Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 08:06 PM EDT

PDB ID	:	4NAH
Title	:	Inhibitors of 4-Phosphopanthetheine Adenylyltransferase (PPAT)
Authors	:	Lahiri, S.D.
Deposited on	:	2013-10-22
Resolution	:	2.38 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 (i) 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 (i)) were used in the production of this report:

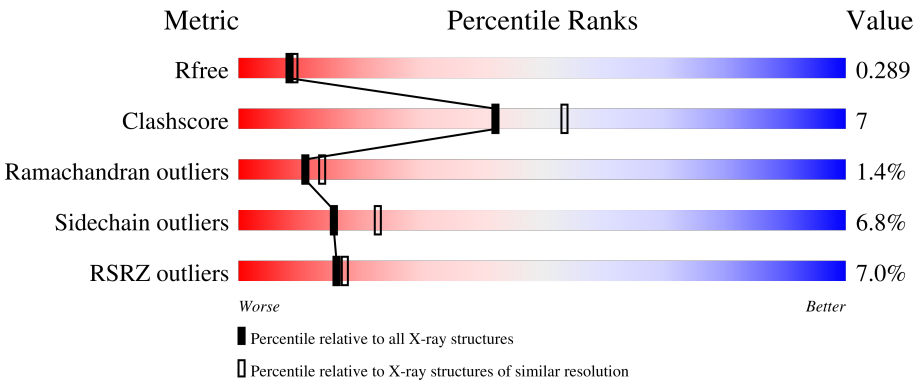
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.38 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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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 <=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	160	2%, 81%, 14%
1	B	160	8%, 85%, 13%
1	C	160	6%, 84%, 13%
1	D	160	4%, 79%, 17%
1	E	160	12%, 74%, 21%

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Mol	Chain	Length	Quality of chain
1	F	160	10% 87% 12% ••

2 Entry composition (i)

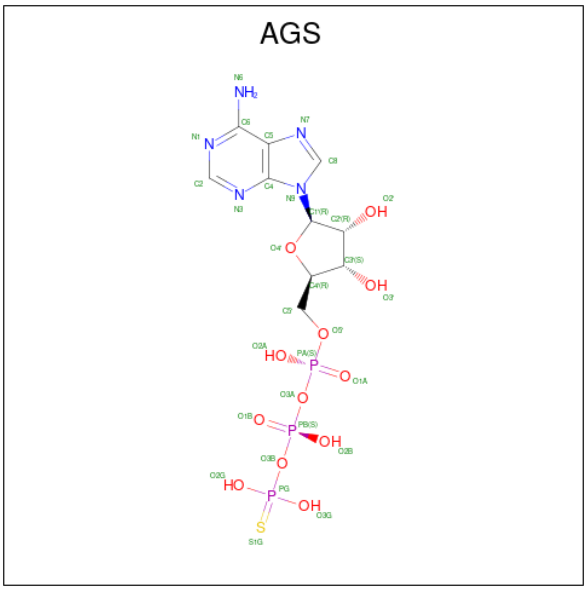
There are 4 unique types of molecules in this entry. The entry contains 8204 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Phosphopantetheine adenylyltransferase.

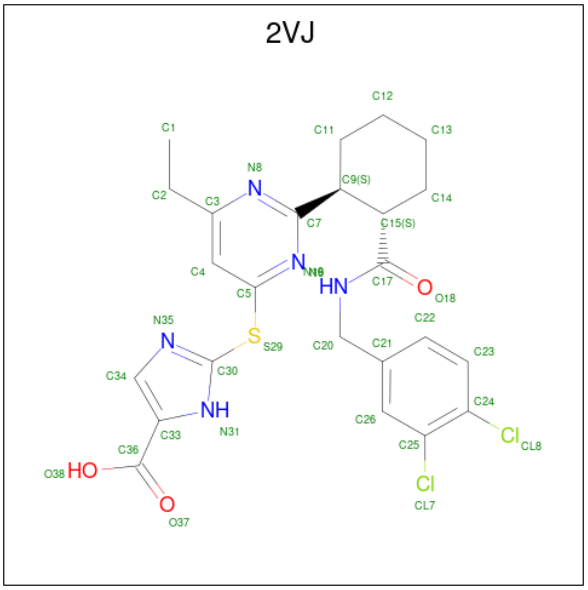
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	159	1285	821	213	244	7	0	1	0
			Total	C	N	O	S			
1	B	160	1290	824	214	245	7	0	0	0
			Total	C	N	O	S			
1	C	160	1290	824	214	245	7	0	0	0
			Total	C	N	O	S			
1	D	159	1285	821	213	244	7	0	1	0
			Total	C	N	O	S			
1	E	160	1290	824	214	245	7	0	0	0
			Total	C	N	O	S			
1	F	160	1290	824	214	245	7	0	0	0

- Molecule 2 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
			Total	C	N	O	P	S		
2	A	1	31	10	5	12	3	1	0	0
2	B	1	31	10	5	12	3	1	0	0
2	C	1	31	10	5	12	3	1	0	0
2	D	1	31	10	5	12	3	1	0	0
2	E	1	31	10	5	12	3	1	0	0
2	F	1	31	10	5	12	3	1	0	0

- Molecule 3 is 2-[(2-{(1S,2S)-2-[(3,4-dichlorobenzyl)carbamoyl]cyclohexyl}-6-ethylpyrimidin-4-yl)sulfanyl]-1H-imidazole-5-carboxylic acid (three-letter code: 2VJ) (formula: $C_{24}H_{25}Cl_2N_5O_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	N	O	S		
3	A	1	35	24	2	5	3	1	0	0
3	A	1	35	24	2	5	3	1	0	0
3	B	1	35	24	2	5	3	1	0	0
3	D	1	35	24	2	5	3	1	0	0
3	F	1	35	24	2	5	3	1	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	N	O	S		
3	F	1	35	24	2	5	3	1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	17	17	17	0	0
4	B	22	22	22	0	0
4	C	13	13	13	0	0
4	D	10	10	10	0	0
4	E	3	3	3	0	0
4	F	13	13	13	0	0

3 Residue-property plots (i)

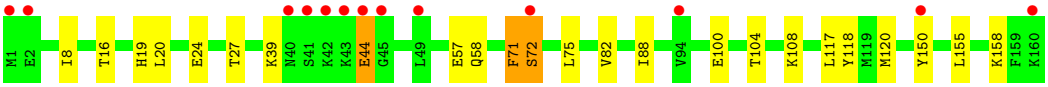
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

Chain A:

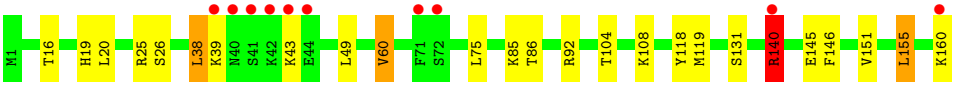
• Molecule 1: Phosphopantetheine adenylyltransferase

Chain B:



• Molecule 1: Phosphopantetheine adenylyltransferase

Chain C:

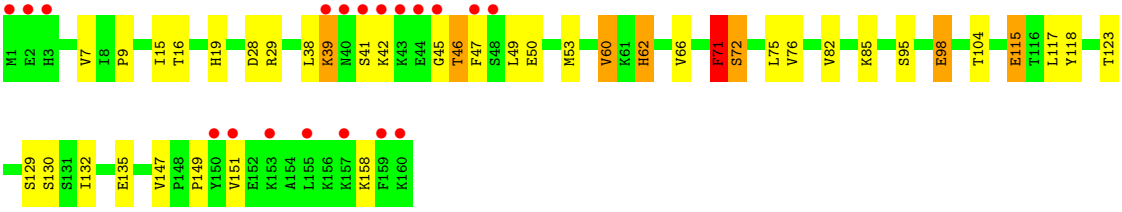


• Molecule 1: Phosphopantetheine adenylyltransferase

Chain D:

• Molecule 1: Phosphopantetheine adenylyltransferase

Chain E:



• Molecule 1: Phosphopantetheine adenylyltransferase

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	68.48Å 105.36Å 79.98Å 90.00° 94.69° 90.00°	Depositor
Resolution (Å)	41.70 – 2.38 41.70 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.1 (41.70-2.38) 99.1 (41.70-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.93 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.216 , 0.292 0.221 , 0.289	Depositor DCC
R_{free} test set	2280 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	36.6	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 43.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8204	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.46% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: AGS, 2VJ

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	0.75	0/1312	0.83	0/1767
1	B	0.78	0/1314	0.87	0/1769
1	C	0.72	0/1314	0.82	2/1769 (0.1%)
1	D	0.79	0/1312	0.86	3/1767 (0.2%)
1	E	0.72	0/1314	0.84	1/1769 (0.1%)
1	F	0.68	0/1314	0.80	1/1769 (0.1%)
All	All	0.74	0/7880	0.84	7/10610 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	155	LEU	CA-CB-CG	7.40	132.33	115.30
1	D	36[A]	CYS	N-CA-CB	-6.30	99.26	110.60
1	D	36[B]	CYS	N-CA-CB	-6.30	99.26	110.60
1	C	25	ARG	NE-CZ-NH2	5.70	123.15	120.30
1	E	71	PHE	C-N-CA	5.51	135.47	121.70
1	D	96	ASP	CB-CG-OD1	5.40	123.16	118.30
1	C	140	ARG	NE-CZ-NH1	5.39	122.99	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	71	PHE	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1285	0	1297	22	0
1	B	1290	0	1304	18	0
1	C	1290	0	1304	16	0
1	D	1285	0	1297	18	0
1	E	1290	0	1304	24	0
1	F	1290	0	1304	13	0
2	A	31	0	12	4	0
2	B	31	0	12	0	0
2	C	31	0	12	1	0
2	D	31	0	12	3	0
2	E	31	0	12	0	0
2	F	31	0	12	1	0
3	A	70	0	49	6	0
3	B	35	0	25	1	0
3	D	35	0	25	3	0
3	F	70	0	49	2	0
4	A	17	0	0	2	0
4	B	22	0	0	1	0
4	C	13	0	0	1	0
4	D	10	0	0	1	0
4	E	3	0	0	0	0
4	F	13	0	0	0	0
All	All	8204	0	8030	111	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 7.

All (111) 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:E:115:GLU:OE2	1:E:117:LEU:HD13	1.42	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:GLU:HB2	1:D:45:GLY:O	1.66	0.96
1:C:38:LEU:H	1:C:38:LEU:HD12	1.42	0.83
1:B:104:THR:HG21	1:B:118:TYR:OH	1.80	0.81
2:D:201:AGS:O3G	2:D:201:AGS:O2B	2.01	0.78
1:A:36[B]:CYS:SG	3:A:203:2VJ:CL7	2.79	0.78
1:C:140:ARG:HB2	1:C:140:ARG:HH11	1.49	0.77
1:A:104:THR:OG1	1:A:118:TYR:OH	2.04	0.76
2:A:201:AGS:O1B	4:A:313:HOH:O	2.05	0.74
1:E:115:GLU:OE2	1:E:117:LEU:CD1	2.30	0.74
1:B:71:PHE:CG	1:B:72:SER:HB2	2.23	0.74
1:E:38:LEU:HD23	1:E:39:LYS:N	2.04	0.73
2:A:201:AGS:O2B	2:A:201:AGS:S1G	2.47	0.73
1:E:9:PRO:HG3	1:E:75:LEU:HD21	1.72	0.72
1:A:7:VAL:HG13	1:A:36[A]:CYS:SG	2.31	0.71
1:C:140:ARG:HB2	1:C:140:ARG:NH1	2.05	0.71
1:E:50:GLU:N	1:E:50:GLU:OE1	2.24	0.70
1:B:104:THR:HG22	4:B:302:HOH:O	1.91	0.69
1:A:135:GLU:OE2	3:A:202:2VJ:C34	2.39	0.69
1:C:104:THR:OG1	1:C:118:TYR:OH	2.09	0.69
1:F:151:VAL:O	1:F:155:LEU:HD23	1.92	0.69
2:A:201:AGS:O2B	3:A:203:2VJ:O38	2.13	0.67
1:B:71:PHE:HA	1:B:72:SER:HB2	1.76	0.66
1:F:16:THR:HA	1:F:147:VAL:HG12	1.79	0.65
1:B:104:THR:CG2	1:B:118:TYR:OH	2.45	0.65
1:B:16:THR:H	1:B:19:HIS:HD2	1.47	0.61
1:B:71:PHE:CD1	1:B:72:SER:HB2	2.36	0.60
1:D:82:VAL:HG12	1:D:82:VAL:O	2.02	0.59
1:F:9:PRO:HG3	1:F:75:LEU:HD21	1.84	0.58
1:F:7:VAL:HG13	1:F:36:CYS:SG	2.43	0.58
1:A:106:MET:O	1:A:106:MET:HE2	2.03	0.58
1:E:45:GLY:O	1:E:47:PHE:N	2.36	0.58
1:B:71:PHE:CA	1:B:72:SER:HB2	2.33	0.58
1:D:3:HIS:CE1	4:D:306:HOH:O	2.56	0.57
1:E:71:PHE:CG	1:E:72:SER:HB2	2.39	0.57
1:F:49:LEU:HD23	1:F:49:LEU:C	2.26	0.56
1:A:106:MET:HE2	1:A:110:LEU:HD13	1.87	0.56
1:C:119:MET:CE	1:E:115:GLU:HG3	2.36	0.55
1:D:104:THR:OG1	1:D:118:TYR:OH	2.24	0.55
1:D:108:LYS:NZ	1:D:115:GLU:OE2	2.38	0.55
3:A:202:2VJ:H4	1:C:75:LEU:CD2	2.38	0.54
1:B:120:MET:HG3	1:F:104:THR:HG21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:THR:OG1	1:E:29:ARG:NH1	2.41	0.54
1:A:16:THR:H	1:A:19:HIS:HD2	1.55	0.53
1:A:129:SER:HB2	2:A:201:AGS:O2G	2.08	0.53
1:C:16:THR:H	1:C:19:HIS:HD2	1.56	0.53
1:E:104:THR:OG1	1:E:118:TYR:OH	2.24	0.53
1:A:42:LYS:O	1:A:43:LYS:CB	2.57	0.53
3:A:202:2VJ:H23	4:A:301:HOH:O	2.08	0.53
1:A:36[B]:CYS:SG	1:A:37:VAL:N	2.82	0.53
1:C:108:LYS:NZ	4:C:307:HOH:O	2.41	0.52
1:D:76:VAL:HG21	1:D:111:ASN:HB3	1.91	0.52
3:D:202:2VJ:C34	1:E:135:GLU:OE2	2.58	0.51
1:F:16:THR:H	1:F:19:HIS:HD2	1.58	0.51
1:F:135:GLU:CD	3:F:202:2VJ:C36	2.78	0.51
1:A:40:ASN:C	1:A:41:SER:O	2.47	0.51
1:E:7:VAL:HG11	1:E:75:LEU:HD11	1.92	0.51
1:A:106:MET:CE	1:A:110:LEU:HD13	2.40	0.50
1:D:16:THR:H	1:D:19:HIS:HD2	1.60	0.50
1:E:7:VAL:HG12	1:E:9:PRO:HD3	1.94	0.49
2:F:201:AGS:O1A	2:F:201:AGS:O3G	2.29	0.49
1:E:82:VAL:HG12	1:E:82:VAL:O	2.12	0.49
1:A:39:LYS:HD3	1:A:40:ASN:HD22	1.77	0.49
1:A:44:GLU:HA	1:A:45:GLY:O	2.13	0.49
1:E:49:LEU:CD2	1:E:53:MET:SD	3.01	0.49
1:A:9:PRO:HG3	1:A:75:LEU:HD21	1.93	0.49
1:A:8:ILE:HG12	1:A:88:ILE:HB	1.95	0.48
1:B:24:GLU:O	1:B:27:THR:HG22	2.13	0.47
1:E:60:VAL:HG21	1:E:66:VAL:HG11	1.96	0.47
1:B:71:PHE:HA	1:B:72:SER:CB	2.42	0.47
1:D:22:ILE:HD11	2:D:201:AGS:H2	1.96	0.47
1:B:118:TYR:HB2	1:F:118:TYR:HB2	1.97	0.47
1:D:33:ILE:HB	1:D:66:VAL:HG22	1.97	0.47
1:D:75:LEU:CD2	3:D:202:2VJ:H4	2.45	0.46
1:A:44:GLU:HB2	1:A:45:GLY:O	2.15	0.46
1:B:8:ILE:HG12	1:B:88:ILE:HB	1.97	0.45
1:C:49:LEU:C	1:C:49:LEU:HD13	2.36	0.45
1:B:16:THR:H	1:B:19:HIS:CD2	2.32	0.45
1:C:145:GLU:HG2	1:C:146:PHE:CE1	2.50	0.45
1:A:75:LEU:CD2	3:A:203:2VJ:H4	2.47	0.45
1:E:129:SER:OG	1:E:132:ILE:HG22	2.17	0.45
1:C:145:GLU:HG2	1:C:146:PHE:CD1	2.52	0.44
1:D:28:ASP:OD2	1:D:29:ARG:NH1	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:71:PHE:HA	1:E:72:SER:HB2	1.99	0.44
1:C:151:VAL:HG12	1:C:155:LEU:HD22	1.99	0.44
1:E:45:GLY:O	1:E:46:THR:C	2.55	0.44
1:A:106:MET:CE	1:A:109:LYS:HB2	2.47	0.44
1:C:38:LEU:HD12	1:C:38:LEU:N	2.22	0.44
1:F:40:ASN:O	1:F:41:SER:C	2.56	0.44
1:A:42:LYS:O	1:A:43:LYS:HB3	2.18	0.43
1:E:71:PHE:HA	1:E:72:SER:CB	2.48	0.43
1:B:58:GLN:HG3	1:B:150:TYR:CZ	2.53	0.43
1:D:75:LEU:HD23	3:D:202:2VJ:H4	1.99	0.43
1:C:60:VAL:O	1:C:60:VAL:CG1	2.65	0.43
1:A:76:VAL:HG21	1:A:110:LEU:HB3	2.01	0.42
1:B:117:LEU:HD13	1:F:117:LEU:HD13	2.01	0.42
1:D:90:GLY:O	2:D:201:AGS:O2'	2.38	0.42
1:A:7:VAL:CG1	1:A:36[A]:CYS:SG	3.05	0.41
1:F:135:GLU:OE1	3:F:202:2VJ:C36	2.68	0.41
1:D:41:SER:HB3	1:D:44:GLU:OE2	2.20	0.41
1:E:98:GLU:OE2	1:F:94:VAL:HB	2.20	0.41
1:B:75:LEU:CD2	3:B:202:2VJ:H4	2.50	0.41
1:B:100:GLU:O	1:B:104:THR:HG23	2.19	0.41
1:D:132:ILE:HD13	1:D:132:ILE:HG21	1.84	0.41
1:C:92:ARG:NH1	2:C:201:AGS:S1G	2.89	0.40
1:E:16:THR:HA	1:E:147:VAL:HG12	2.02	0.40
1:D:47:PHE:HZ	1:D:155:LEU:HD13	1.87	0.40
1:D:160:LYS:HD3	1:D:160:LYS:C	2.42	0.40
1:E:15:ILE:HG13	1:E:19:HIS:HB2	2.03	0.40
1:D:43:LYS:N	1:D:44:GLU:OE1	2.54	0.40
1:E:158:LYS:O	1:E:158:LYS:HD2	2.20	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	158/160 (99%)	150 (95%)	5 (3%)	3 (2%)	8 9
1	B	158/160 (99%)	154 (98%)	2 (1%)	2 (1%)	12 15
1	C	158/160 (99%)	148 (94%)	8 (5%)	2 (1%)	12 15
1	D	158/160 (99%)	148 (94%)	8 (5%)	2 (1%)	12 15
1	E	158/160 (99%)	146 (92%)	8 (5%)	4 (2%)	5 5
1	F	158/160 (99%)	153 (97%)	5 (3%)	0	100 100
All	All	948/960 (99%)	899 (95%)	36 (4%)	13 (1%)	11 14

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	44	GLU
1	B	72	SER
1	C	39	LYS
1	E	46	THR
1	E	72	SER
1	A	41	SER
1	A	43	LYS
1	A	45	GLY
1	C	140	ARG
1	D	43	LYS
1	D	44	GLU
1	E	62	HIS
1	E	71	PHE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	147/147 (100%)	137 (93%)	10 (7%)	16 23
1	B	147/147 (100%)	139 (95%)	8 (5%)	22 33
1	C	147/147 (100%)	137 (93%)	10 (7%)	16 23
1	D	147/147 (100%)	136 (92%)	11 (8%)	13 19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	147/147 (100%)	132 (90%)	15 (10%)	7 9
1	F	147/147 (100%)	141 (96%)	6 (4%)	30 45
All	All	882/882 (100%)	822 (93%)	60 (7%)	16 23

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
1	A	39	LYS
1	A	42	LYS
1	A	55	LEU
1	A	61	LYS
1	A	80	GLU
1	A	103	LEU
1	A	110	LEU
1	A	140	ARG
1	A	155	LEU
1	B	20	LEU
1	B	39	LYS
1	B	44	GLU
1	B	57	GLU
1	B	82	VAL
1	B	108	LYS
1	B	155	LEU
1	B	158	LYS
1	C	20	LEU
1	C	26	SER
1	C	38	LEU
1	C	43	LYS
1	C	60	VAL
1	C	85	LYS
1	C	131	SER
1	C	140	ARG
1	C	155	LEU
1	C	160	LYS
1	D	44	GLU
1	D	67	LYS
1	D	72	SER
1	D	76	VAL
1	D	111	ASN
1	D	135	GLU

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Mol	Chain	Res	Type
1	D	145	GLU
1	D	155	LEU
1	D	157	LYS
1	D	158	LYS
1	D	160	LYS
1	E	28	ASP
1	E	39	LYS
1	E	41	SER
1	E	42	LYS
1	E	60	VAL
1	E	62	HIS
1	E	76	VAL
1	E	85	LYS
1	E	95	SER
1	E	98	GLU
1	E	115	GLU
1	E	123	THR
1	E	130	SER
1	E	149	PRO
1	E	151	VAL
1	F	28	ASP
1	F	41	SER
1	F	53	MET
1	F	72	SER
1	F	145	GLU
1	F	155	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	HIS
1	A	40	ASN
1	B	19	HIS
1	B	107	ASN
1	C	19	HIS
1	C	40	ASN
1	C	124	ASN
1	D	19	HIS
1	D	81	GLN
1	D	111	ASN
1	D	124	ASN
1	E	19	HIS

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Mol	Chain	Res	Type
1	E	62	HIS
1	E	70	GLN
1	E	81	GLN
1	F	19	HIS
1	F	124	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	AGS	E	201	-	26,33,33	1.65	7 (26%)	26,52,52	1.84	5 (19%)
2	AGS	D	201	-	26,33,33	1.34	3 (11%)	26,52,52	1.98	5 (19%)
2	AGS	F	201	-	26,33,33	1.58	3 (11%)	26,52,52	1.83	7 (26%)
3	2VJ	A	203	-	35,38,38	1.44	3 (8%)	42,53,53	2.23	11 (26%)
2	AGS	A	201	-	26,33,33	1.38	5 (19%)	26,52,52	2.10	6 (23%)
3	2VJ	A	202	-	35,38,38	1.06	4 (11%)	42,53,53	2.10	12 (28%)
3	2VJ	F	203	-	35,38,38	1.10	3 (8%)	42,53,53	1.84	12 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	AGS	B	201	-	26,33,33	1.56	6 (23%)	26,52,52	1.80	6 (23%)
3	2VJ	B	202	-	35,38,38	1.66	4 (11%)	42,53,53	2.57	18 (42%)
2	AGS	C	201	-	26,33,33	1.68	6 (23%)	26,52,52	1.75	3 (11%)
3	2VJ	D	202	-	35,38,38	1.43	7 (20%)	42,53,53	2.43	13 (30%)
3	2VJ	F	202	-	35,38,38	1.52	6 (17%)	42,53,53	1.86	10 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AGS	E	201	-	-	3/17/38/38	0/3/3/3
2	AGS	D	201	-	-	3/17/38/38	0/3/3/3
2	AGS	F	201	-	-	7/17/38/38	0/3/3/3
3	2VJ	A	203	-	-	0/17/34/34	0/4/4/4
2	AGS	A	201	-	-	7/17/38/38	0/3/3/3
3	2VJ	A	202	-	-	0/17/34/34	0/4/4/4
3	2VJ	F	203	-	-	0/17/34/34	0/4/4/4
2	AGS	B	201	-	-	2/17/38/38	0/3/3/3
3	2VJ	B	202	-	-	0/17/34/34	0/4/4/4
2	AGS	C	201	-	-	1/17/38/38	0/3/3/3
3	2VJ	D	202	-	-	0/17/34/34	0/4/4/4
3	2VJ	F	202	-	-	0/17/34/34	0/4/4/4

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	202	2VJ	C33-C36	-6.70	1.41	1.50
3	A	203	2VJ	C33-C36	-5.44	1.43	1.50
3	F	202	2VJ	C33-C36	-5.08	1.43	1.50
3	D	202	2VJ	C33-C36	-4.94	1.43	1.50
2	F	201	AGS	O4'-C1'	4.43	1.47	1.41
3	F	203	2VJ	C33-C36	-4.22	1.44	1.50
3	F	202	2VJ	C5-S29	-4.02	1.72	1.77
3	A	203	2VJ	C30-S29	3.94	1.81	1.75
2	E	201	AGS	PG-O2G	3.85	1.67	1.54
2	B	201	AGS	C4-N3	-3.84	1.30	1.35
2	C	201	AGS	C4-N3	-3.78	1.30	1.35
2	B	201	AGS	PG-O2G	3.72	1.67	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	201	AGS	PG-O3G	3.55	1.66	1.54
2	C	201	AGS	PG-O3G	3.55	1.66	1.54
2	A	201	AGS	PB-O1B	3.42	1.63	1.50
2	C	201	AGS	PB-O1B	3.27	1.62	1.50
2	E	201	AGS	PB-O1B	3.00	1.61	1.50
2	E	201	AGS	C4-N3	-2.99	1.31	1.35
2	D	201	AGS	PA-O1A	2.99	1.61	1.50
3	F	202	2VJ	C5-N6	-2.80	1.31	1.33
3	A	202	2VJ	C33-C36	-2.78	1.46	1.50
3	D	202	2VJ	C3-N8	-2.74	1.30	1.34
2	E	201	AGS	O4'-C1'	2.74	1.44	1.41
2	B	201	AGS	C2-N3	2.73	1.36	1.32
2	D	201	AGS	O4'-C1'	2.66	1.44	1.41
2	B	201	AGS	PG-O3G	2.65	1.63	1.54
3	F	202	2VJ	C7-N6	-2.64	1.29	1.34
2	A	201	AGS	C8-N7	-2.64	1.30	1.34
3	D	202	2VJ	C25-CL7	2.59	1.79	1.73
2	C	201	AGS	PG-S1G	-2.59	1.85	1.90
3	F	202	2VJ	O38-C36	2.54	1.38	1.30
3	B	202	2VJ	C5-S29	-2.50	1.74	1.77
2	F	201	AGS	C8-N7	-2.49	1.30	1.34
3	D	202	2VJ	O38-C36	2.48	1.38	1.30
3	B	202	2VJ	O38-C36	2.37	1.37	1.30
2	E	201	AGS	C8-N7	-2.37	1.30	1.34
2	A	201	AGS	PG-O2G	2.35	1.62	1.54
2	C	201	AGS	C8-N7	-2.35	1.30	1.34
2	A	201	AGS	PG-O3G	2.35	1.62	1.54
2	D	201	AGS	C8-N7	-2.34	1.30	1.34
3	A	202	2VJ	O38-C36	2.33	1.37	1.30
3	A	202	2VJ	C34-C33	2.31	1.41	1.37
3	F	202	2VJ	C15-C9	-2.27	1.52	1.55
2	C	201	AGS	PG-O2G	2.22	1.62	1.54
3	A	203	2VJ	C7-N6	-2.21	1.30	1.34
2	E	201	AGS	PG-O3G	2.19	1.62	1.54
3	F	203	2VJ	C30-S29	2.17	1.78	1.75
3	A	202	2VJ	C7-N6	-2.14	1.30	1.34
3	D	202	2VJ	C7-N8	-2.12	1.30	1.34
3	D	202	2VJ	C5-S29	-2.10	1.74	1.77
3	F	203	2VJ	O38-C36	2.09	1.36	1.30
2	E	201	AGS	PA-O1A	2.08	1.58	1.50
3	B	202	2VJ	C7-N6	-2.08	1.30	1.34
3	D	202	2VJ	C7-N6	-2.08	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	AGS	PA-O1A	2.07	1.58	1.50
2	B	201	AGS	O4'-C1'	2.06	1.44	1.41
2	B	201	AGS	C8-N7	-2.05	1.31	1.34

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	202	2VJ	C4-C5-S29	-9.94	113.20	123.98
3	D	202	2VJ	C4-C5-S29	-8.74	114.50	123.98
2	D	201	AGS	PA-O3A-PB	-7.57	106.86	132.83
3	A	203	2VJ	C4-C5-N6	-7.06	118.61	123.55
3	A	202	2VJ	C4-C5-N6	-6.55	118.98	123.55
3	F	202	2VJ	C4-C5-S29	-6.33	117.12	123.98
2	A	201	AGS	PA-O3A-PB	-6.25	111.39	132.83
2	C	201	AGS	PA-O3A-PB	-5.90	112.58	132.83
3	A	203	2VJ	C30-S29-C5	5.67	114.49	102.27
3	D	202	2VJ	C9-C7-N6	5.62	122.76	117.00
2	B	201	AGS	PA-O3A-PB	-5.60	113.60	132.83
2	E	201	AGS	PA-O3A-PB	-5.53	113.86	132.83
3	F	203	2VJ	C25-C26-C21	-5.00	117.05	120.46
2	A	201	AGS	N3-C2-N1	-4.73	121.29	128.68
3	B	202	2VJ	C20-C21-C26	-4.35	111.24	120.64
3	F	202	2VJ	C9-C7-N8	4.28	121.39	117.00
3	F	203	2VJ	C4-C5-N6	-4.10	120.69	123.55
3	A	202	2VJ	C4-C5-S29	-4.03	119.61	123.98
3	D	202	2VJ	C9-C15-C17	-4.01	105.62	111.21
3	A	202	2VJ	C4-C3-N8	-4.01	118.65	122.90
3	B	202	2VJ	C23-C24-CL8	3.99	126.41	118.41
2	D	201	AGS	N3-C2-N1	-3.96	122.48	128.68
3	D	202	2VJ	C4-C3-N8	-3.93	118.73	122.90
3	A	203	2VJ	C23-C24-CL8	3.85	126.13	118.41
3	A	202	2VJ	C11-C9-C7	-3.81	103.78	111.88
3	A	203	2VJ	C25-C24-CL8	-3.80	111.58	120.85
3	F	202	2VJ	C25-C26-C21	-3.73	117.92	120.46
3	D	202	2VJ	O38-C36-C33	3.69	123.08	114.69
3	B	202	2VJ	N8-C7-N6	-3.66	120.72	126.00
3	B	202	2VJ	C9-C7-N6	3.64	120.73	117.00
2	A	201	AGS	O4'-C1'-C2'	-3.64	101.61	106.93
3	F	203	2VJ	C4-C5-S29	-3.64	120.03	123.98
2	B	201	AGS	C4-C5-N7	-3.61	105.63	109.40
3	F	202	2VJ	C4-C3-N8	-3.61	119.08	122.90
3	A	202	2VJ	O38-C36-C33	3.56	122.80	114.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	201	AGS	C5'-C4'-C3'	-3.56	101.85	115.18
2	E	201	AGS	O2G-PG-O3B	3.55	116.49	104.64
3	B	202	2VJ	C9-C15-C17	-3.52	106.31	111.21
3	A	202	2VJ	O38-C36-O37	-3.51	115.55	123.35
3	A	203	2VJ	C20-C21-C26	-3.41	113.26	120.64
3	D	202	2VJ	C12-C11-C9	-3.39	106.97	111.63
2	F	201	AGS	PA-O5'-C5'	-3.38	101.86	121.68
3	B	202	2VJ	C20-C21-C22	3.33	127.82	120.91
3	D	202	2VJ	C4-C5-N6	-3.30	121.24	123.55
2	C	201	AGS	N3-C2-N1	-3.23	123.63	128.68
3	A	203	2VJ	N8-C7-N6	-3.22	121.35	126.00
3	B	202	2VJ	C2-C3-C4	-3.19	116.13	122.58
2	F	201	AGS	O5'-C5'-C4'	3.14	119.80	108.99
2	A	201	AGS	O2G-PG-O3B	3.14	115.12	104.64
2	E	201	AGS	N3-C2-N1	-3.13	123.79	128.68
2	C	201	AGS	O3G-PG-O3B	3.12	115.06	104.64
2	B	201	AGS	C3'-C2'-C1'	-3.06	96.37	100.98
2	E	201	AGS	C4-C5-N7	-3.04	106.23	109.40
2	F	201	AGS	N3-C2-N1	-3.04	123.93	128.68
3	A	203	2VJ	C13-C12-C11	-3.03	105.23	111.42
3	A	202	2VJ	N8-C7-N6	-3.03	121.63	126.00
3	F	202	2VJ	C11-C9-C7	-2.99	105.52	111.88
3	A	203	2VJ	C20-C21-C22	2.95	127.03	120.91
3	F	203	2VJ	C11-C9-C7	-2.88	105.76	111.88
3	A	202	2VJ	C9-C7-N8	2.85	119.92	117.00
3	B	202	2VJ	C11-C9-C15	-2.83	105.25	109.84
3	D	202	2VJ	C9-C7-N8	-2.80	114.13	117.00
3	B	202	2VJ	C12-C13-C14	-2.74	105.82	111.42
3	B	202	2VJ	O38-C36-C33	2.74	120.92	114.69
3	F	203	2VJ	C4-C3-N8	-2.73	120.00	122.90
2	F	201	AGS	PA-O3A-PB	-2.67	123.65	132.83
3	A	202	2VJ	C25-C26-C21	-2.66	118.64	120.46
3	B	202	2VJ	C25-C24-CL8	-2.64	114.39	120.85
2	B	201	AGS	O2G-PG-O3B	2.64	113.47	104.64
3	F	203	2VJ	C22-C23-C24	-2.63	116.20	120.00
3	D	202	2VJ	C20-C21-C22	-2.61	115.50	120.91
2	F	201	AGS	C2'-C3'-C4'	-2.58	97.64	102.64
3	A	203	2VJ	C9-C7-N8	2.56	119.62	117.00
2	D	201	AGS	PA-O5'-C5'	-2.53	106.85	121.68
3	F	203	2VJ	O38-C36-C33	2.53	120.44	114.69
2	F	201	AGS	O2A-PA-O5'	-2.51	96.09	107.75
3	F	203	2VJ	N8-C7-N6	-2.48	122.42	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	203	2VJ	C26-C25-C24	2.45	123.54	120.21
3	F	202	2VJ	C2-C3-C4	-2.39	117.74	122.58
3	A	202	2VJ	C22-C23-C24	-2.38	116.56	120.00
3	A	202	2VJ	C22-C21-C26	2.36	121.84	118.54
3	B	202	2VJ	O37-C36-C33	-2.34	116.50	121.24
3	B	202	2VJ	C11-C9-C7	-2.34	106.91	111.88
3	F	203	2VJ	C9-C7-N8	2.27	119.33	117.00
3	F	202	2VJ	C14-C15-C17	-2.26	105.93	111.13
3	B	202	2VJ	C13-C12-C11	-2.25	106.82	111.42
3	A	203	2VJ	C4-C3-N8	-2.24	120.52	122.90
3	F	203	2VJ	O38-C36-O37	-2.24	118.37	123.35
2	A	201	AGS	O4'-C4'-C3'	2.24	109.54	105.11
3	D	202	2VJ	O18-C17-C15	-2.23	119.04	121.73
2	A	201	AGS	C2'-C3'-C4'	-2.22	98.33	102.64
2	D	201	AGS	C4-C5-N7	-2.19	107.11	109.40
3	B	202	2VJ	C23-C22-C21	-2.19	118.01	121.03
3	B	202	2VJ	S29-C5-N6	2.14	124.73	116.44
3	B	202	2VJ	C4-C5-N6	-2.13	122.06	123.55
3	F	202	2VJ	C14-C15-C9	-2.13	107.20	109.58
2	B	201	AGS	N3-C2-N1	-2.12	125.36	128.68
3	A	202	2VJ	C23-C24-C25	2.12	123.96	120.01
3	F	203	2VJ	C12-C11-C9	-2.10	108.74	111.63
3	A	203	2VJ	C12-C13-C14	-2.09	107.15	111.42
3	F	202	2VJ	N8-C7-N6	-2.09	122.99	126.00
2	B	201	AGS	PA-O5'-C5'	-2.04	109.70	121.68
3	F	202	2VJ	C22-C21-C26	2.03	121.39	118.54
3	D	202	2VJ	C13-C12-C11	-2.03	107.28	111.42
2	D	201	AGS	C3'-C2'-C1'	2.02	104.03	100.98
2	E	201	AGS	O2A-PA-O5'	2.02	117.14	107.75
3	D	202	2VJ	S29-C5-N6	2.01	124.22	116.44
3	D	202	2VJ	N8-C7-N6	-2.01	123.10	126.00

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	AGS	PB-O3B-PG-O2G
2	A	201	AGS	C5'-O5'-PA-O2A
2	D	201	AGS	O4'-C4'-C5'-O5'
2	E	201	AGS	C5'-O5'-PA-O3A
2	D	201	AGS	C3'-C4'-C5'-O5'
2	F	201	AGS	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	F	201	AGS	O4'-C4'-C5'-O5'
2	A	201	AGS	O4'-C4'-C5'-O5'
2	F	201	AGS	C5'-O5'-PA-O3A
2	E	201	AGS	PA-O3A-PB-O1B
2	A	201	AGS	C5'-O5'-PA-O1A
2	E	201	AGS	C5'-O5'-PA-O1A
2	F	201	AGS	C5'-O5'-PA-O2A
2	F	201	AGS	PA-O3A-PB-O2B
2	D	201	AGS	C4'-C5'-O5'-PA
2	A	201	AGS	PB-O3B-PG-O3G
2	F	201	AGS	PB-O3B-PG-O2G
2	F	201	AGS	PB-O3B-PG-O3G
2	A	201	AGS	C3'-C4'-C5'-O5'
2	A	201	AGS	C5'-O5'-PA-O3A
2	B	201	AGS	C5'-O5'-PA-O3A
2	C	201	AGS	C5'-O5'-PA-O3A
2	B	201	AGS	C5'-O5'-PA-O1A

There are no ring outliers.

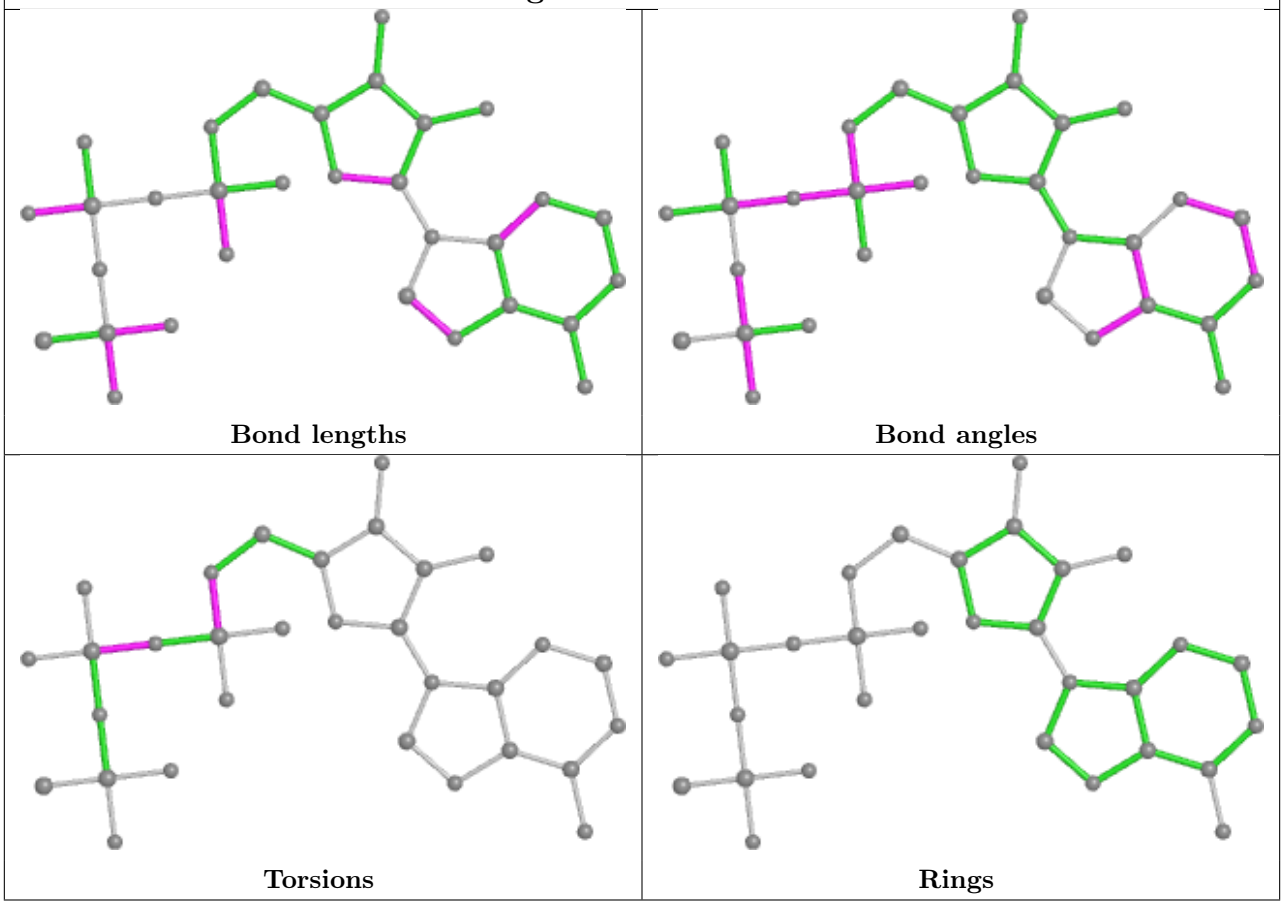
9 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	201	AGS	3	0
2	F	201	AGS	1	0
3	A	203	2VJ	3	0
2	A	201	AGS	4	0
3	A	202	2VJ	3	0
3	B	202	2VJ	1	0
2	C	201	AGS	1	0
3	D	202	2VJ	3	0
3	F	202	2VJ	2	0

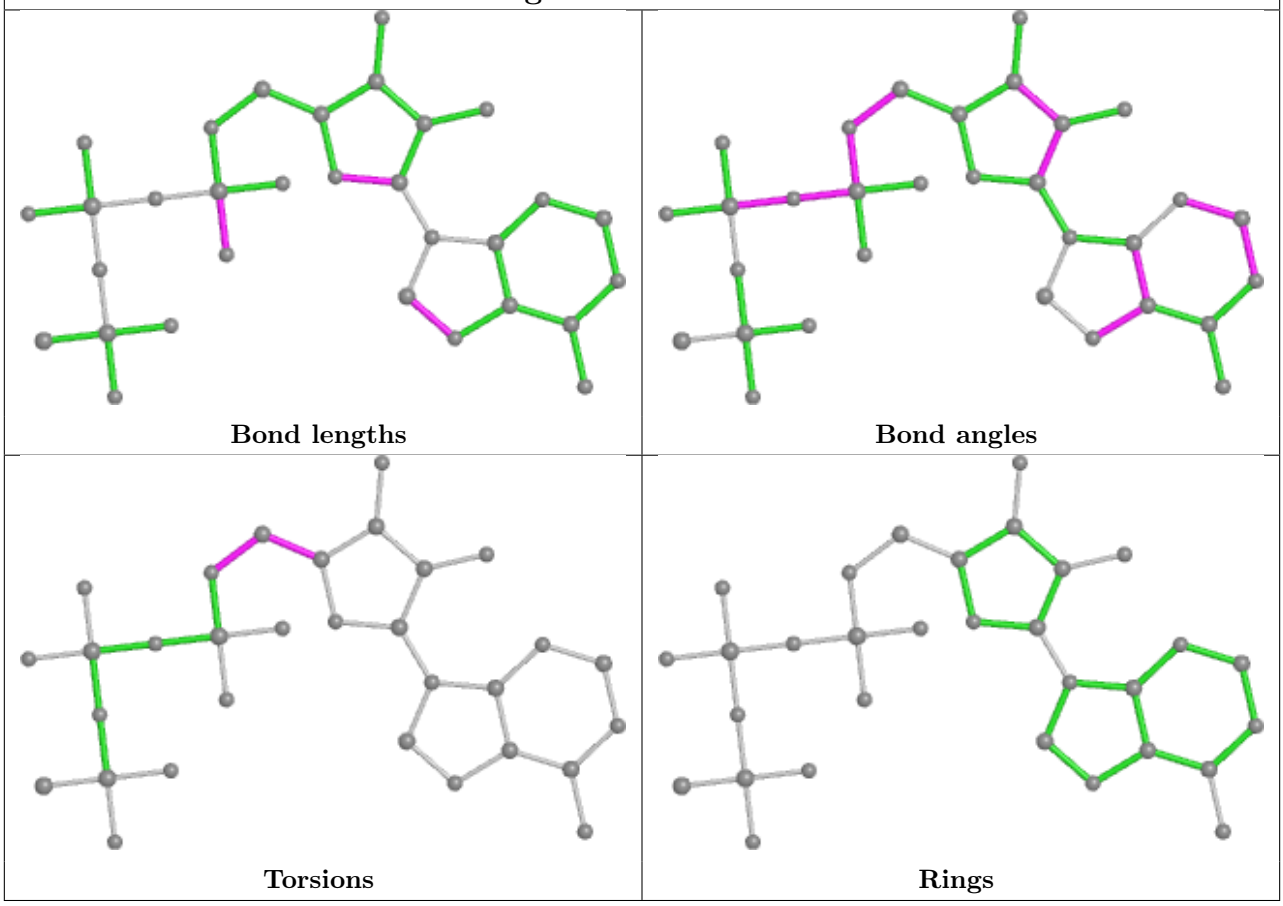
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

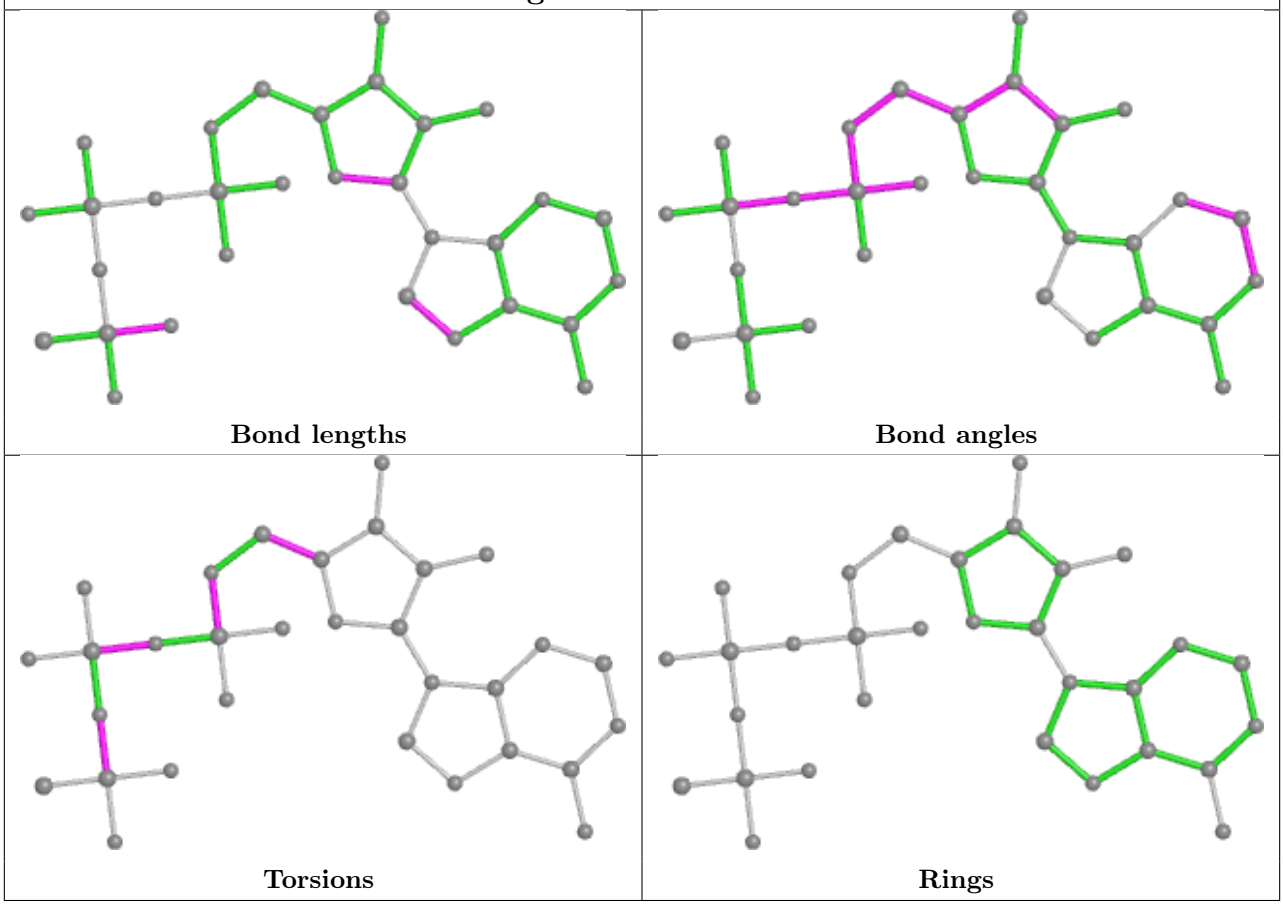
Ligand AGS E 201



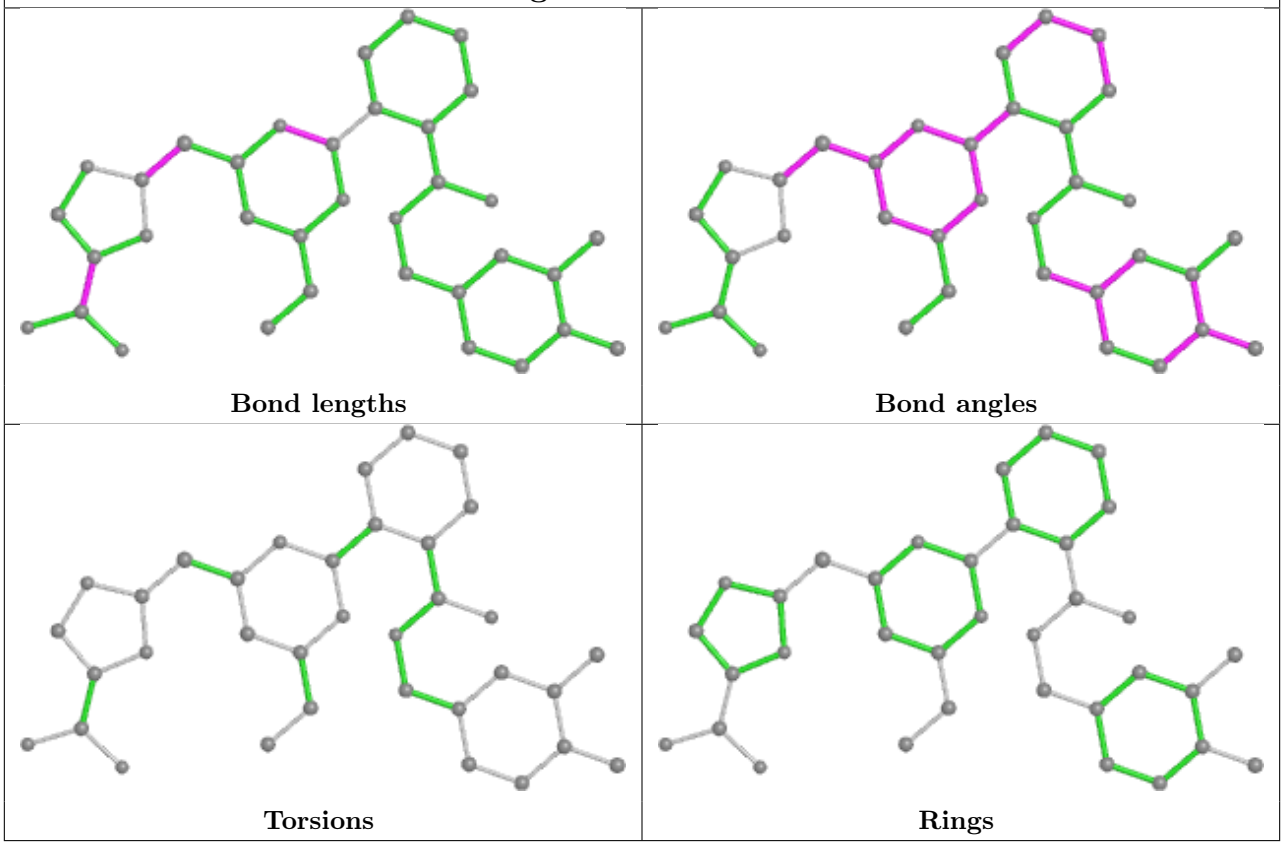
Ligand AGS D 201



Ligand AGS F 201



Ligand 2VJ A 203



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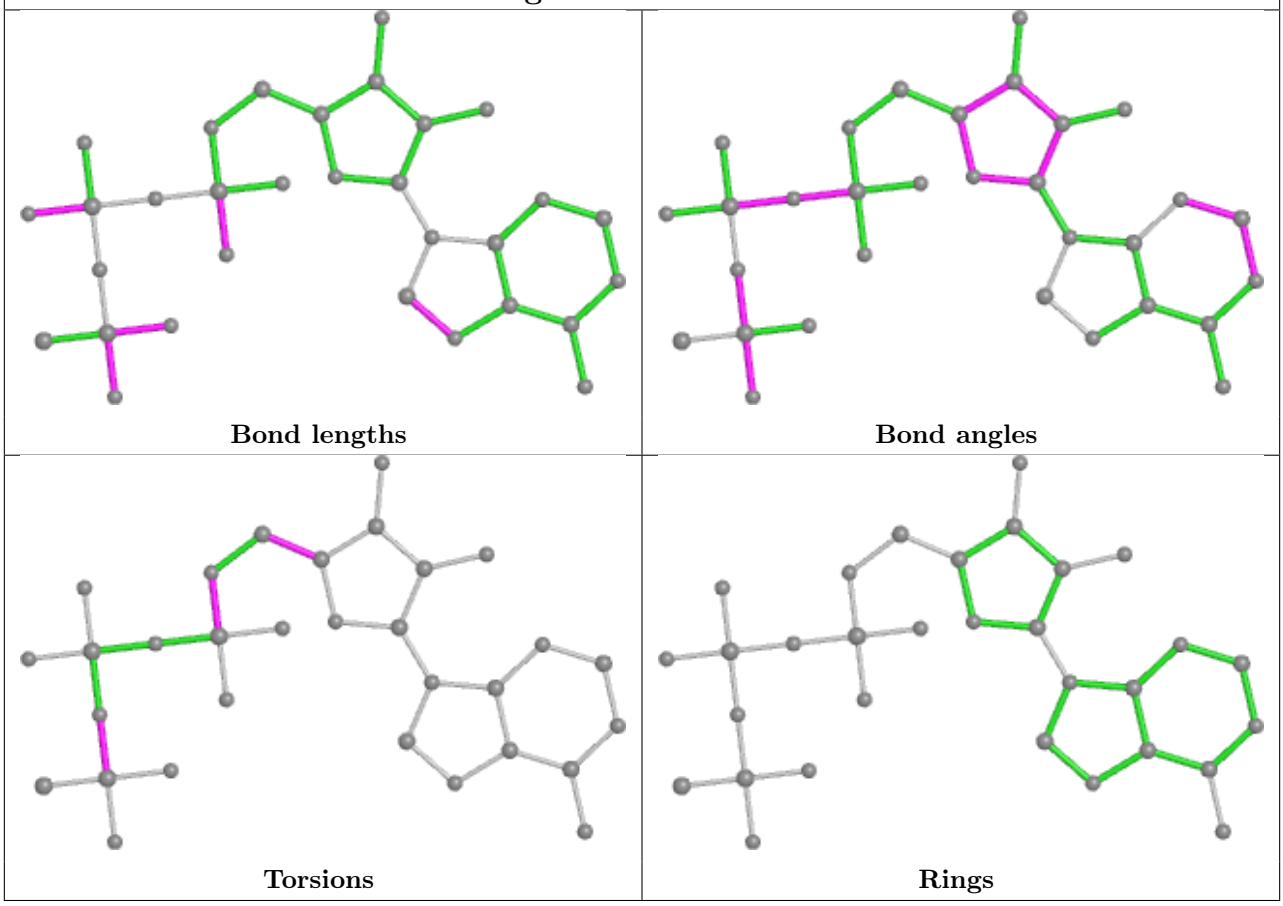
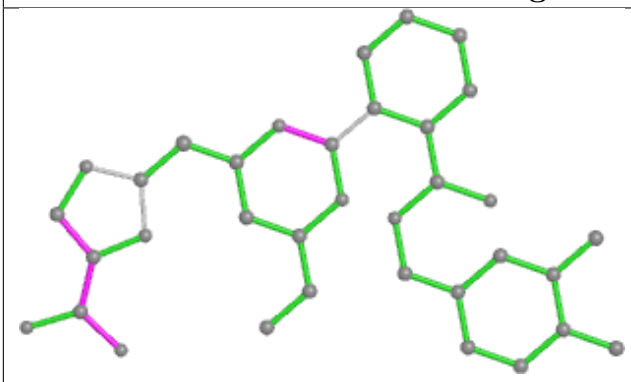
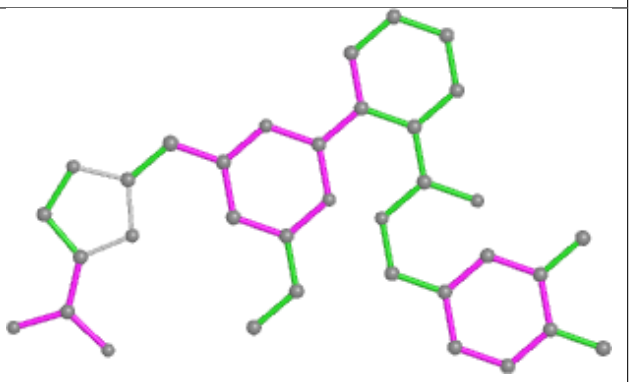


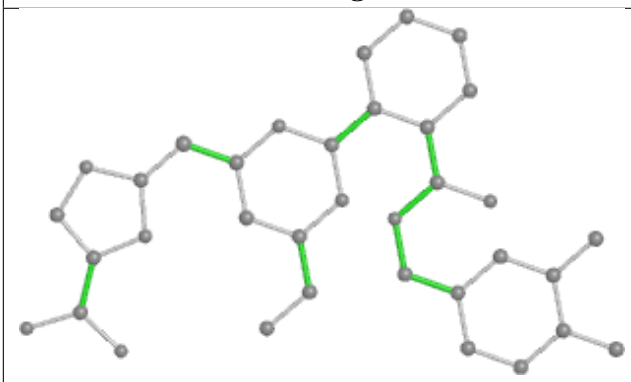
Ligand 2VJ A 202



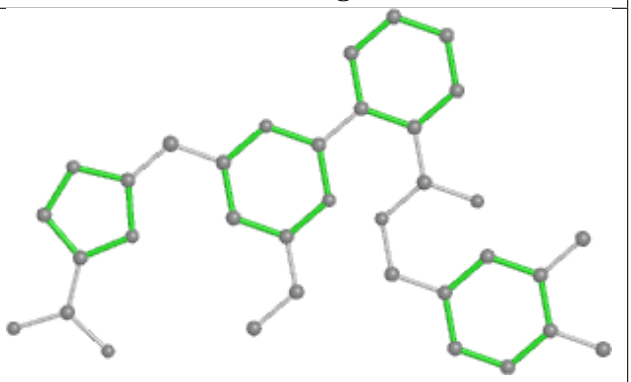
Bond lengths



Bond angles

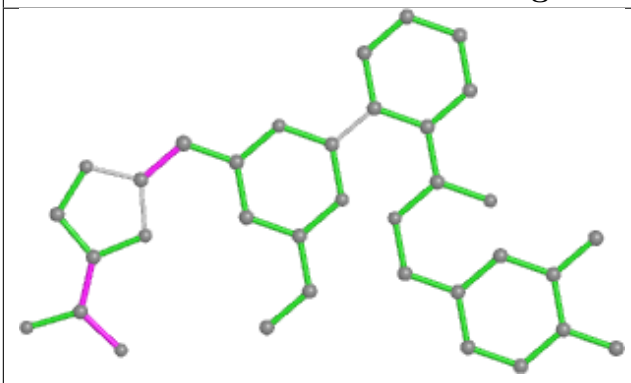


Torsions

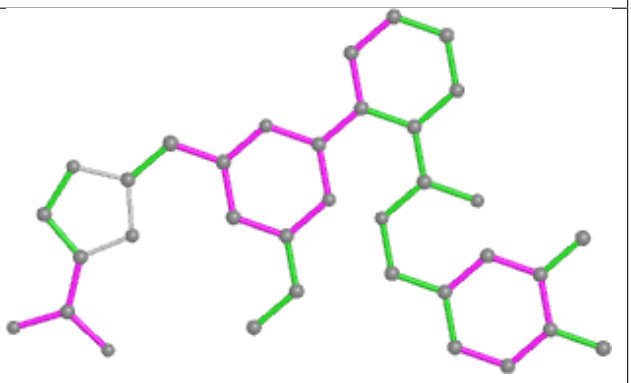


Rings

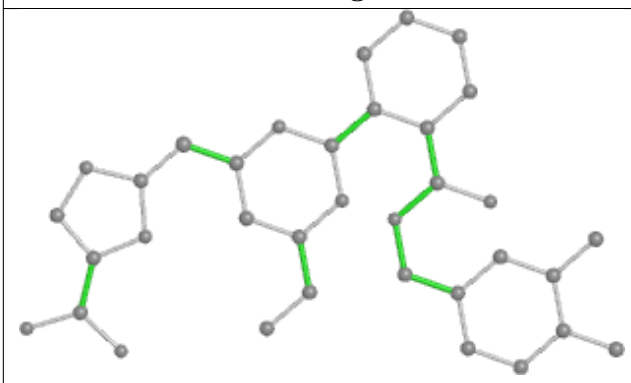
Ligand 2VJ F 203



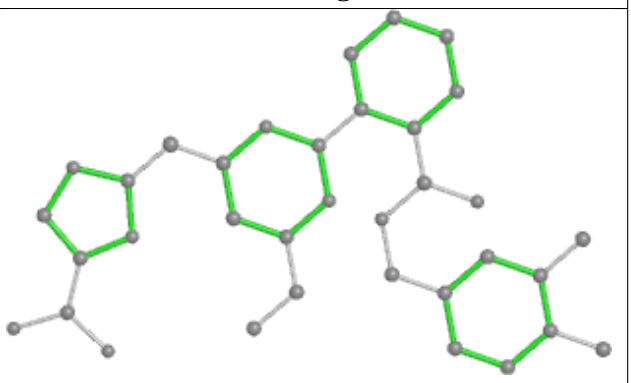
Bond lengths



Bond angles

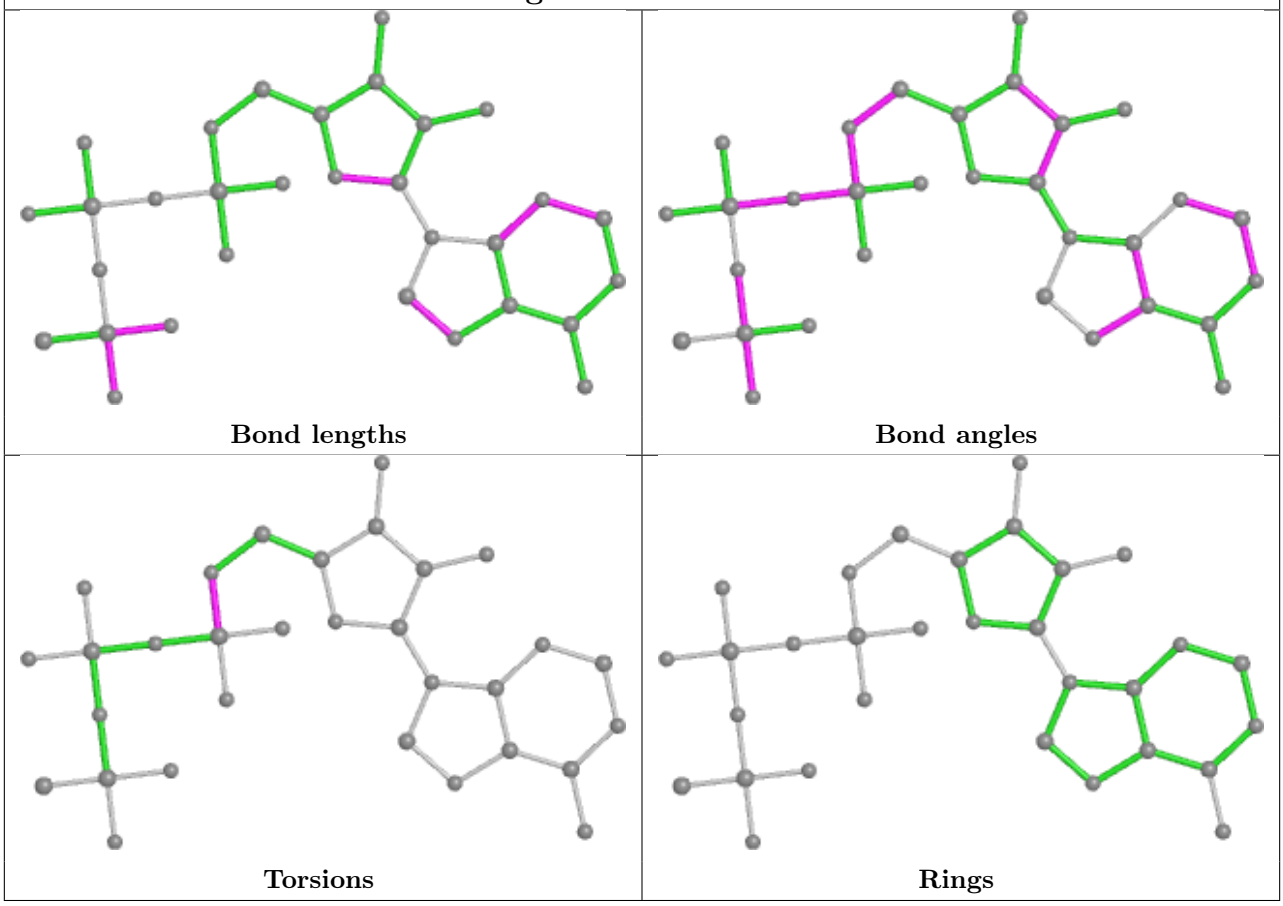


Torsions

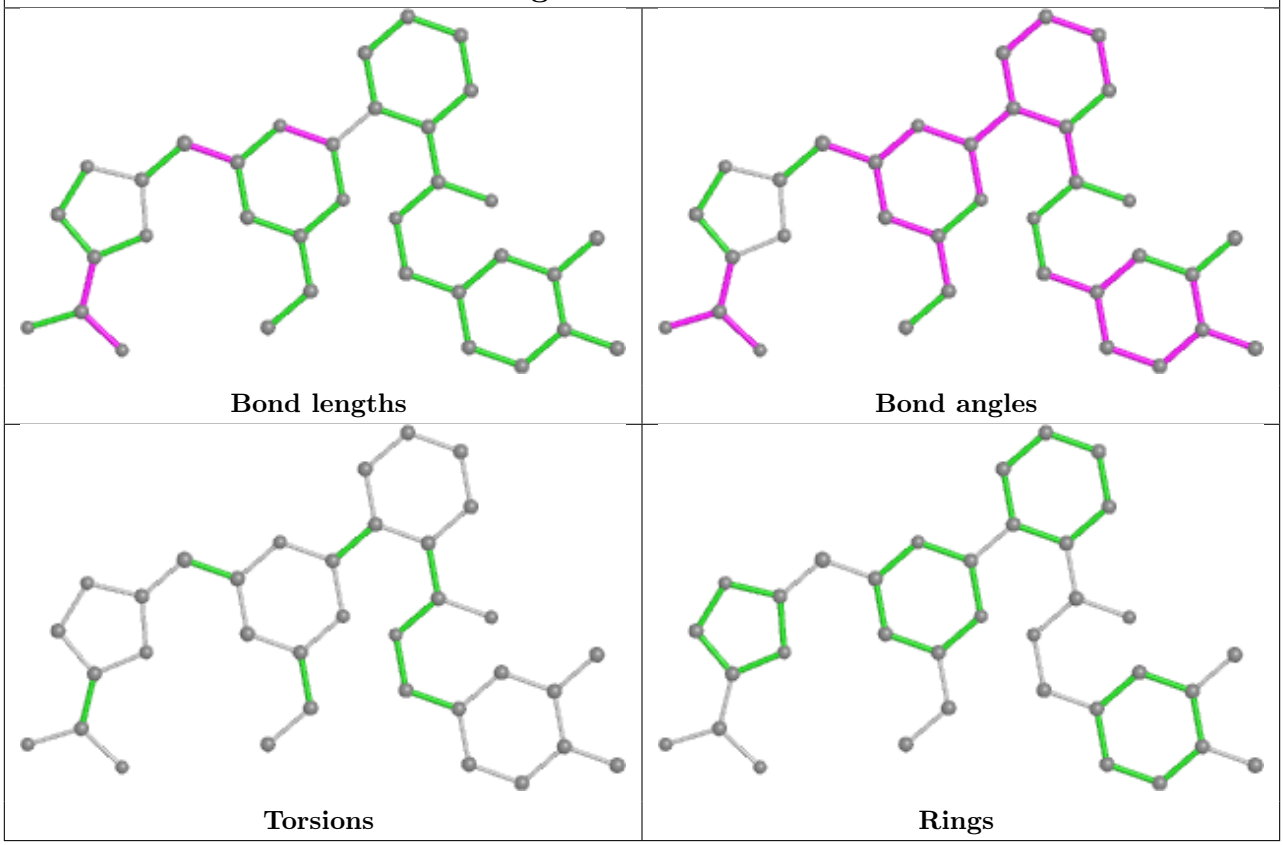


Rings

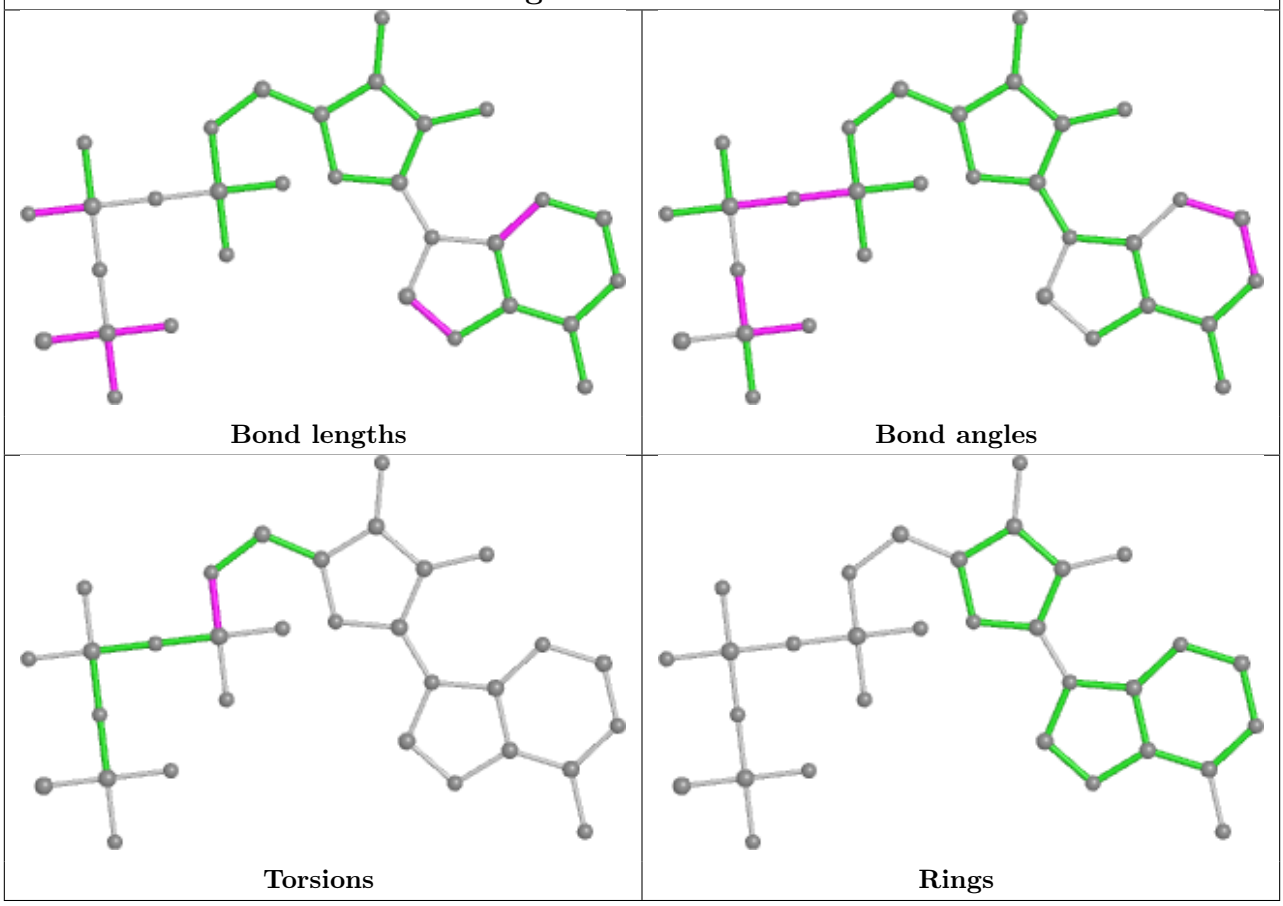
Ligand AGS B 201



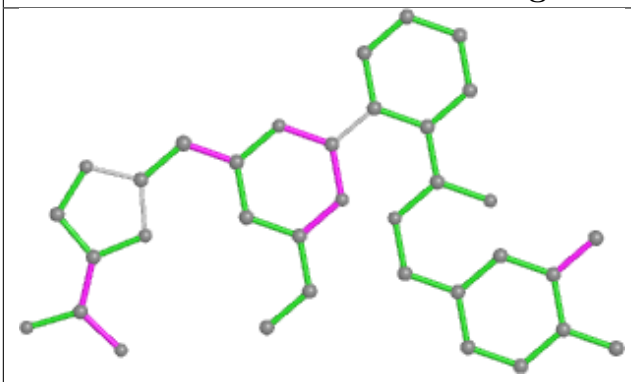
Ligand 2VJ B 202



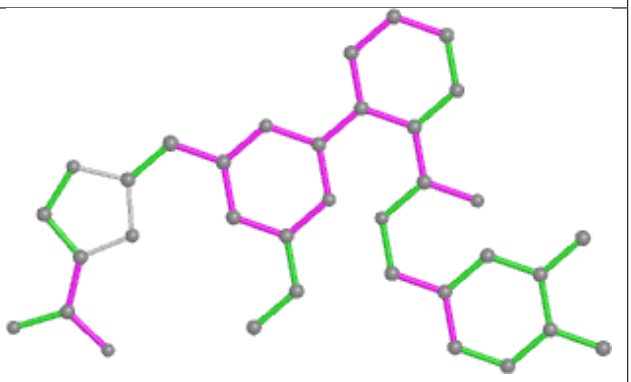
Ligand AGS C 201



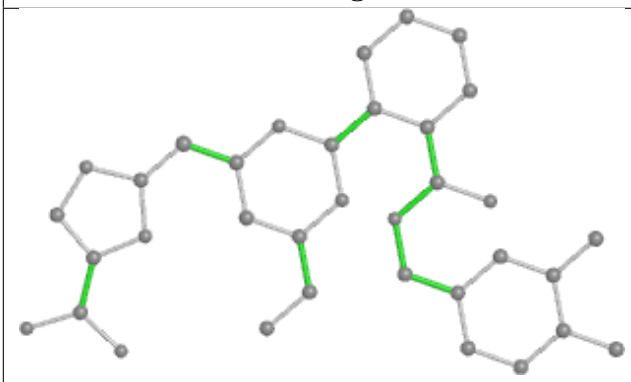
Ligand 2VJ D 202



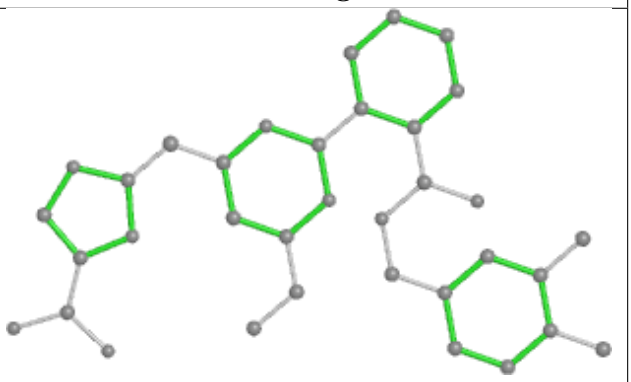
Bond lengths



Bond angles

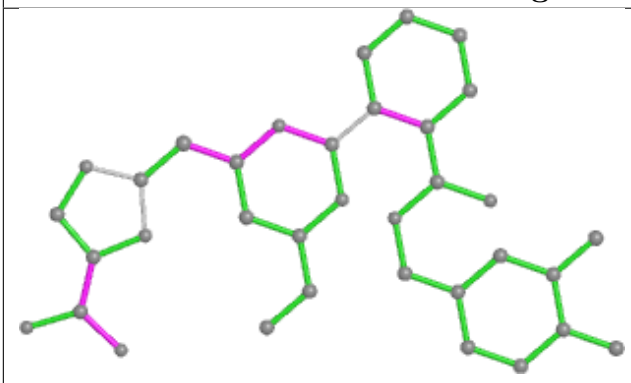


Torsions

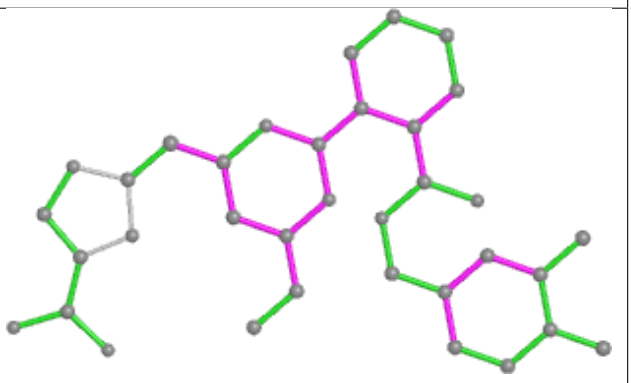


Rings

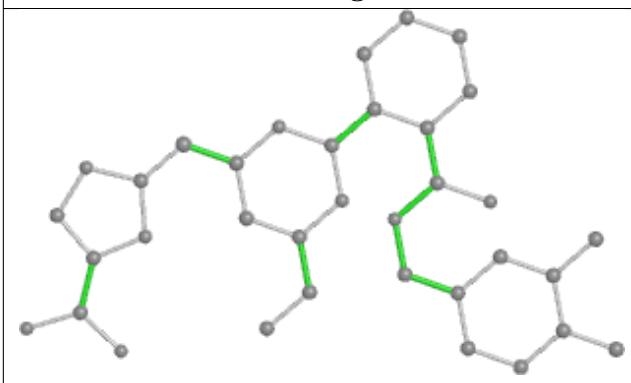
Ligand 2VJ F 202



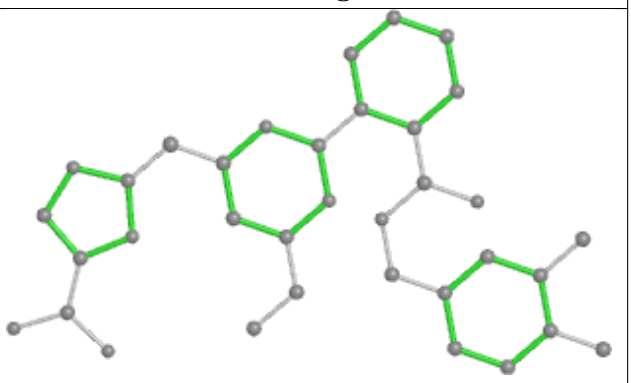
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	159/160 (99%)	0.21	3 (1%)	66	68	21, 35, 50, 50	0
1	B	160/160 (100%)	0.39	13 (8%)	12	13	20, 33, 50, 50	0
1	C	160/160 (100%)	0.40	10 (6%)	20	21	22, 38, 50, 50	0
1	D	159/160 (99%)	0.36	6 (3%)	40	43	20, 38, 50, 50	0
1	E	160/160 (100%)	0.79	19 (11%)	4	5	27, 46, 50, 50	0
1	F	160/160 (100%)	0.47	16 (10%)	7	8	22, 39, 50, 50	0
All	All	958/960 (99%)	0.44	67 (6%)	16	17	20, 38, 50, 50	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	40	ASN	6.3
1	E	1	MET	6.1
1	E	160	LYS	6.0
1	B	1	MET	5.4
1	E	40	ASN	5.3
1	C	160	LYS	4.7
1	C	39	LYS	4.4
1	D	42	LYS	4.2
1	B	2	GLU	4.1
1	F	40	ASN	4.0
1	E	42	LYS	3.9
1	D	43	LYS	3.8
1	B	160	LYS	3.8
1	B	44	GLU	3.7
1	E	157	LYS	3.6
1	A	43	LYS	3.6
1	A	44	GLU	3.5
1	E	43	LYS	3.5
1	F	44	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	38	LEU	3.4
1	E	2	GLU	3.3
1	C	43	LYS	3.3
1	F	160	LYS	3.3
1	E	41	SER	3.3
1	F	42	LYS	3.3
1	C	41	SER	3.2
1	C	44	GLU	3.2
1	E	151	VAL	3.2
1	C	72	SER	3.1
1	C	140	ARG	3.0
1	F	39	LYS	3.0
1	C	42	LYS	2.9
1	A	42	LYS	2.8
1	E	44	GLU	2.8
1	F	157	LYS	2.8
1	E	39	LYS	2.8
1	F	41	SER	2.8
1	E	47	PHE	2.7
1	B	43	LYS	2.7
1	E	159	PHE	2.7
1	B	42	LYS	2.6
1	D	40	ASN	2.6
1	B	150	TYR	2.6
1	E	150	TYR	2.5
1	F	155	LEU	2.5
1	B	41	SER	2.4
1	F	72	SER	2.4
1	F	145	GLU	2.4
1	B	40	ASN	2.4
1	E	3	HIS	2.4
1	F	46	THR	2.3
1	D	2	GLU	2.3
1	B	49	LEU	2.3
1	C	71	PHE	2.3
1	E	45	GLY	2.2
1	E	48	SER	2.2
1	F	153	LYS	2.2
1	D	160	LYS	2.2
1	E	153	LYS	2.1
1	D	150	TYR	2.1
1	F	150	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	94	VAL	2.1
1	B	72	SER	2.1
1	B	45	GLY	2.1
1	E	155	LEU	2.1
1	F	156	LYS	2.1
1	F	43	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

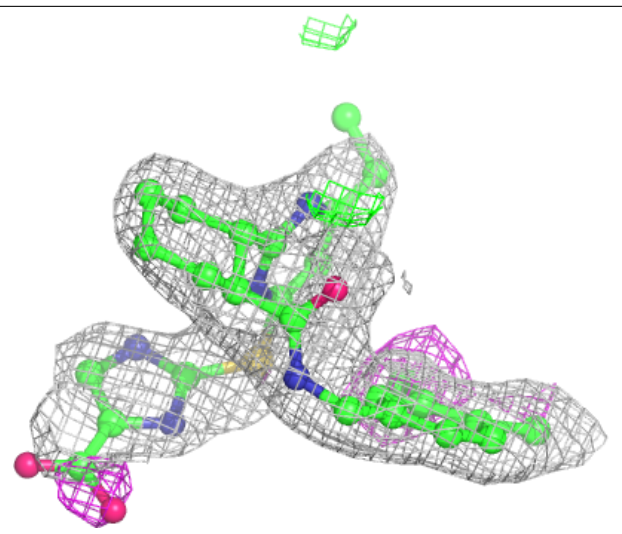
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

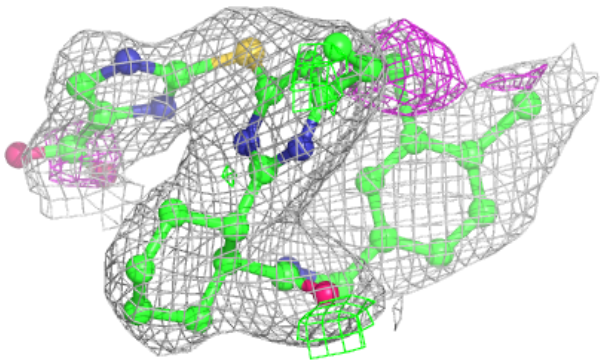
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	2VJ	F	202	35/35	0.81	0.21	35,44,50,50	0
3	2VJ	D	202	35/35	0.82	0.19	25,39,50,50	0
3	2VJ	F	203	35/35	0.83	0.17	32,39,50,50	0
3	2VJ	A	203	35/35	0.85	0.20	25,35,50,50	0
3	2VJ	A	202	35/35	0.86	0.19	30,40,50,50	0
3	2VJ	B	202	35/35	0.88	0.16	24,31,50,50	0
2	AGS	F	201	31/31	0.88	0.17	34,42,50,50	0
2	AGS	A	201	31/31	0.88	0.15	26,37,50,50	0
2	AGS	D	201	31/31	0.88	0.17	24,33,50,50	0
2	AGS	E	201	31/31	0.89	0.16	28,42,50,50	0
2	AGS	C	201	31/31	0.91	0.15	32,40,50,50	0
2	AGS	B	201	31/31	0.93	0.15	21,29,50,50	0

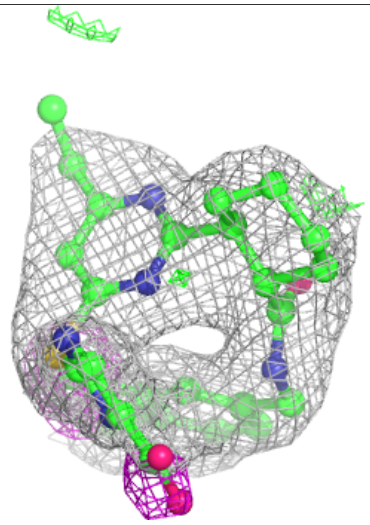
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 2VJ F 202:

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

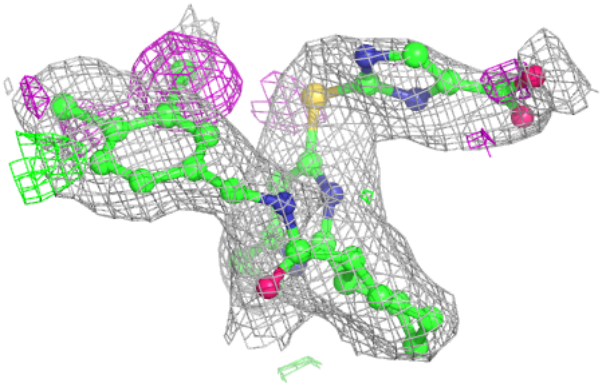


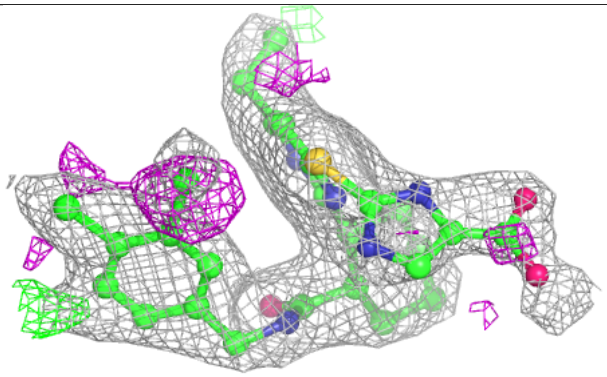


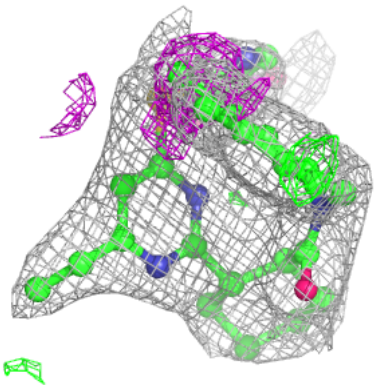


Electron density around 2VJ D 202:

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

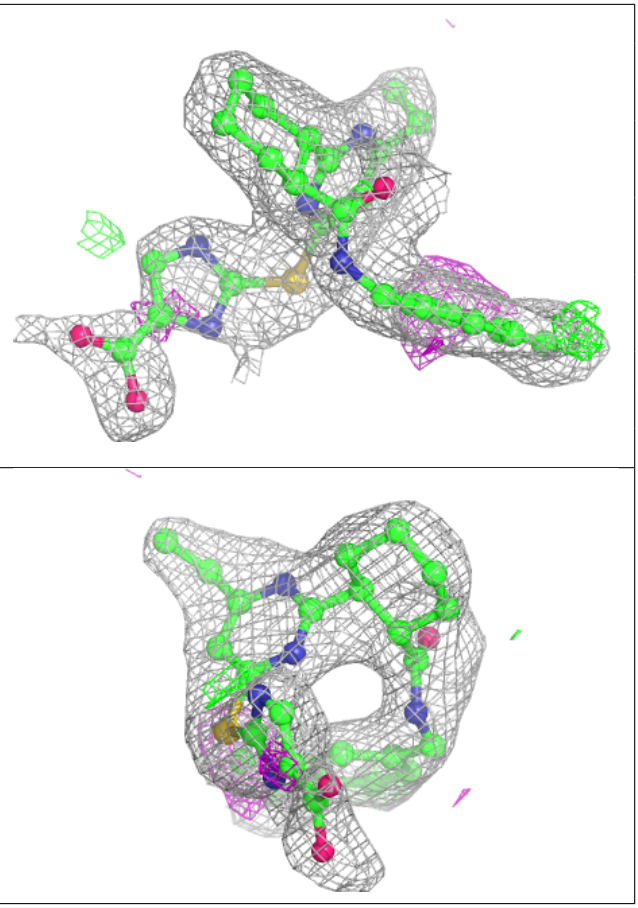






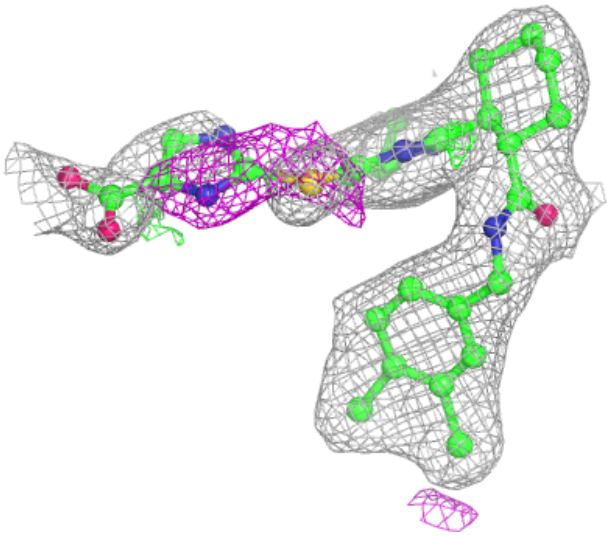
Electron density around 2VJ F 203:

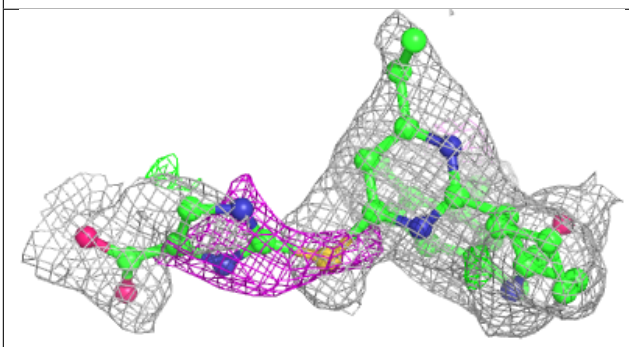
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

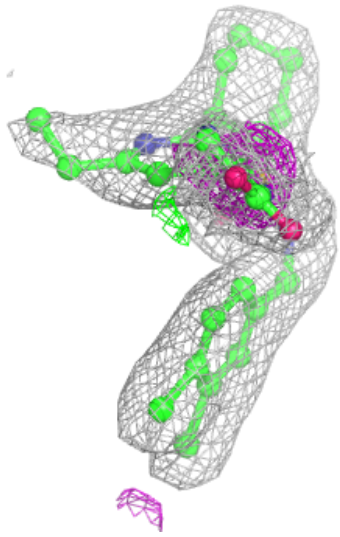


Electron density around 2VJ A 203:

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

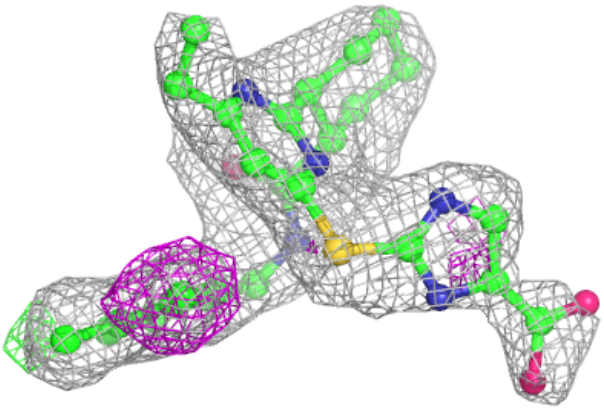


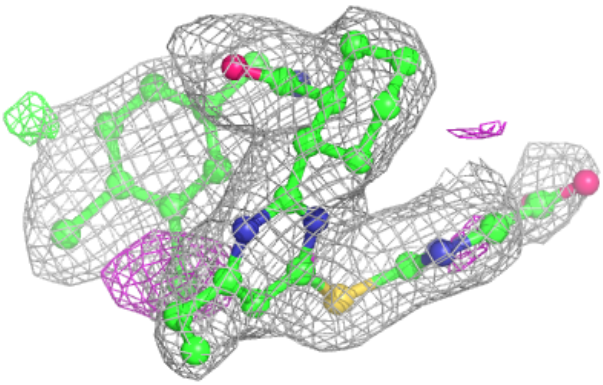


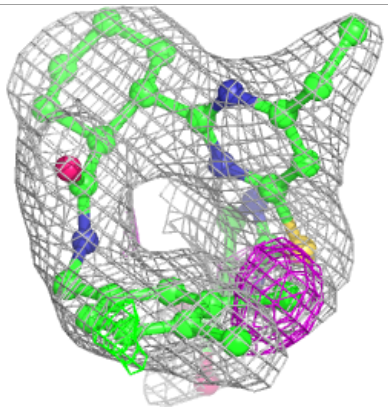


Electron density around 2VJ A 202:

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

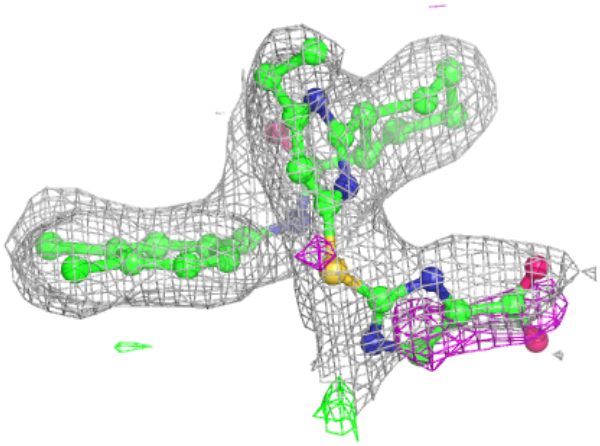


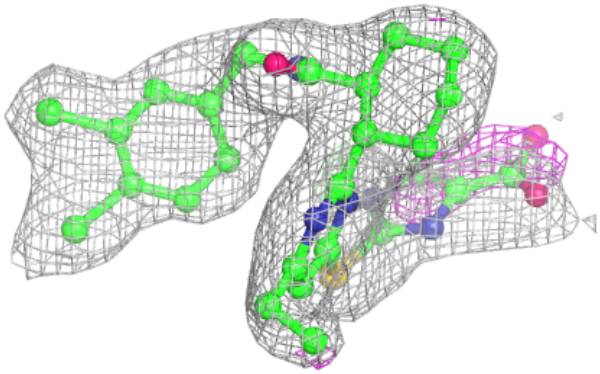


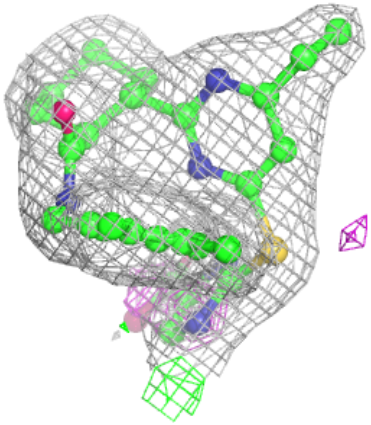


Electron density around 2VJ B 202:

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

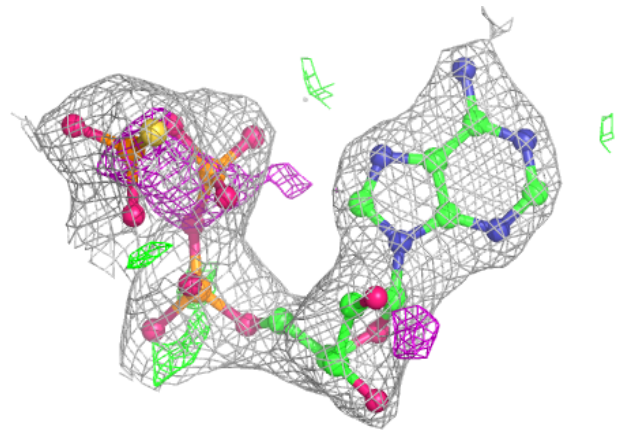


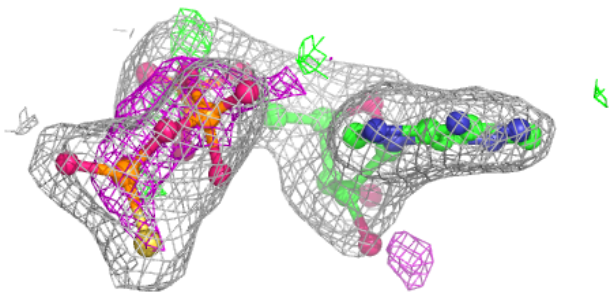


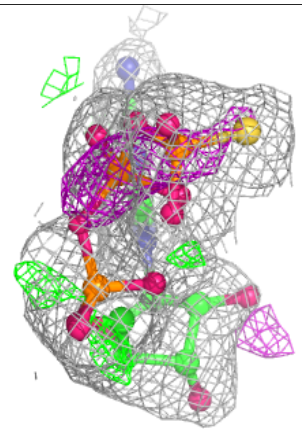


Electron density around AGS F 201:

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

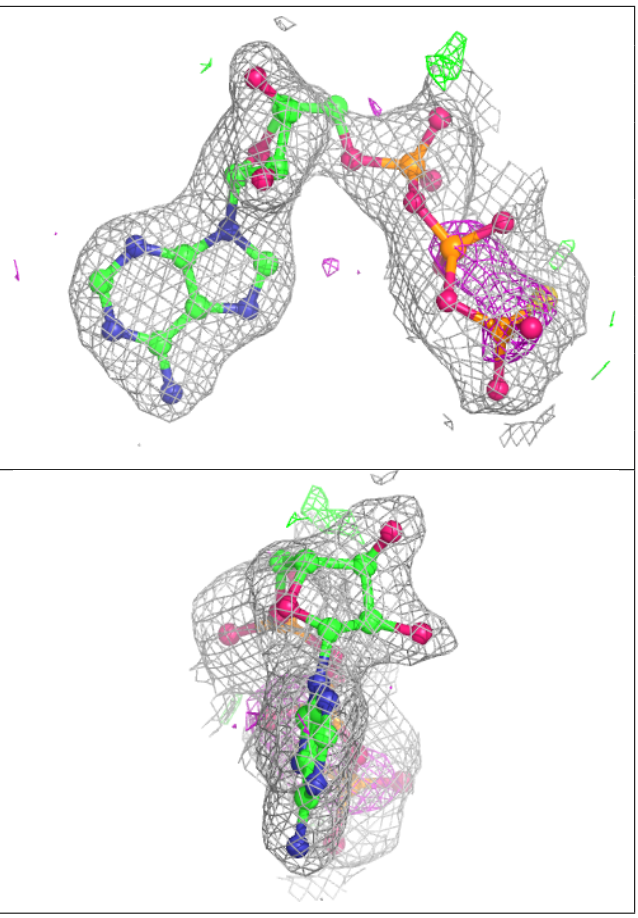






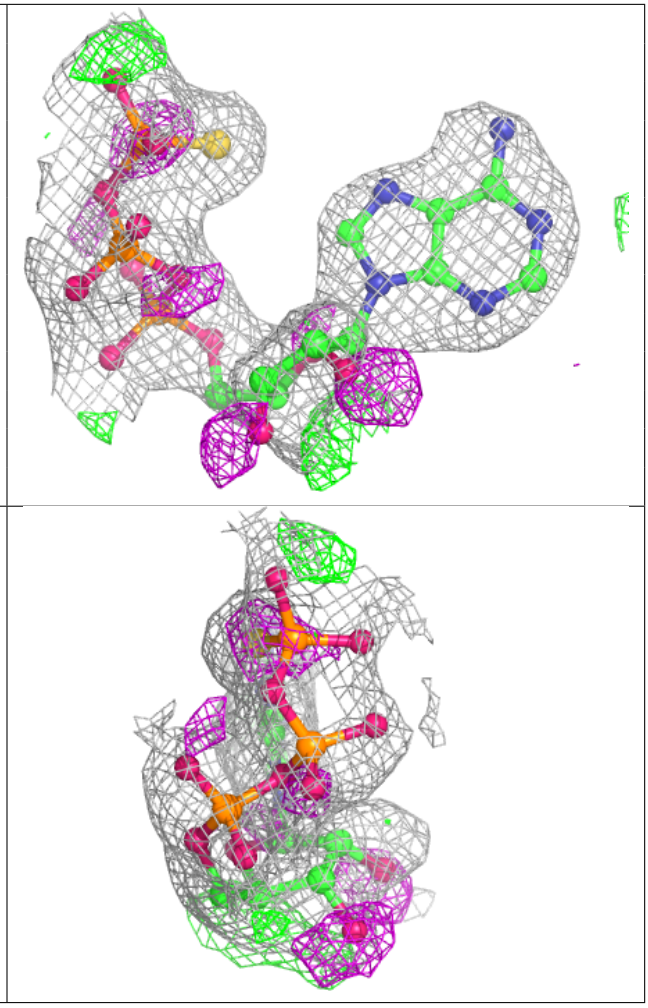
Electron density around AGS A 201:

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



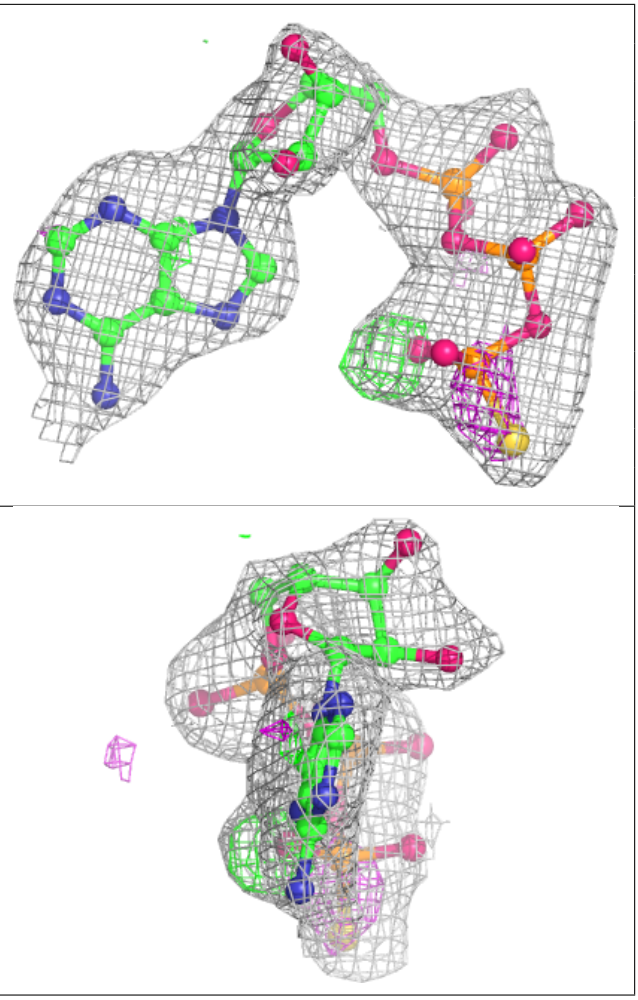
Electron density around AGS D 201:

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



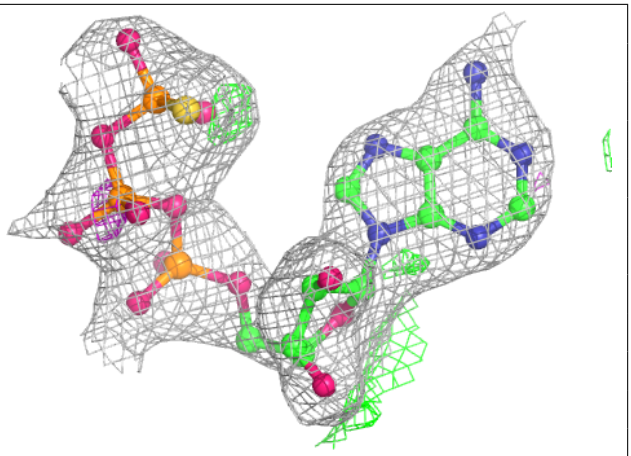
Electron density around AGS E 201:

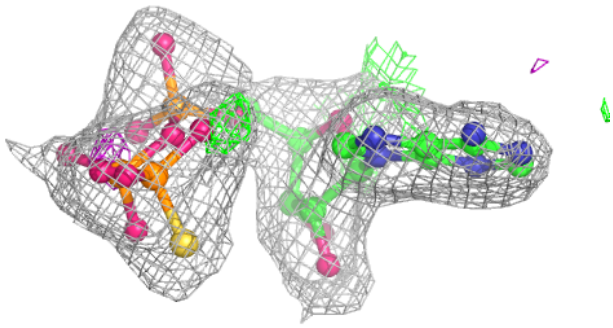
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

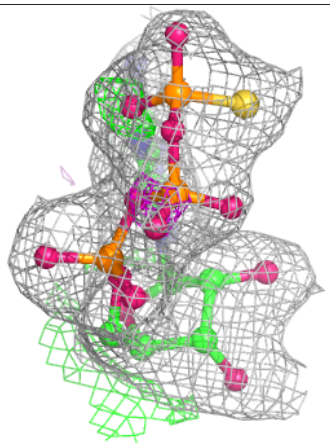


Electron density around AGS C 201:

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

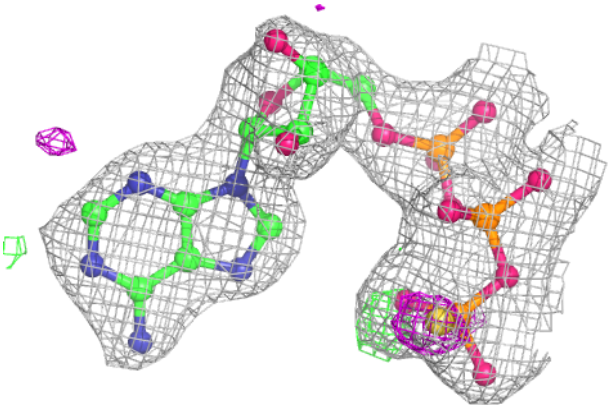


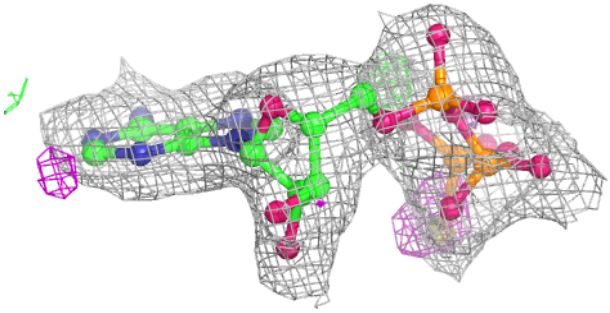


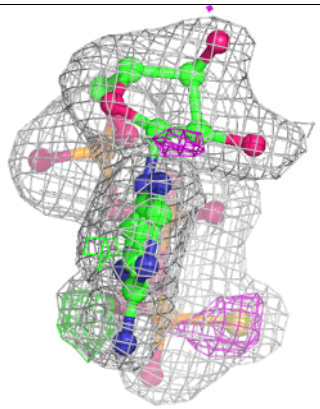


Electron density around AGS B 201:

$2mF_o$-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.