5'-PA-O1A
4	A	600	AGS	C5'-O5'-PA-O1A

There are no ring outliers.

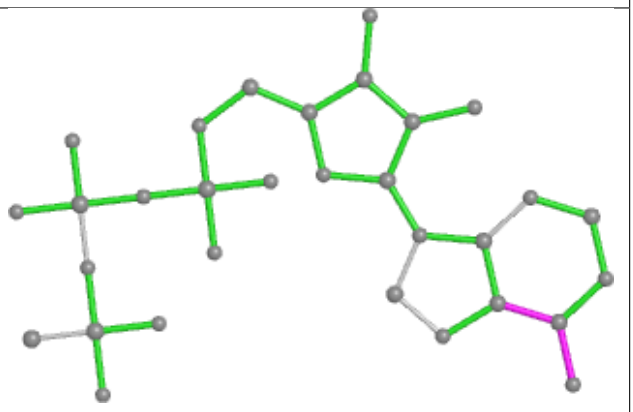
No monomer is involved in short contacts.

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

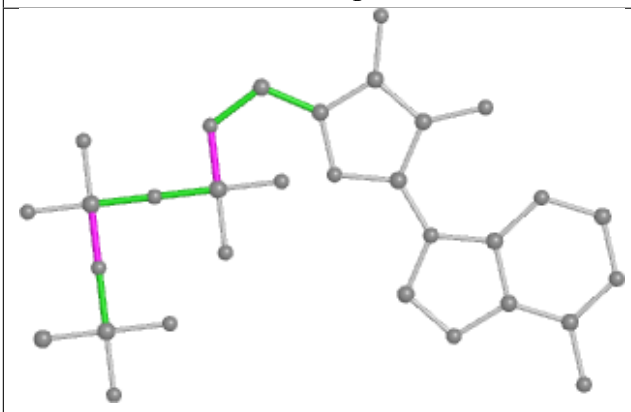
Ligand AGS C 600



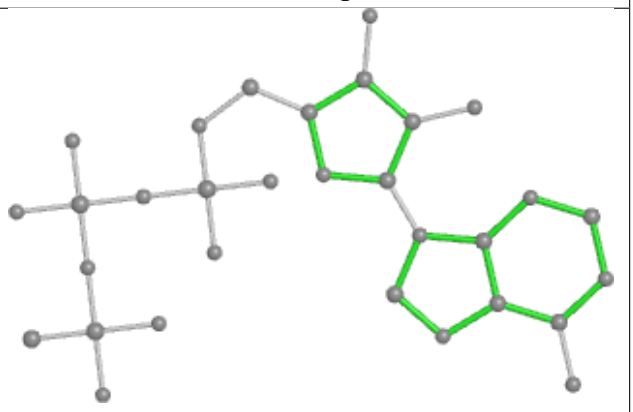
Bond lengths



Bond angles

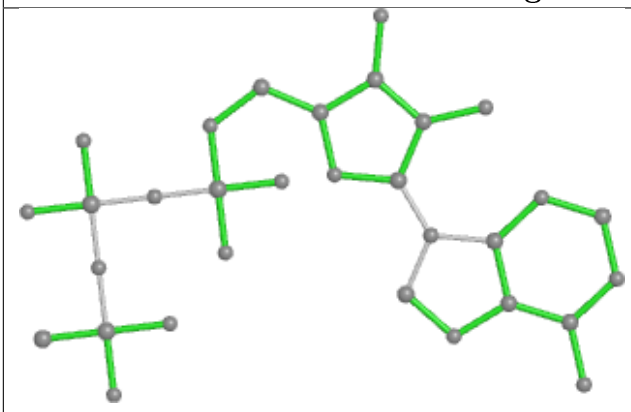


Torsions

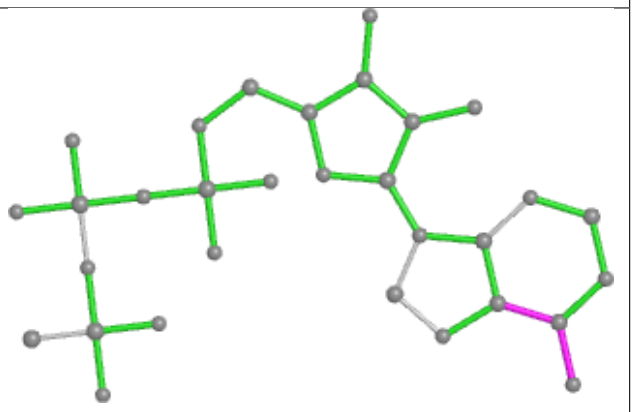


Rings

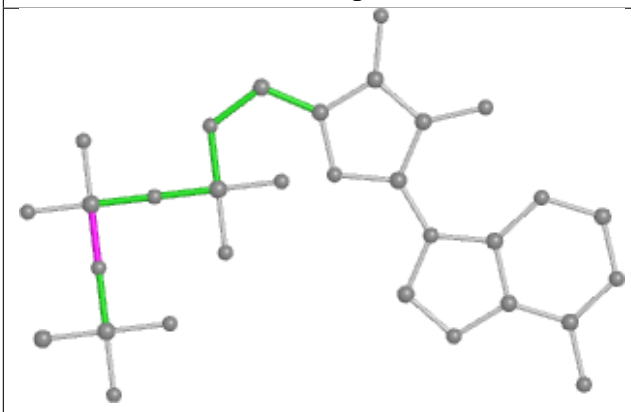
Ligand AGS B 600



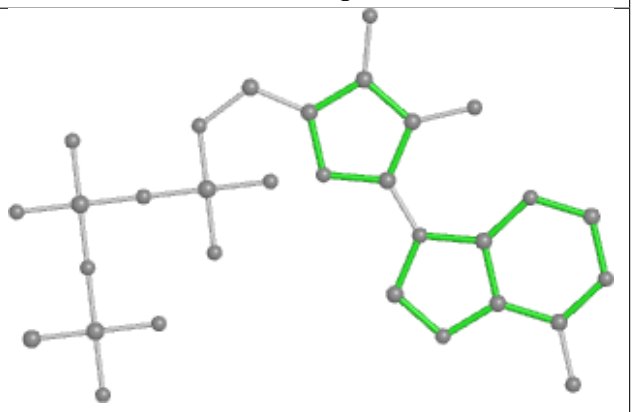
Bond lengths



Bond angles

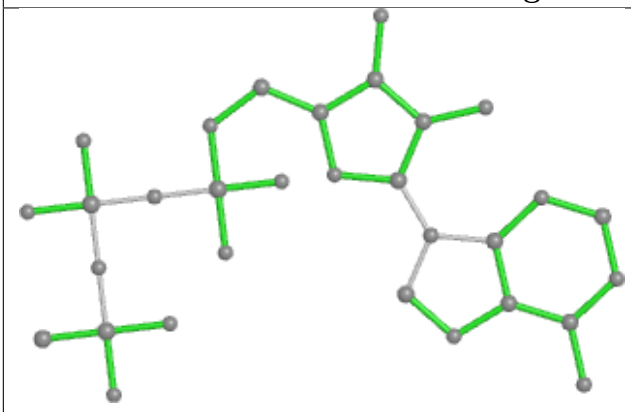


Torsions

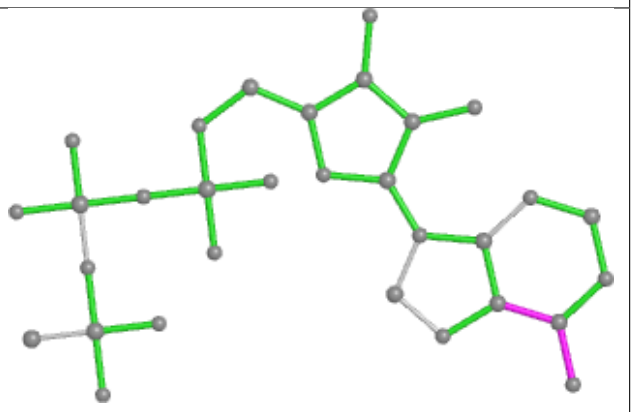


Rings

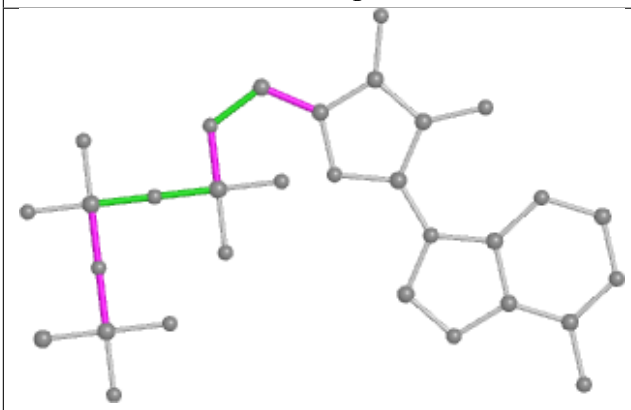
Ligand AGS D 600



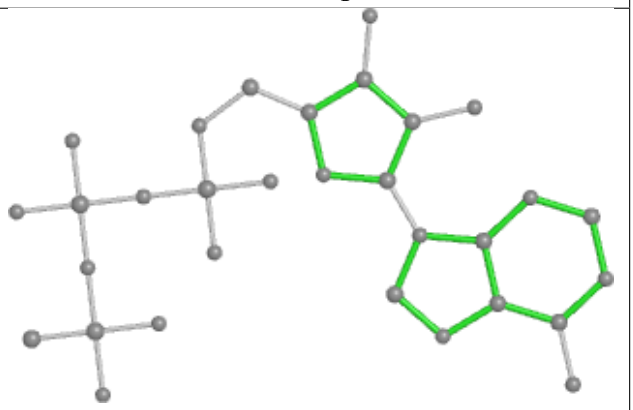
Bond lengths



Bond angles

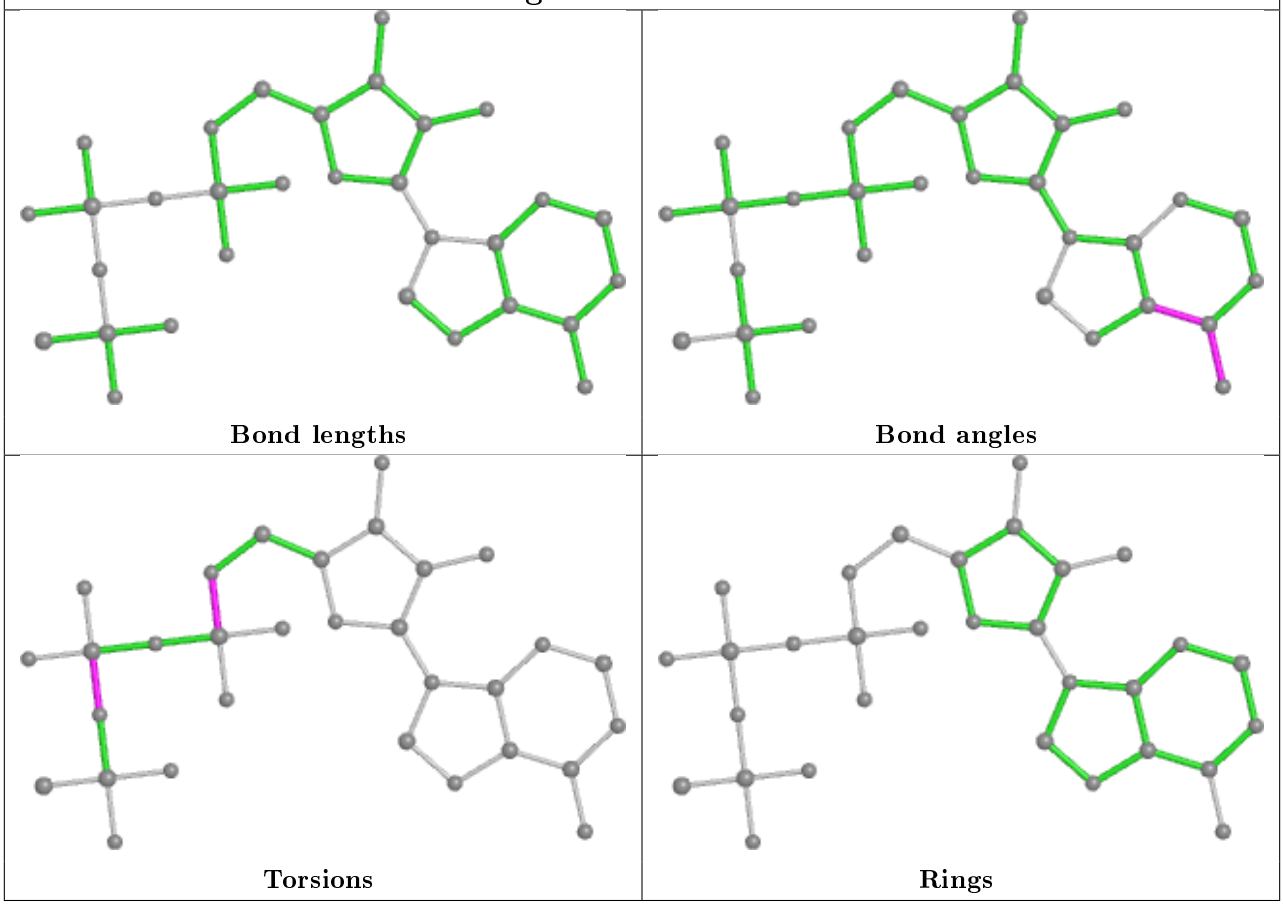


Torsions



Rings

Ligand AGS A 600



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, 95^{th} 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%)	0.49	68 (11%) 4 6	73, 177, 277, 287	0
1	C	569/587 (96%)	0.71	90 (15%) 2 3	99, 206, 269, 277	0
2	B	573/599 (95%)	0.29	46 (8%) 12 14	76, 151, 276, 280	0
2	D	573/599 (95%)	0.93	109 (19%) 1 1	103, 188, 267, 276	0
3	E	115/118 (97%)	1.85	33 (28%) 0 0	154, 195, 215, 225	0
3	F	115/118 (97%)	2.41	47 (40%) 0 0	181, 230, 248, 257	0
All	All	2514/2608 (96%)	0.75	393 (15%) 2 3	73, 188, 271, 287	0

All (393) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	289	ASP	33.6
1	A	265	ASN	20.7
3	E	73	ASP	19.2
3	E	72	ASP	17.6
3	F	74	ALA	17.0
1	C	265	ASN	16.7
2	D	288	LYS	16.4
3	F	73	ASP	15.6
2	D	287	LEU	15.4
3	F	12	VAL	15.3
1	A	266	GLN	14.3
3	E	76	ASN	13.6
3	F	11	LEU	13.4
1	A	264	ASN	13.1
2	D	290	ILE	12.5
2	B	289	ASP	12.1
1	C	399	THR	12.0
3	F	10	GLY	11.9
3	F	13	GLN	11.0

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Mol	Chain	Res	Type	RSRZ
2	D	284	TRP	11.0
2	B	60	ILE	10.9
1	A	243	PHE	10.6
3	E	8	GLY	10.5
1	C	264	ASN	10.4
3	F	83	ASN	10.4
1	C	280	MET	10.2
2	B	288	LYS	10.1
1	A	238	PHE	10.0
2	D	262	VAL	10.0
3	E	77	THR	9.9
3	E	74	ALA	9.9
3	F	17	SER	9.9
3	F	72	ASP	9.5
2	B	287	LEU	9.2
2	D	409	ARG	9.2
1	A	242	LEU	9.1
3	E	75	LYS	9.0
3	F	19	THR	8.8
1	C	326	PRO	8.7
3	E	9	GLY	8.6
3	F	75	LYS	8.6
3	F	21	SER	8.5
2	B	61	GLY	8.3
3	F	81	GLN	8.3
3	E	28	ASP	8.3
2	D	178	ILE	8.2
2	D	337	GLU	8.1
2	D	594	VAL	8.0
2	D	285	LEU	8.0
1	C	251	MET	7.9
1	C	244	ILE	7.9
1	C	240	LEU	7.9
1	A	247	VAL	7.9
1	C	266	GLN	7.9
3	F	29	ILE	7.7
1	C	381	ARG	7.7
1	C	243	PHE	7.6
1	C	284	PHE	7.5
2	D	58	TYR	7.5
1	C	402	LEU	7.5
1	C	528	ILE	7.4

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Mol	Chain	Res	Type	RSRZ
1	C	233	PHE	7.4
2	D	340	LYS	7.3
3	F	68	THR	7.2
3	E	105	TRP	7.1
3	E	106	GLY	7.1
1	C	328	VAL	7.1
1	A	249	MET	7.1
1	C	237	VAL	7.0
1	A	251	MET	7.0
1	C	327	ASN	6.9
2	D	271	ASN	6.9
3	F	18	LEU	6.9
1	A	260	VAL	6.9
1	C	247	VAL	6.8
2	D	275	PHE	6.7
3	E	68	THR	6.7
3	F	70	SER	6.6
1	C	262	VAL	6.4
1	C	321	ASN	6.4
2	D	416	GLY	6.4
3	F	30	SER	6.3
1	C	396	ASP	6.2
2	B	178	ILE	6.2
1	C	238	PHE	6.2
2	D	369	PRO	6.2
3	E	17	SER	6.2
2	D	574	ASP	6.2
1	A	46	ARG	6.1
3	F	76	ASN	6.0
1	A	286	LEU	6.0
2	B	59	LEU	5.8
2	D	361	TRP	5.8
2	B	62	LYS	5.8
2	B	285	LEU	5.8
1	C	234	SER	5.8
1	A	250	GLY	5.7
1	A	241	PRO	5.7
2	D	264	PRO	5.7
2	D	293	VAL	5.7
1	C	397	VAL	5.6
1	C	14	PHE	5.6
1	C	277	ASN	5.6

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Mol	Chain	Res	Type	RSRZ
1	C	236	ILE	5.6
1	A	240	LEU	5.6
1	A	287	MET	5.6
1	C	380	PRO	5.5
2	D	411	GLN	5.5
1	C	263	ARG	5.5
2	D	259	PHE	5.5
2	D	286	ALA	5.4
1	A	261	LEU	5.4
3	F	9	GLY	5.4
2	D	270	VAL	5.3
2	D	151	LEU	5.3
1	A	244	ILE	5.3
2	D	267	MET	5.3
1	A	277	ASN	5.3
1	C	76	PHE	5.2
3	E	10	GLY	5.2
3	E	31	PHE	5.2
2	D	593	LEU	5.1
1	A	246	ILE	5.1
1	A	200	LEU	5.1
1	C	404	ASP	5.0
3	F	28	ASP	5.0
1	C	260	VAL	5.0
1	C	400	VAL	5.0
2	D	414	VAL	5.0
3	F	7	SER	5.0
2	D	342	ASP	4.9
2	D	263	LEU	4.9
2	D	341	ASP	4.9
1	C	317	GLU	4.9
2	B	284	TRP	4.9
1	C	568	GLN	4.8
2	B	290	ILE	4.8
1	A	258	GLY	4.8
3	F	31	PHE	4.8
2	D	266	LEU	4.8
1	A	253	ALA	4.8
1	C	75	VAL	4.8
2	D	258	ILE	4.8
2	B	83	LEU	4.7
2	B	292	THR	4.7

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Mol	Chain	Res	Type	RSRZ
2	D	417	ILE	4.7
1	C	379	ILE	4.7
1	C	258	GLY	4.6
3	E	7	SER	4.6
1	A	254	VAL	4.6
2	D	261	GLY	4.6
1	C	403	LYS	4.6
2	D	370	VAL	4.6
2	B	63	THR	4.6
3	E	83	ASN	4.5
2	D	40	ILE	4.5
2	D	338	GLU	4.5
1	A	283	MET	4.5
1	C	398	ARG	4.5
3	E	29	ILE	4.4
3	E	70	SER	4.4
3	F	69	ILE	4.4
1	A	252	ILE	4.4
2	D	487	ASP	4.4
3	F	112	THR	4.4
1	C	318	GLU	4.4
2	D	251	LYS	4.3
2	D	254	THR	4.3
2	D	283	GLY	4.3
1	A	47	GLY	4.3
1	C	286	LEU	4.3
1	A	248	ASN	4.3
1	C	166	ILE	4.2
2	B	57	PRO	4.2
1	C	405	LEU	4.2
1	A	31	SER	4.2
2	B	340	LYS	4.1
1	A	257	PHE	4.1
3	F	104	TYR	4.1
2	B	260	SER	4.1
1	C	249	MET	4.0
3	F	79	SER	4.0
1	A	236	ILE	4.0
1	A	551	HIS	4.0
2	D	280	GLY	4.0
2	D	59	LEU	3.9
3	E	30	SER	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	79	TYR	3.9
1	A	239	ALA	3.9
1	C	406	ARG	3.9
2	D	62	LYS	3.9
2	D	311	ASN	3.9
2	D	272	ASN	3.9
3	E	107	GLN	3.9
3	E	27	ARG	3.9
1	A	273	MET	3.9
3	E	71	ARG	3.8
1	A	280	MET	3.8
1	A	397	VAL	3.8
1	C	283	MET	3.8
1	A	399	THR	3.8
1	A	284	PHE	3.8
2	D	336	LEU	3.8
1	C	267	MET	3.8
3	F	8	GLY	3.7
1	C	329	GLU	3.7
2	D	39	LEU	3.7
2	D	55	LEU	3.7
1	A	245	PHE	3.7
2	D	57	PRO	3.7
2	B	417	ILE	3.7
3	E	45	ARG	3.7
1	C	395	LEU	3.7
2	D	408	ASP	3.7
2	D	410	GLY	3.7
3	F	16	GLY	3.6
1	A	395	LEU	3.6
2	D	268	ASN	3.6
1	A	48	ASP	3.6
2	D	291	ILE	3.6
1	C	439	ILE	3.6
1	C	71	ILE	3.6
2	D	150	VAL	3.6
1	A	396	ASP	3.6
1	A	270	GLY	3.6
2	D	269	MET	3.5
2	B	56	SER	3.5
1	A	150	SER	3.5
2	B	591	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
2	D	591	TYR	3.5
1	C	517	LYS	3.4
3	F	15	GLY	3.4
2	D	99	LYS	3.4
2	D	103	THR	3.4
1	C	384	ASP	3.3
1	C	437	ASP	3.3
2	B	37	PHE	3.3
2	B	291	ILE	3.2
3	F	20	LEU	3.2
1	A	417	VAL	3.2
1	C	527	LYS	3.2
2	B	294	GLY	3.2
3	F	99	LEU	3.2
1	C	255	LEU	3.2
3	E	81	GLN	3.2
3	F	82	MET	3.1
1	C	248	ASN	3.1
1	C	241	PRO	3.1
2	D	255	LYS	3.1
1	A	398	ARG	3.1
1	C	273	MET	3.1
2	D	573	HIS	3.1
1	C	401	LYS	3.1
2	D	98	GLY	3.1
1	A	65	ILE	3.0
2	D	488	ASN	3.0
1	C	287	MET	3.0
2	D	37	PHE	3.0
2	B	339	GLU	3.0
3	E	21	SER	3.0
1	A	290	GLY	3.0
2	B	64	ILE	3.0
1	A	35	LEU	3.0
1	C	250	GLY	2.9
2	B	461	ILE	2.9
3	F	24	ALA	2.9
2	B	79	TYR	2.9
1	C	261	LEU	2.9
2	D	83	LEU	2.9
3	F	97	ALA	2.8
2	B	319	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	38	ARG	2.8
1	C	550	THR	2.8
1	C	526	GLN	2.8
1	C	259	GLY	2.8
3	F	114	SER	2.8
3	F	98	SER	2.8
2	D	413	LEU	2.8
2	D	372	LYS	2.8
2	D	120	LEU	2.8
1	A	51	LEU	2.8
2	B	80	MET	2.8
1	C	254	VAL	2.8
2	D	402	MET	2.7
2	B	348	LEU	2.7
2	B	422	ILE	2.7
3	E	94	TYR	2.7
2	D	339	GLU	2.7
2	B	262	VAL	2.7
2	D	82	ILE	2.7
1	A	227	ARG	2.7
2	D	549	ARG	2.7
1	C	46	ARG	2.7
2	D	100	ILE	2.7
1	A	263	ARG	2.7
1	A	328	VAL	2.7
2	D	459	GLU	2.7
1	C	319	ALA	2.7
3	E	11	LEU	2.7
2	D	568	VAL	2.7
2	D	348	LEU	2.7
2	B	286	ALA	2.6
3	F	27	ARG	2.6
2	B	99	LYS	2.6
1	C	245	PHE	2.6
1	A	153	VAL	2.6
1	C	230	ILE	2.6
2	B	338	GLU	2.6
3	F	77	THR	2.6
1	A	52	VAL	2.6
1	C	48	ASP	2.6
1	C	569	PHE	2.6
1	C	74	THR	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	60	ILE	2.6
1	C	231	SER	2.5
3	E	79	SER	2.5
2	B	264	PRO	2.5
2	B	263	LEU	2.5
2	D	490	GLU	2.5
1	A	528	ILE	2.5
2	D	101	MET	2.5
2	D	308	ARG	2.5
1	C	417	VAL	2.5
2	D	36	THR	2.5
1	C	276	THR	2.5
3	E	69	ILE	2.5
2	B	95	TRP	2.5
2	D	119	LYS	2.5
1	A	44	ILE	2.5
2	D	314	SER	2.5
3	F	101	GLY	2.5
1	A	552	LYS	2.4
2	B	315	ASN	2.4
2	D	296	ILE	2.4
1	C	177	GLY	2.4
1	A	267	MET	2.4
3	F	113	VAL	2.4
1	A	256	TRP	2.4
2	D	233	THR	2.3
3	E	14	ALA	2.3
1	A	529	PRO	2.3
3	F	100	PRO	2.3
2	D	461	ILE	2.3
2	D	310	LEU	2.3
1	A	279	LEU	2.3
2	D	224	SER	2.3
2	D	260	SER	2.3
2	D	470	SER	2.3
2	B	179	LEU	2.3
2	D	442	SER	2.3
2	D	524	THR	2.2
2	D	54	VAL	2.2
1	A	61	ILE	2.2
2	D	563	ARG	2.2
3	E	108	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	153	VAL	2.2
1	C	232	ALA	2.2
2	B	442	SER	2.2
1	C	176	LYS	2.2
2	D	192	LEU	2.2
3	F	102	LEU	2.2
2	D	468	THR	2.2
1	C	503	ILE	2.2
1	C	242	LEU	2.1
1	C	509	LEU	2.1
3	F	45	ARG	2.1
1	C	502	PRO	2.1
2	B	281	PHE	2.1
1	A	233	PHE	2.1
1	C	29	ASP	2.1
2	D	292	THR	2.1
2	D	257	GLN	2.1
1	C	229	ILE	2.1
2	D	407	VAL	2.1
1	A	237	VAL	2.1
2	D	69	VAL	2.1
3	E	12	VAL	2.1
2	D	154	SER	2.1
2	B	342	ASP	2.1
1	A	255	LEU	2.1
2	D	265	PRO	2.0
2	D	273	LEU	2.0
2	D	454	PRO	2.0
2	B	261	GLY	2.0
2	D	551	ASN	2.0
2	B	204	TYR	2.0
3	F	34	VAL	2.0
2	D	473	PHE	2.0
3	F	23	ALA	2.0
3	F	32	PHE	2.0
1	A	74	THR	2.0
2	B	312	GLU	2.0
2	D	112	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 carbohydrates in this entry.

6.4 Ligands (i)

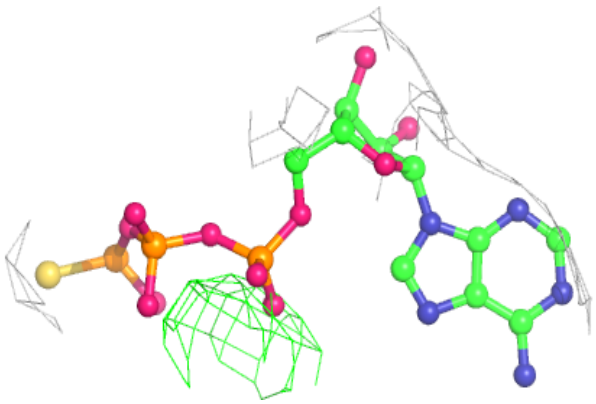
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

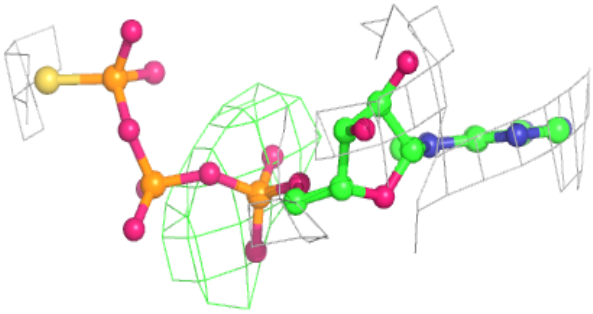
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	AGS	D	600	31/31	0.93	0.20	157,163,169,169	0
5	MG	B	601	1/1	0.94	0.25	76,76,76,76	0
4	AGS	A	600	31/31	0.96	0.21	120,124,126,127	0
4	AGS	C	600	31/31	0.97	0.18	150,155,163,164	0
5	MG	C	601	1/1	0.97	0.22	143,143,143,143	0
5	MG	D	601	1/1	0.97	0.25	121,121,121,121	0
5	MG	A	601	1/1	0.98	0.28	87,87,87,87	0
4	AGS	B	600	31/31	0.98	0.24	94,97,100,102	0

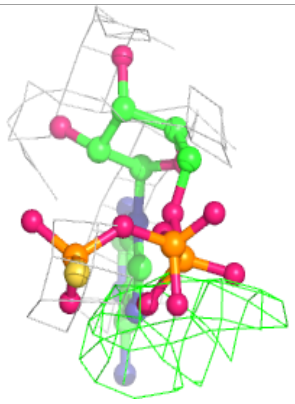
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

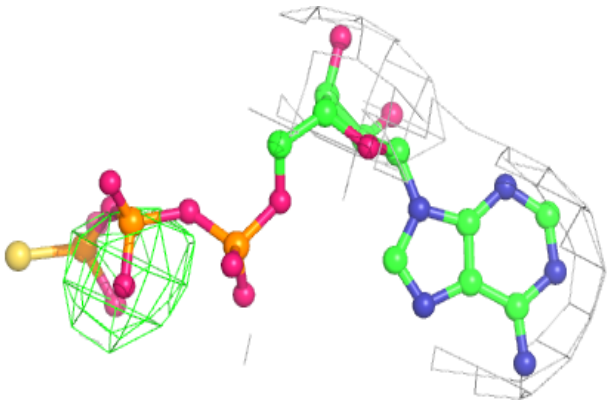


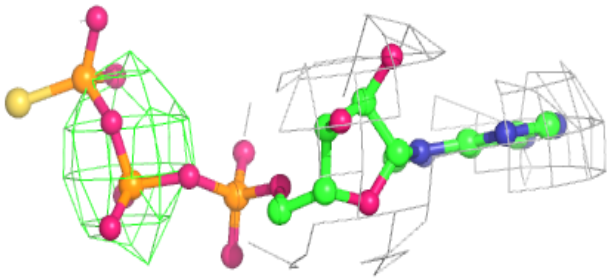


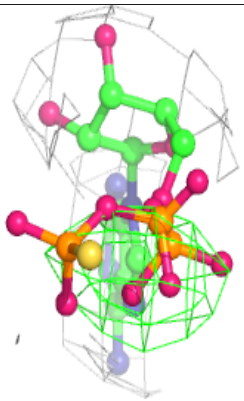


Electron density around AGS A 600:

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

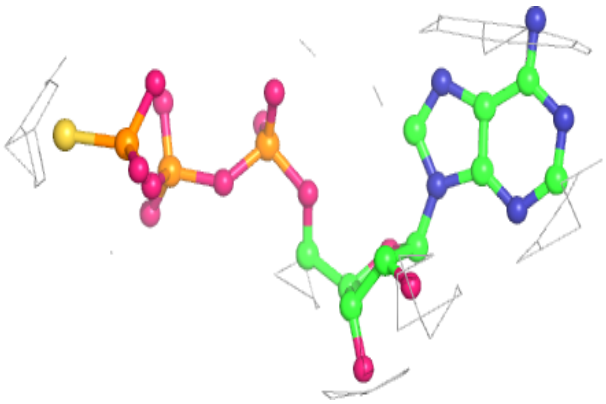


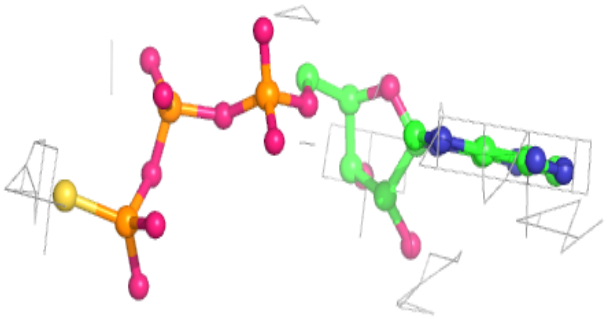




Electron density around AGS C 600:

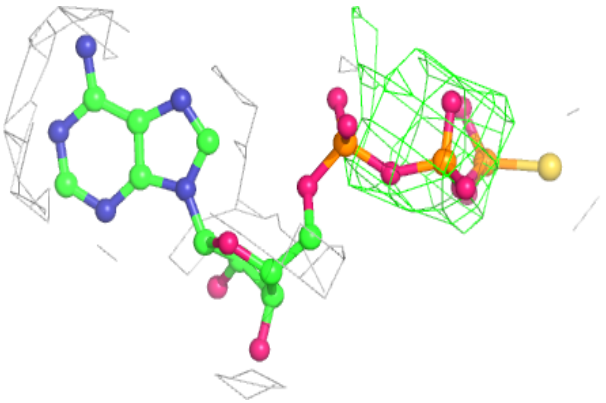
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

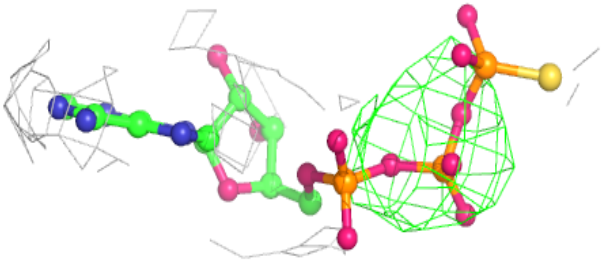


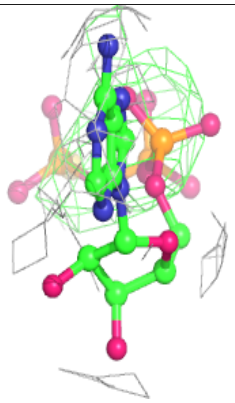


Electron density around AGS B 600:

$2mF_o$-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.