Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 03:21 PM BST

PDB ID	:	5M2X
Title	:	Crystal structure of the full-length Zika virus NS5 protein (Human isolate Z1106033)
Authors	:	Ferrero, D.S.; Ruiz-Arroyo, V.M.; Soler, N.; Uson, I.; Verdaguer, N.
Deposited on	:	2016-10-13
Resolution	:	4.99 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:

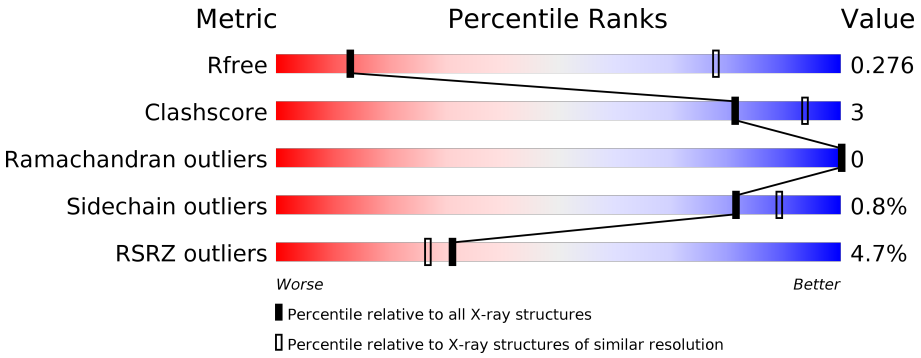
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.99 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	1140 (6.20-3.80)
Clashscore	141614	1000 (6.16-3.82)
Ramachandran outliers	138981	1146 (6.20-3.80)
Sidechain outliers	138945	1122 (6.20-3.80)
RSRZ outliers	127900	1010 (6.22-3.72)

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	914	5% 89% 8% ·
1	B	914	6% 90% 7% ·
1	C	914	6% 90% 6% ·
1	D	914	3% 89% 7% ·
1	E	914	3% 89% 8% ·
1	F	914	4% 89% 7% ·

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	D	1002	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 42817 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 NS5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	883	Total	C	N	O	S	0	0	0
			7097	4463	1286	1302	46			
1	B	882	Total	C	N	O	S	0	0	0
			7090	4459	1285	1300	46			
1	C	883	Total	C	N	O	S	0	0	0
			7097	4463	1286	1302	46			
1	D	883	Total	C	N	O	S	0	0	0
			7097	4463	1286	1302	46			
1	E	883	Total	C	N	O	S	0	0	0
			7097	4463	1286	1302	46			
1	F	883	Total	C	N	O	S	0	0	0
			7097	4463	1286	1302	46			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP A0A1B2ZC85
A	904	GLY	-	expression tag	UNP A0A1B2ZC85
A	905	SER	-	expression tag	UNP A0A1B2ZC85
A	906	SER	-	expression tag	UNP A0A1B2ZC85
A	907	SER	-	expression tag	UNP A0A1B2ZC85
A	908	HIS	-	expression tag	UNP A0A1B2ZC85
A	909	HIS	-	expression tag	UNP A0A1B2ZC85
A	910	HIS	-	expression tag	UNP A0A1B2ZC85
A	911	HIS	-	expression tag	UNP A0A1B2ZC85
A	912	HIS	-	expression tag	UNP A0A1B2ZC85
A	913	HIS	-	expression tag	UNP A0A1B2ZC85
B	0	MET	-	initiating methionine	UNP A0A1B2ZC85
B	904	GLY	-	expression tag	UNP A0A1B2ZC85
B	905	SER	-	expression tag	UNP A0A1B2ZC85
B	906	SER	-	expression tag	UNP A0A1B2ZC85
B	907	SER	-	expression tag	UNP A0A1B2ZC85
B	908	HIS	-	expression tag	UNP A0A1B2ZC85

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Chain	Residue	Modelled	Actual	Comment	Reference
B	909	HIS	-	expression tag	UNP A0A1B2ZC85
B	910	HIS	-	expression tag	UNP A0A1B2ZC85
B	911	HIS	-	expression tag	UNP A0A1B2ZC85
B	912	HIS	-	expression tag	UNP A0A1B2ZC85
B	913	HIS	-	expression tag	UNP A0A1B2ZC85
C	0	MET	-	initiating methionine	UNP A0A1B2ZC85
C	904	GLY	-	expression tag	UNP A0A1B2ZC85
C	905	SER	-	expression tag	UNP A0A1B2ZC85
C	906	SER	-	expression tag	UNP A0A1B2ZC85
C	907	SER	-	expression tag	UNP A0A1B2ZC85
C	908	HIS	-	expression tag	UNP A0A1B2ZC85
C	909	HIS	-	expression tag	UNP A0A1B2ZC85
C	910	HIS	-	expression tag	UNP A0A1B2ZC85
C	911	HIS	-	expression tag	UNP A0A1B2ZC85
C	912	HIS	-	expression tag	UNP A0A1B2ZC85
C	913	HIS	-	expression tag	UNP A0A1B2ZC85
D	0	MET	-	initiating methionine	UNP A0A1B2ZC85
D	904	GLY	-	expression tag	UNP A0A1B2ZC85
D	905	SER	-	expression tag	UNP A0A1B2ZC85
D	906	SER	-	expression tag	UNP A0A1B2ZC85
D	907	SER	-	expression tag	UNP A0A1B2ZC85
D	908	HIS	-	expression tag	UNP A0A1B2ZC85
D	909	HIS	-	expression tag	UNP A0A1B2ZC85
D	910	HIS	-	expression tag	UNP A0A1B2ZC85
D	911	HIS	-	expression tag	UNP A0A1B2ZC85
D	912	HIS	-	expression tag	UNP A0A1B2ZC85
D	913	HIS	-	expression tag	UNP A0A1B2ZC85
E	0	MET	-	initiating methionine	UNP A0A1B2ZC85
E	904	GLY	-	expression tag	UNP A0A1B2ZC85
E	905	SER	-	expression tag	UNP A0A1B2ZC85
E	906	SER	-	expression tag	UNP A0A1B2ZC85
E	907	SER	-	expression tag	UNP A0A1B2ZC85
E	908	HIS	-	expression tag	UNP A0A1B2ZC85
E	909	HIS	-	expression tag	UNP A0A1B2ZC85
E	910	HIS	-	expression tag	UNP A0A1B2ZC85
E	911	HIS	-	expression tag	UNP A0A1B2ZC85
E	912	HIS	-	expression tag	UNP A0A1B2ZC85
E	913	HIS	-	expression tag	UNP A0A1B2ZC85
F	0	MET	-	initiating methionine	UNP A0A1B2ZC85
F	904	GLY	-	expression tag	UNP A0A1B2ZC85
F	905	SER	-	expression tag	UNP A0A1B2ZC85
F	906	SER	-	expression tag	UNP A0A1B2ZC85

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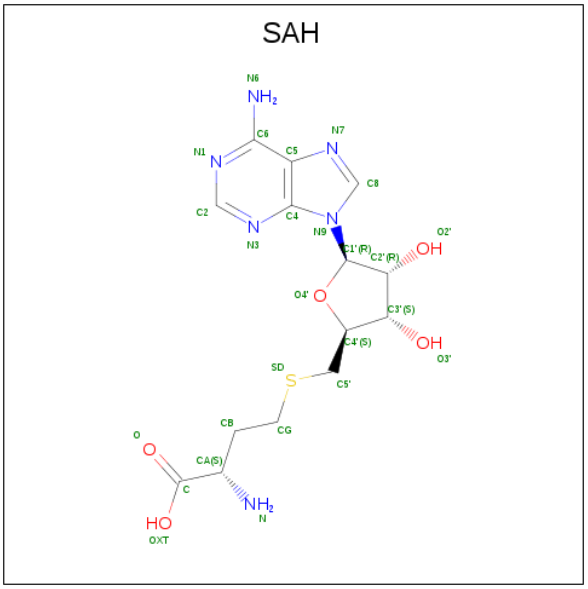
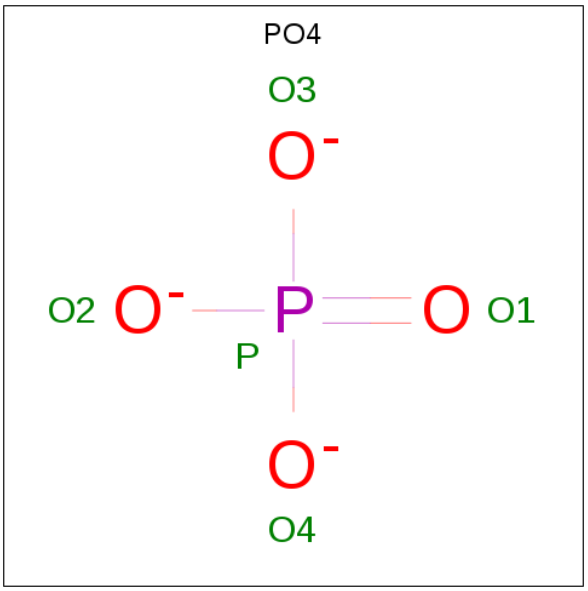
Chain	Residue	Modelled	Actual	Comment	Reference
F	907	SER	-	expression tag	UNP A0A1B2ZC85
F	908	HIS	-	expression tag	UNP A0A1B2ZC85
F	909	HIS	-	expression tag	UNP A0A1B2ZC85
F	910	HIS	-	expression tag	UNP A0A1B2ZC85
F	911	HIS	-	expression tag	UNP A0A1B2ZC85
F	912	HIS	-	expression tag	UNP A0A1B2ZC85
F	913	HIS	-	expression tag	UNP A0A1B2ZC85

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	C	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	E	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	F	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0
3	E	1	Total O P 5 4 1	0	0
3	E	1	Total O P 5 4 1	0	0
3	F	1	Total O P 5 4 1	0	0
3	F	1	Total O P 5 4 1	0	0
3	F	1	Total O P 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total O P 5 4 1	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

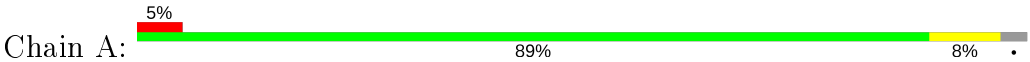
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	2	Total Zn 2 2	0	0
4	E	2	Total Zn 2 2	0	0
4	B	1	Total Zn 1 1	0	0
4	C	2	Total Zn 2 2	0	0
4	A	2	Total Zn 2 2	0	0
4	F	2	Total Zn 2 2	0	0

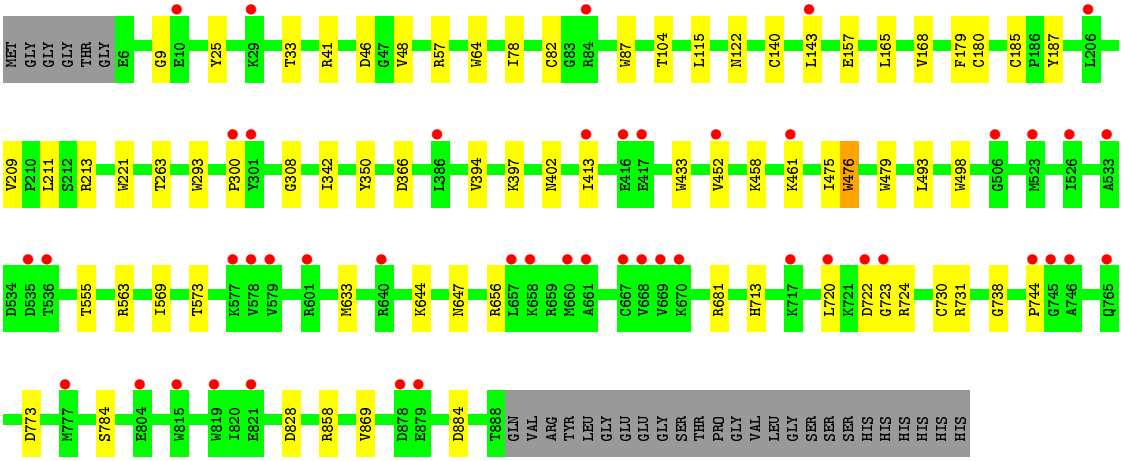
3 Residue-property plots (i)

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: NS5

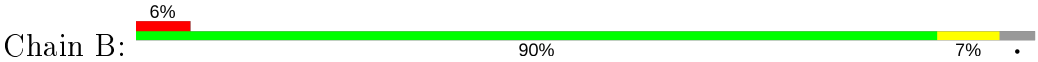
Chain A:

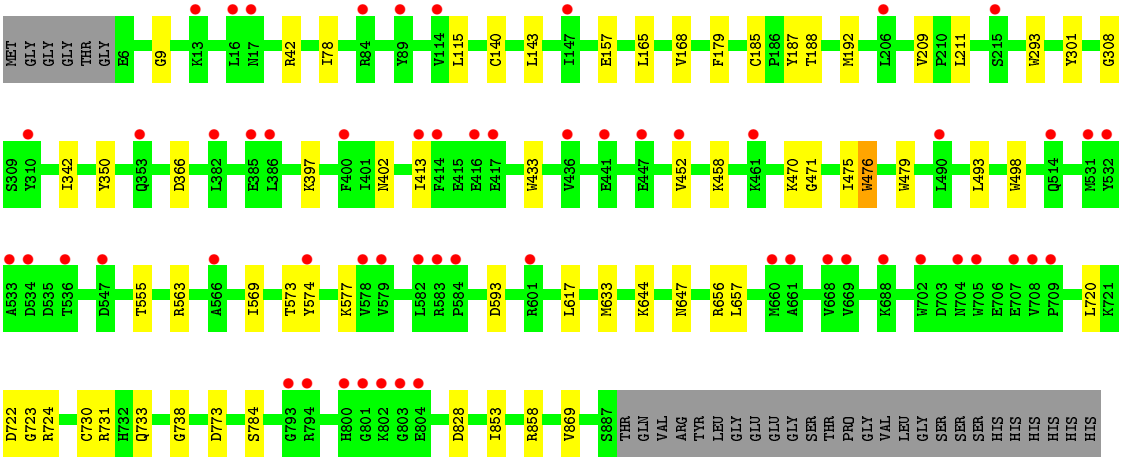




- Molecule 1: NS5

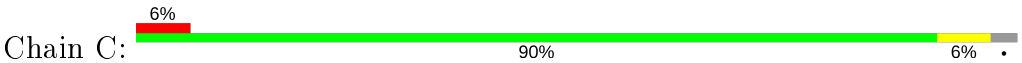
Chain B:

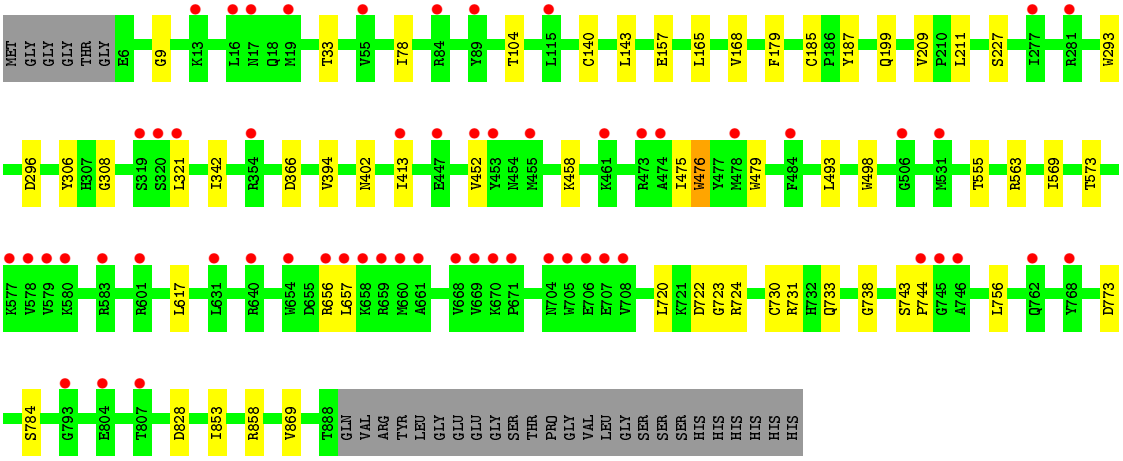




- Molecule 1: NS5

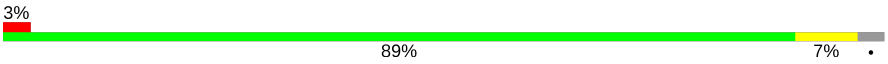
Chain C:

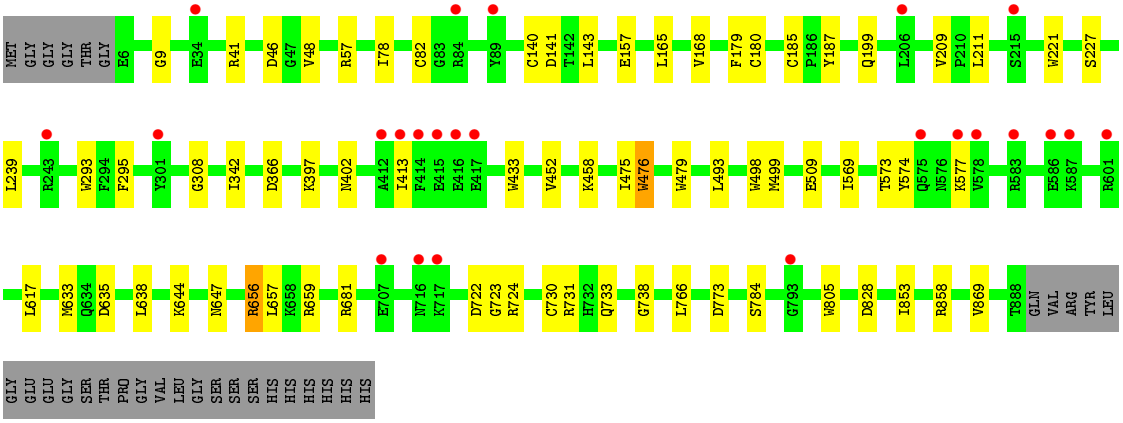




• Molecule 1: NS5

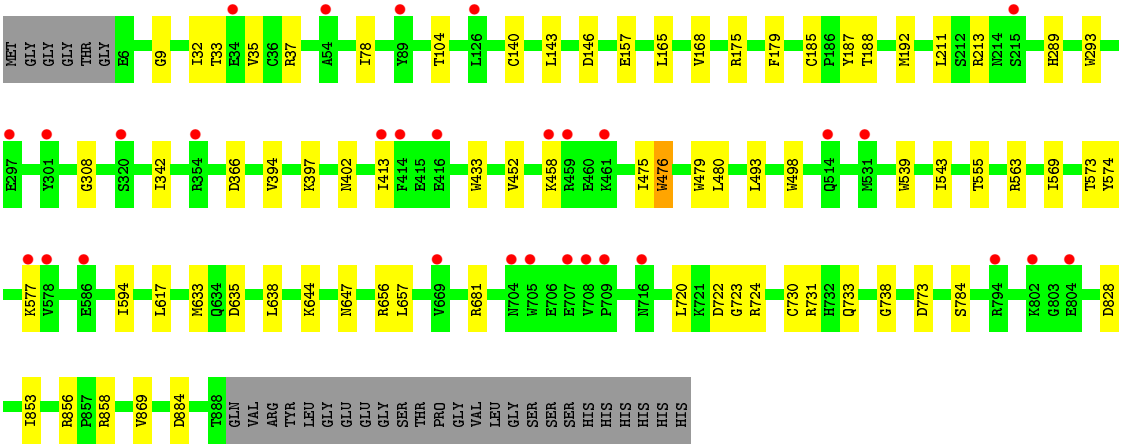
Chain D:





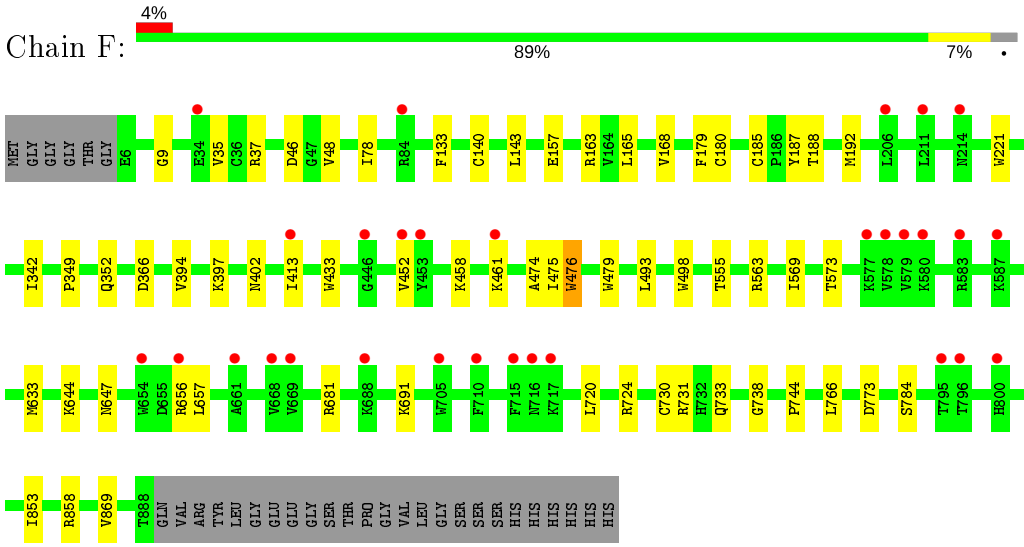
• Molecule 1: NS5

Chain E:



• Molecule 1: NS5

Chain F:


4%
89%
7%
MET GLY GLY GLY THR GLY E6 G9 E34 V35 C36 R37 D46 G47 V48 I78 R84 F133 C140 L143 E157 R163 V164 L165 V168 F179 C180 C185 P186 Y187 T188 M192 L206 L211 N214 W221 W293 Y301 G308
I342 P349 Q352 D366 V394 K397 N402 I413 W433 G446 V452 Y453 K458 K461 A474 I475 W476 W479 L493 W498 T555 R563 I569 T573 K577 V578 V579 K580 R583 K587 T590 D593 L617
M633 K644 N647 W654 D655 R656 L657 A661 V668 V669 R681 K688 K691 W705 F710 F715 N716 K717 L720 R724 C730 R731 H732 Q733 G738 P744 L766 D773 S784 T795 T796 H800 E804 W805 E827 D828
I853 R858 V869 T888 GLN VAL ARG TYR LEU GLY GLU GLU GLY SER THR PRO GLY VAL LEU GLY SER SER SER HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	191.06Å 192.06Å 407.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.52 – 4.99 49.52 – 4.99	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.52-4.99) 97.1 (49.52-4.99)	Depositor EDS
R_{merge}	0.75	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.67 (at 5.10Å)	Xtriage
Refinement program	PHENIX (1.11_2567: ???)	Depositor
R, R_{free}	0.227 , 0.276 0.227 , 0.276	Depositor DCC
R_{free} test set	3279 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	110.6	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 216.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.32$, $< L^2 > = 0.15$	Xtriage
Estimated twinning fraction	0.166 for k,h,-l	Xtriage
Reported twinning fraction	0.842 for H, K, L 0.158 for K, H, -L	Depositor
Outliers	0 of 65689 reflections	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	42817	wwPDB-VP
Average B, all atoms (Å^2)	160.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% 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: ZN, SAH, PO4

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	0.24	0/7262	0.44	0/9813
1	B	0.24	0/7255	0.44	0/9803
1	C	0.24	0/7262	0.43	0/9813
1	D	0.24	0/7262	0.44	0/9813
1	E	0.24	0/7262	0.44	0/9813
1	F	0.24	0/7262	0.44	0/9813
All	All	0.24	0/43565	0.44	0/58868

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	7097	0	6997	42	0
1	B	7090	0	6992	33	0
1	C	7097	0	6997	30	0
1	D	7097	0	6997	40	0
1	E	7097	0	6997	39	0
1	F	7097	0	6998	37	0
2	A	26	0	19	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	26	0	19	1	0
2	C	26	0	19	2	0
2	D	26	0	19	2	0
2	E	26	0	19	3	0
2	F	26	0	19	0	0
3	A	10	0	0	1	0
3	B	10	0	0	0	0
3	C	5	0	0	0	0
3	D	20	0	0	0	0
3	E	10	0	0	0	0
3	F	20	0	0	1	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
All	All	42817	0	42092	223	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 (223) 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:C:104:THR:HA	2:C:1001:SAH:H2	1.64	0.78
1:A:104:THR:HA	2:A:1001:SAH:H2	1.67	0.77
1:D:141:ASP:OD1	1:E:175:ARG:NH2	2.23	0.69
1:D:569:ILE:O	1:D:573:THR:HB	1.94	0.68
1:A:165:LEU:HA	1:A:168:VAL:HG22	1.78	0.65
1:F:569:ILE:O	1:F:573:THR:HB	1.97	0.64
1:A:569:ILE:O	1:A:573:THR:HB	1.96	0.64
1:C:165:LEU:HA	1:C:168:VAL:HG22	1.80	0.63
1:F:165:LEU:HA	1:F:168:VAL:HG22	1.80	0.62
1:D:165:LEU:HA	1:D:168:VAL:HG22	1.80	0.61
1:E:165:LEU:HA	1:E:168:VAL:HG22	1.81	0.61
1:B:733:GLN:NE2	1:B:773:ASP:HB2	2.15	0.61
1:F:733:GLN:NE2	1:F:773:ASP:HB2	2.16	0.61
1:B:165:LEU:HA	1:B:168:VAL:HG22	1.82	0.60
1:A:784:SER:HB3	1:A:869:VAL:HG13	1.83	0.60
1:E:569:ILE:O	1:E:573:THR:HB	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:THR:HG21	1:A:300:PRO:HG3	1.84	0.59
1:B:569:ILE:O	1:B:573:THR:HB	2.01	0.59
1:F:784:SER:HB3	1:F:869:VAL:HG13	1.85	0.58
1:C:569:ILE:O	1:C:573:THR:HB	2.03	0.57
1:E:784:SER:HB3	1:E:869:VAL:HG13	1.87	0.57
1:C:733:GLN:NE2	1:C:773:ASP:HB2	2.19	0.57
1:C:784:SER:HB3	1:C:869:VAL:HG13	1.88	0.56
1:B:724:ARG:HD3	1:B:828:ASP:HB3	1.86	0.56
1:C:458:LYS:HD2	1:C:475:ILE:HD11	1.88	0.56
1:B:784:SER:HB3	1:B:869:VAL:HG13	1.88	0.55
1:A:25:TYR:OH	1:B:42:ARG:NH2	2.40	0.55
1:F:458:LYS:HD2	1:F:475:ILE:HD11	1.89	0.55
1:D:458:LYS:HD2	1:D:475:ILE:HD11	1.89	0.55
1:D:784:SER:HB3	1:D:869:VAL:HG13	1.90	0.54
1:E:476:TRP:N	1:E:476:TRP:CD1	2.75	0.54
1:E:157:GLU:HB3	1:E:185:CYS:HB2	1.88	0.54
1:F:476:TRP:N	1:F:476:TRP:CD1	2.75	0.54
1:A:476:TRP:CD1	1:A:476:TRP:N	2.75	0.54
1:C:476:TRP:CD1	1:C:476:TRP:N	2.75	0.54
1:E:458:LYS:HD2	1:E:475:ILE:HD11	1.90	0.54
1:E:733:GLN:NE2	1:E:773:ASP:HB2	2.22	0.54
1:C:724:ARG:HD3	1:C:828:ASP:HB3	1.90	0.53
1:B:78:ILE:HD12	1:B:140:CYS:HB3	1.89	0.53
1:B:476:TRP:N	1:B:476:TRP:CD1	2.77	0.53
1:D:476:TRP:CD1	1:D:476:TRP:N	2.76	0.53
1:A:104:THR:HA	2:A:1001:SAH:C2	2.39	0.53
1:A:78:ILE:HD12	1:A:140:CYS:HB3	1.90	0.53
1:E:724:ARG:HD3	1:E:828:ASP:HB3	1.90	0.53
1:E:617:LEU:HD22	1:E:657:LEU:HD11	1.92	0.52
1:B:458:LYS:HD2	1:B:475:ILE:HD11	1.92	0.52
1:A:458:LYS:HD2	1:A:475:ILE:HD11	1.92	0.52
1:E:78:ILE:HD12	1:E:140:CYS:HB3	1.91	0.52
1:A:82:CYS:O	2:A:1001:SAH:HA	2.11	0.51
1:D:773:ASP:OD1	1:D:858:ARG:NE	2.29	0.50
1:F:720:LEU:HD12	1:F:724:ARG:HB2	1.92	0.50
1:D:569:ILE:O	1:D:573:THR:CB	2.58	0.50
1:F:78:ILE:HD12	1:F:140:CYS:HB3	1.93	0.50
1:D:293:TRP:CZ2	1:D:308:GLY:HA3	2.46	0.50
1:A:41:ARG:HH22	1:A:57:ARG:NH2	2.10	0.50
1:A:569:ILE:O	1:A:573:THR:CB	2.60	0.49
1:E:293:TRP:CH2	1:E:594:ILE:HD13	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:720:LEU:HD12	1:B:724:ARG:HB2	1.95	0.49
1:D:82:CYS:O	2:D:1001:SAH:N	2.45	0.49
1:B:493:LEU:HA	1:B:498:TRP:CD1	2.48	0.49
1:F:569:ILE:O	1:F:573:THR:CB	2.60	0.49
1:D:733:GLN:NE2	1:D:773:ASP:HB2	2.28	0.48
1:C:744:PRO:HD3	1:C:756:LEU:HD22	1.94	0.48
1:D:730:CYS:SG	1:D:731:ARG:N	2.87	0.48
1:E:104:THR:HA	2:E:1001:SAH:H2	1.94	0.48
1:A:493:LEU:HA	1:A:498:TRP:CD1	2.48	0.48
1:E:493:LEU:HA	1:E:498:TRP:CD1	2.48	0.48
1:C:209:VAL:HG12	1:C:211:LEU:H	1.79	0.48
1:D:78:ILE:HD12	1:D:140:CYS:HB3	1.94	0.48
1:C:293:TRP:CZ2	1:C:308:GLY:HA3	2.48	0.48
1:B:617:LEU:HD22	1:B:657:LEU:HD11	1.96	0.48
1:F:617:LEU:HD22	1:F:657:LEU:HD11	1.96	0.48
1:F:493:LEU:HA	1:F:498:TRP:CD1	2.48	0.48
1:C:321:LEU:HB2	1:C:743:SER:HB3	1.96	0.47
1:E:143:LEU:O	1:E:179:PHE:HA	2.14	0.47
1:D:41:ARG:HH22	1:D:57:ARG:NH2	2.11	0.47
1:A:724:ARG:HD3	1:A:828:ASP:HB3	1.96	0.47
1:C:9:GLY:HA3	1:C:187:TYR:HB2	1.96	0.47
1:E:32:ILE:HD13	1:E:213:ARG:HA	1.96	0.47
1:A:720:LEU:HD12	1:A:724:ARG:HB2	1.97	0.47
1:E:730:CYS:SG	1:E:731:ARG:N	2.88	0.47
1:F:724:ARG:HD3	1:F:828:ASP:HB3	1.96	0.47
1:F:633:MET:HE2	1:F:633:MET:HB3	1.72	0.47
1:E:413:ILE:HD13	1:E:452:VAL:HB	1.95	0.46
1:F:293:TRP:CZ2	1:F:308:GLY:HA3	2.50	0.46
1:F:644:LYS:HA	1:F:647:ASN:HB2	1.96	0.46
1:C:78:ILE:HD12	1:C:140:CYS:HB3	1.97	0.46
1:A:46:ASP:HB2	1:A:48:VAL:HG23	1.97	0.46
1:B:633:MET:HB3	1:B:633:MET:HE2	1.69	0.46
1:D:493:LEU:HA	1:D:498:TRP:CD1	2.49	0.46
1:E:644:LYS:HA	1:E:647:ASN:HB2	1.96	0.46
1:F:143:LEU:O	1:F:179:PHE:HA	2.15	0.46
1:C:143:LEU:O	1:C:179:PHE:HA	2.16	0.46
1:D:853:ILE:HA	1:D:858:ARG:HD3	1.98	0.46
1:A:122:ASN:HB2	1:A:300:PRO:HB3	1.98	0.46
1:E:33:THR:HB	1:E:211:LEU:HD23	1.97	0.46
1:A:9:GLY:HA3	1:A:187:TYR:HB2	1.98	0.45
1:A:644:LYS:HA	1:A:647:ASN:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:730:CYS:SG	1:A:731:ARG:N	2.89	0.45
1:B:730:CYS:SG	1:B:731:ARG:N	2.89	0.45
1:C:493:LEU:HA	1:C:498:TRP:CD1	2.51	0.45
1:D:342:ILE:HD12	1:D:738:GLY:HA3	1.98	0.45
1:C:617:LEU:HD22	1:C:657:LEU:HD11	1.99	0.45
1:C:773:ASP:OD1	1:C:858:ARG:NE	2.32	0.45
1:A:143:LEU:O	1:A:179:PHE:HA	2.17	0.45
1:B:342:ILE:HD12	1:B:738:GLY:HA3	1.98	0.45
1:F:730:CYS:SG	1:F:731:ARG:N	2.89	0.45
1:D:724:ARG:HD3	1:D:828:ASP:HB3	1.98	0.45
1:E:773:ASP:OD1	1:E:858:ARG:NE	2.28	0.45
1:A:773:ASP:OD1	1:A:858:ARG:NE	2.26	0.45
1:B:143:LEU:O	1:B:179:PHE:HA	2.16	0.45
1:C:342:ILE:HD12	1:C:738:GLY:HA3	1.98	0.45
1:D:633:MET:HE1	1:D:681:ARG:CZ	2.47	0.45
1:B:293:TRP:CZ2	1:B:308:GLY:HA3	2.52	0.45
1:D:397:LYS:HG3	1:D:433:TRP:CH2	2.52	0.45
1:E:853:ILE:HA	1:E:858:ARG:HD3	1.98	0.45
1:A:157:GLU:HB3	1:A:185:CYS:HB2	1.98	0.45
1:A:555:THR:O	1:A:563:ARG:HD3	2.17	0.45
1:D:413:ILE:HD13	1:D:452:VAL:HB	1.98	0.45
1:D:574:TYR:O	1:D:577:LYS:NZ	2.44	0.45
1:E:342:ILE:HD12	1:E:738:GLY:HA3	1.98	0.45
1:A:397:LYS:HE3	1:A:433:TRP:CE2	2.52	0.45
1:E:574:TYR:O	1:E:577:LYS:NZ	2.47	0.45
1:C:296:ASP:N	1:C:306:TYR:OH	2.49	0.44
1:C:853:ILE:HA	1:C:858:ARG:HD3	1.99	0.44
1:D:9:GLY:HA3	1:D:187:TYR:HB2	1.98	0.44
1:E:146:ASP:HB3	2:E:1001:SAH:HG1	1.98	0.44
1:A:64:TRP:CE3	1:A:209:VAL:HG13	2.51	0.44
1:A:397:LYS:HG3	1:A:433:TRP:CH2	2.52	0.44
1:A:87:TRP:CD1	2:A:1001:SAH:O	2.70	0.44
1:E:569:ILE:O	1:E:573:THR:CB	2.66	0.44
1:F:773:ASP:OD1	1:F:858:ARG:NE	2.25	0.44
1:B:413:ILE:HD13	1:B:452:VAL:HB	1.98	0.44
1:C:157:GLU:HB3	1:C:185:CYS:HB2	1.98	0.44
1:F:352:GLN:HE22	1:F:474:ALA:HA	1.83	0.44
1:F:691:LYS:NZ	3:F:1003:PO4:O3	2.50	0.44
1:A:713:HIS:NE2	1:A:731:ARG:HD2	2.33	0.43
1:F:461:LYS:HE3	1:F:744:PRO:HG3	1.99	0.43
1:F:853:ILE:HA	1:F:858:ARG:HD3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:MET:HB3	1:A:633:MET:HE2	1.69	0.43
1:B:397:LYS:HE3	1:B:433:TRP:CE2	2.53	0.43
1:F:342:ILE:HD12	1:F:738:GLY:HA3	2.00	0.43
1:B:397:LYS:HG3	1:B:433:TRP:CH2	2.54	0.43
1:C:722:ASP:OD1	1:C:723:GLY:N	2.52	0.43
1:E:633:MET:HE1	1:E:681:ARG:CZ	2.48	0.43
1:B:209:VAL:HG12	1:B:211:LEU:H	1.83	0.43
1:C:555:THR:O	1:C:563:ARG:HD3	2.18	0.43
1:D:293:TRP:HE1	1:D:295:PHE:HE1	1.66	0.43
1:D:656:ARG:HA	1:D:659:ARG:HD2	2.01	0.43
1:E:722:ASP:OD1	1:E:723:GLY:N	2.52	0.43
1:F:349:PRO:HG2	1:F:590:THR:HG21	2.00	0.43
1:F:46:ASP:HB2	1:F:48:VAL:HG23	2.01	0.43
1:B:722:ASP:OD1	1:B:723:GLY:N	2.52	0.43
1:B:853:ILE:HA	1:B:858:ARG:HD3	2.00	0.43
1:B:555:THR:O	1:B:563:ARG:HD3	2.19	0.43
1:D:617:LEU:HD22	1:D:657:LEU:HD11	2.01	0.43
1:F:633:MET:HE1	1:F:681:ARG:CZ	2.49	0.43
1:E:289:HIS:O	1:E:293:TRP:HB2	2.19	0.43
1:A:115:LEU:HB3	1:A:350:TYR:OH	2.19	0.42
1:A:722:ASP:OD1	1:A:723:GLY:N	2.51	0.42
1:B:9:GLY:HA3	1:B:187:TYR:HB2	2.01	0.42
1:F:157:GLU:HB3	1:F:185:CYS:HB2	1.99	0.42
1:B:157:GLU:HB3	1:B:185:CYS:HB2	1.99	0.42
1:C:413:ILE:HD13	1:C:452:VAL:HB	2.00	0.42
1:C:569:ILE:O	1:C:573:THR:CB	2.67	0.42
1:A:213:ARG:NH2	3:A:1003:PO4:O1	2.53	0.42
1:D:143:LEU:O	1:D:179:PHE:HA	2.19	0.42
1:E:555:THR:O	1:E:563:ARG:HD3	2.18	0.42
1:E:9:GLY:HA3	1:E:187:TYR:HB2	2.02	0.42
1:F:180:CYS:HA	1:F:221:TRP:O	2.19	0.42
1:B:115:LEU:HB3	1:B:350:TYR:OH	2.19	0.42
1:C:720:LEU:HD12	1:C:724:ARG:HB2	2.01	0.42
1:F:9:GLY:HA3	1:F:187:TYR:HB2	2.02	0.42
1:A:633:MET:HE1	1:A:681:ARG:CZ	2.49	0.42
1:B:569:ILE:O	1:B:573:THR:CB	2.65	0.42
1:A:342:ILE:HD12	1:A:738:GLY:HA3	2.01	0.42
2:B:1001:SAH:H4'	2:B:1001:SAH:HG2	1.96	0.42
1:B:188:THR:O	1:B:192:MET:HG2	2.19	0.42
1:D:157:GLU:HB3	1:D:185:CYS:HB2	2.00	0.42
1:E:397:LYS:HE3	1:E:433:TRP:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1001:SAH:H2'	2:E:1001:SAH:H8	1.88	0.42
1:E:539:TRP:NE1	1:E:543:ILE:HD11	2.34	0.42
1:C:199:GLN:NE2	1:C:227:SER:O	2.52	0.42
1:C:730:CYS:SG	1:C:731:ARG:N	2.93	0.42
1:A:122:ASN:CB	1:A:300:PRO:HB3	2.49	0.42
2:C:1001:SAH:H8	2:C:1001:SAH:H2'	1.76	0.42
1:E:293:TRP:CZ2	1:E:308:GLY:HA3	2.55	0.42
1:C:33:THR:HB	1:C:211:LEU:HD23	2.01	0.42
1:D:644:LYS:HA	1:D:647:ASN:HB2	2.01	0.42
1:F:413:ILE:HD13	1:F:452:VAL:HB	2.01	0.41
1:B:644:LYS:HA	1:B:647:ASN:HB2	2.01	0.41
1:D:199:GLN:NE2	1:D:227:SER:O	2.54	0.41
1:D:633:MET:HE2	1:D:633:MET:HB3	1.72	0.41
1:F:397:LYS:HE3	1:F:433:TRP:CE2	2.55	0.41
1:A:413:ILE:HD13	1:A:452:VAL:HB	2.03	0.41
1:D:766:LEU:HD23	1:D:805:TRP:HE3	1.84	0.41
1:E:35:VAL:HG23	1:E:37:ARG:HG2	2.01	0.41
1:A:33:THR:HB	1:A:211:LEU:HD23	2.02	0.41
1:F:188:THR:O	1:F:192:MET:HG2	2.20	0.41
1:D:499:MET:HB2	1:D:509:GLU:HB2	2.02	0.41
1:F:35:VAL:HG23	1:F:37:ARG:HG2	2.03	0.41
2:D:1001:SAH:HG2	2:D:1001:SAH:H4'	1.88	0.41
1:E:720:LEU:HD12	1:E:724:ARG:HB2	2.02	0.41
1:A:180:CYS:HA	1:A:221:TRP:O	2.21	0.41
1:F:133:PHE:CE1	1:F:163:ARG:HG2	2.55	0.41
1:F:397:LYS:HG3	1:F:433:TRP:CH2	2.56	0.41
1:D:239:LEU:HA	1:D:239:LEU:HD12	1.89	0.41
1:D:635:ASP:HA	1:D:638:LEU:O	2.21	0.41
1:E:635:ASP:HA	1:E:638:LEU:O	2.21	0.41
1:D:46:ASP:HB2	1:D:48:VAL:HG23	2.02	0.41
1:D:209:VAL:HG12	1:D:211:LEU:H	1.86	0.41
1:D:180:CYS:HA	1:D:221:TRP:O	2.20	0.41
1:E:480:LEU:HA	1:E:480:LEU:HD12	1.92	0.40
1:D:722:ASP:OD1	1:D:723:GLY:N	2.54	0.40
1:E:188:THR:O	1:E:192:MET:HG2	2.21	0.40
1:F:555:THR:O	1:F:563:ARG:HD3	2.21	0.40
1:A:293:TRP:CZ2	1:A:308:GLY:HA3	2.56	0.40
1:D:397:LYS:HE3	1:D:433:TRP:CE2	2.57	0.40
1:F:766:LEU:HD23	1:F:805:TRP:HE3	1.84	0.40
1:A:461:LYS:HE3	1:A:744:PRO:HG3	2.03	0.40
1:B:301:TYR:OH	1:B:593:ASP:OD2	2.27	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:470:LYS:HG2	1:B:471:GLY:N	2.37	0.40
1:B:574:TYR:O	1:B:577:LYS:NZ	2.52	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	881/914 (96%)	819 (93%)	62 (7%)	0	100	100
1	B	880/914 (96%)	822 (93%)	58 (7%)	0	100	100
1	C	881/914 (96%)	821 (93%)	60 (7%)	0	100	100
1	D	881/914 (96%)	817 (93%)	64 (7%)	0	100	100
1	E	881/914 (96%)	820 (93%)	61 (7%)	0	100	100
1	F	881/914 (96%)	819 (93%)	62 (7%)	0	100	100
All	All	5285/5484 (96%)	4918 (93%)	367 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	756/779 (97%)	749 (99%)	7 (1%)	78	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	755/779 (97%)	750 (99%)	5 (1%)	84 90
1	C	756/779 (97%)	750 (99%)	6 (1%)	81 89
1	D	756/779 (97%)	751 (99%)	5 (1%)	84 90
1	E	756/779 (97%)	748 (99%)	8 (1%)	73 85
1	F	756/779 (97%)	750 (99%)	6 (1%)	81 89
All	All	4535/4674 (97%)	4498 (99%)	37 (1%)	81 89

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	366	ASP
1	A	394	VAL
1	A	402	ASN
1	A	476	TRP
1	A	479	TRP
1	A	656	ARG
1	A	884	ASP
1	B	366	ASP
1	B	402	ASN
1	B	476	TRP
1	B	479	TRP
1	B	656	ARG
1	C	366	ASP
1	C	394	VAL
1	C	402	ASN
1	C	476	TRP
1	C	479	TRP
1	C	656	ARG
1	D	366	ASP
1	D	402	ASN
1	D	476	TRP
1	D	479	TRP
1	D	656	ARG
1	E	366	ASP
1	E	394	VAL
1	E	402	ASN
1	E	476	TRP
1	E	479	TRP
1	E	656	ARG
1	E	856	ARG

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Mol	Chain	Res	Type
1	E	884	ASP
1	F	366	ASP
1	F	394	VAL
1	F	402	ASN
1	F	476	TRP
1	F	479	TRP
1	F	656	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	238	GLN
1	F	765	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 32 ligands modelled in this entry, 11 are monoatomic - leaving 21 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	$\#\|Z\|>2$
2	SAH	A	1001	-	21,28,28	1.05	1 (4%)	20,40,40	1.65	4 (20%)
3	PO4	F	1004	-	4,4,4	0.91	0	6,6,6	0.46	0
2	SAH	C	1001	-	21,28,28	1.05	1 (4%)	20,40,40	1.66	4 (20%)
2	SAH	D	1001	-	21,28,28	1.05	1 (4%)	20,40,40	1.66	4 (20%)
3	PO4	E	1003	-	4,4,4	0.90	0	6,6,6	0.43	0
3	PO4	B	1002	-	4,4,4	0.91	0	6,6,6	0.46	0
3	PO4	A	1003	-	4,4,4	0.90	0	6,6,6	0.55	0
3	PO4	D	1005	-	4,4,4	0.91	0	6,6,6	0.44	0
2	SAH	B	1001	-	21,28,28	1.05	1 (4%)	20,40,40	1.66	4 (20%)
3	PO4	F	1005	-	4,4,4	0.91	0	6,6,6	0.46	0
3	PO4	D	1002	-	4,4,4	0.92	0	6,6,6	0.43	0
3	PO4	E	1002	-	4,4,4	0.92	0	6,6,6	0.42	0
3	PO4	C	1002	-	4,4,4	0.92	0	6,6,6	0.43	0
3	PO4	F	1002	-	4,4,4	0.92	0	6,6,6	0.46	0
2	SAH	F	1001	-	21,28,28	1.05	1 (4%)	20,40,40	1.66	4 (20%)
3	PO4	F	1003	-	4,4,4	0.92	0	6,6,6	0.39	0
3	PO4	D	1004	-	4,4,4	0.90	0	6,6,6	0.48	0
3	PO4	D	1003	-	4,4,4	0.92	0	6,6,6	0.42	0
3	PO4	B	1003	-	4,4,4	0.91	0	6,6,6	0.45	0
2	SAH	E	1001	-	21,28,28	1.05	1 (4%)	20,40,40	1.66	4 (20%)
3	PO4	A	1002	-	4,4,4	0.91	0	6,6,6	0.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SAH	A	1001	-	-	4/7/31/31	0/3/3/3
2	SAH	D	1001	-	-	4/7/31/31	0/3/3/3
2	SAH	F	1001	-	-	4/7/31/31	0/3/3/3
2	SAH	B	1001	-	-	3/7/31/31	0/3/3/3
2	SAH	C	1001	-	-	2/7/31/31	0/3/3/3
2	SAH	E	1001	-	-	6/7/31/31	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1001	SAH	C5-C4	2.51	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1001	SAH	C5-C4	2.50	1.47	1.40
2	E	1001	SAH	C5-C4	2.50	1.47	1.40
2	A	1001	SAH	C5-C4	2.50	1.47	1.40
2	B	1001	SAH	C5-C4	2.50	1.47	1.40
2	D	1001	SAH	C5-C4	2.49	1.47	1.40

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1001	SAH	C3'-C2'-C1'	3.41	106.12	100.98
2	B	1001	SAH	C3'-C2'-C1'	3.40	106.09	100.98
2	F	1001	SAH	C3'-C2'-C1'	3.39	106.09	100.98
2	A	1001	SAH	C3'-C2'-C1'	3.39	106.08	100.98
2	C	1001	SAH	C3'-C2'-C1'	3.38	106.07	100.98
2	E	1001	SAH	C3'-C2'-C1'	3.38	106.06	100.98
2	F	1001	SAH	N3-C2-N1	-3.20	123.67	128.68
2	A	1001	SAH	N3-C2-N1	-3.19	123.70	128.68
2	C	1001	SAH	N3-C2-N1	-3.19	123.70	128.68
2	B	1001	SAH	N3-C2-N1	-3.17	123.72	128.68
2	D	1001	SAH	N3-C2-N1	-3.16	123.74	128.68
2	E	1001	SAH	N3-C2-N1	-3.16	123.74	128.68
2	C	1001	SAH	C4-C5-N7	-2.73	106.55	109.40
2	D	1001	SAH	C4-C5-N7	-2.72	106.56	109.40
2	F	1001	SAH	C4-C5-N7	-2.72	106.57	109.40
2	E	1001	SAH	C4-C5-N7	-2.71	106.57	109.40
2	B	1001	SAH	C4-C5-N7	-2.71	106.57	109.40
2	A	1001	SAH	C4-C5-N7	-2.69	106.59	109.40
2	B	1001	SAH	C5'-SD-CG	2.41	109.49	102.27
2	D	1001	SAH	C5'-SD-CG	2.41	109.48	102.27
2	E	1001	SAH	C5'-SD-CG	2.41	109.48	102.27
2	A	1001	SAH	C5'-SD-CG	2.40	109.48	102.27
2	F	1001	SAH	C5'-SD-CG	2.40	109.45	102.27
2	C	1001	SAH	C5'-SD-CG	2.39	109.43	102.27

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1001	SAH	C-CA-CB-CG
2	E	1001	SAH	O4'-C4'-C5'-SD
2	E	1001	SAH	C3'-C4'-C5'-SD
2	D	1001	SAH	O4'-C4'-C5'-SD

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Mol	Chain	Res	Type	Atoms
2	D	1001	SAH	C3'-C4'-C5'-SD
2	B	1001	SAH	O4'-C4'-C5'-SD
2	B	1001	SAH	C3'-C4'-C5'-SD
2	A	1001	SAH	C-CA-CB-CG
2	C	1001	SAH	C-CA-CB-CG
2	F	1001	SAH	C-CA-CB-CG
2	F	1001	SAH	O4'-C4'-C5'-SD
2	F	1001	SAH	C3'-C4'-C5'-SD
2	E	1001	SAH	CA-CB-CG-SD
2	A	1001	SAH	CA-CB-CG-SD
2	E	1001	SAH	N-CA-CB-CG
2	C	1001	SAH	N-CA-CB-CG
2	A	1001	SAH	CB-CG-SD-C5'
2	F	1001	SAH	CB-CG-SD-C5'
2	E	1001	SAH	CB-CG-SD-C5'
2	D	1001	SAH	C4'-C5'-SD-CG
2	B	1001	SAH	C4'-C5'-SD-CG
2	D	1001	SAH	N-CA-CB-CG
2	A	1001	SAH	N-CA-CB-CG

There are no ring outliers.

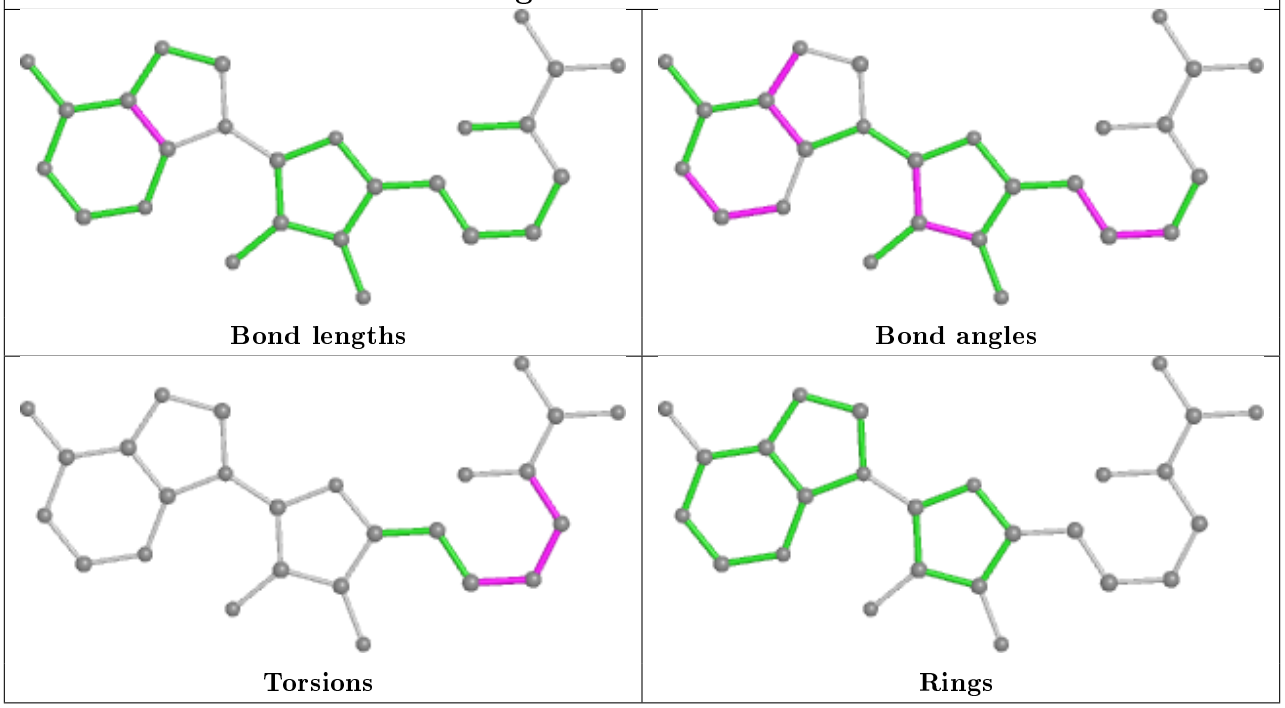
7 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	SAH	4	0
2	C	1001	SAH	2	0
2	D	1001	SAH	2	0
3	A	1003	PO4	1	0
2	B	1001	SAH	1	0
3	F	1003	PO4	1	0
2	E	1001	SAH	3	0

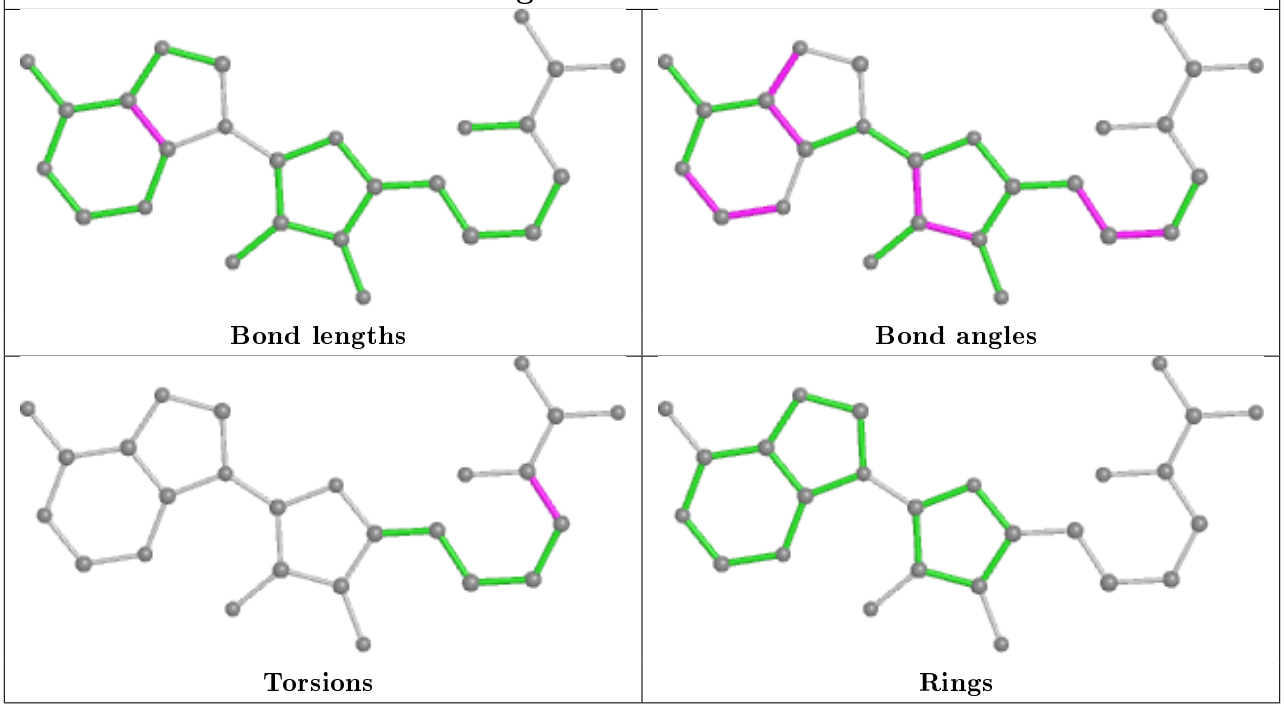
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

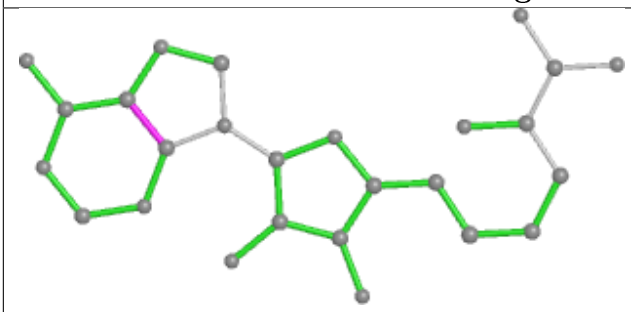
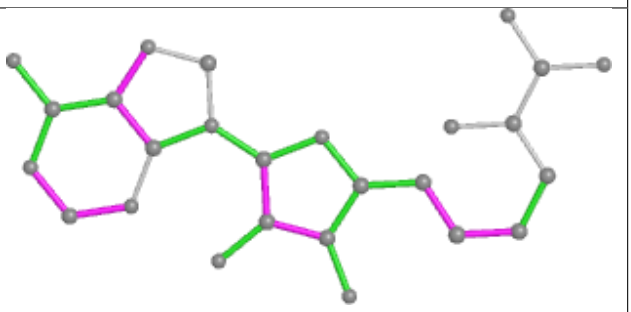
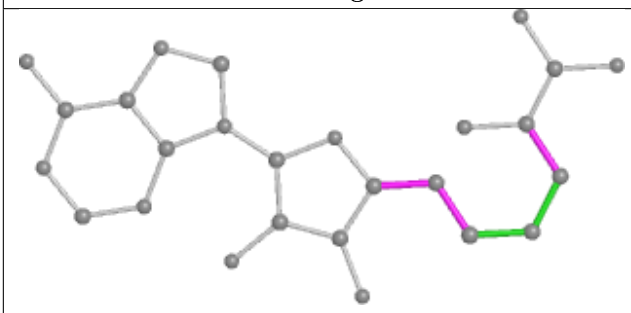
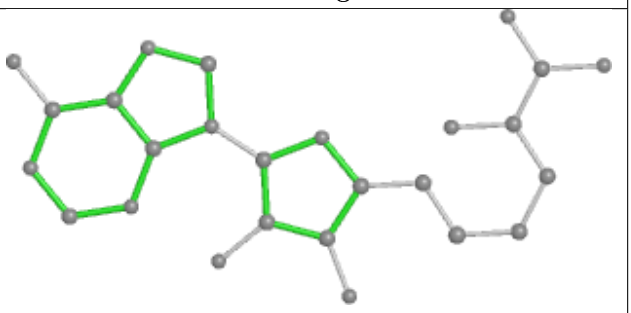
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

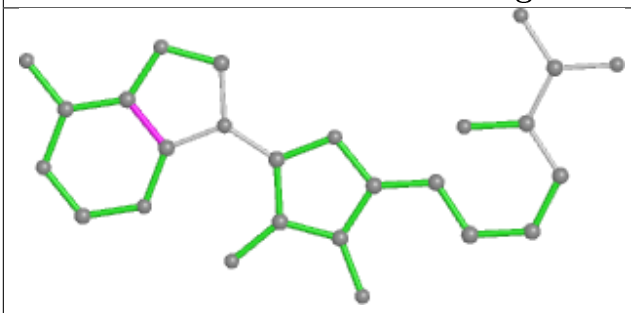
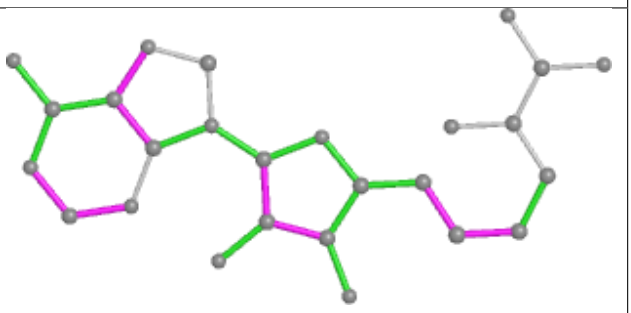
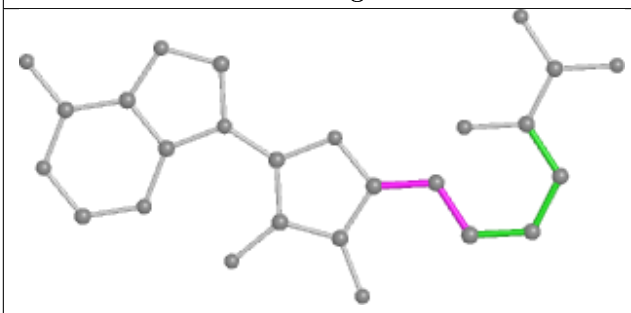
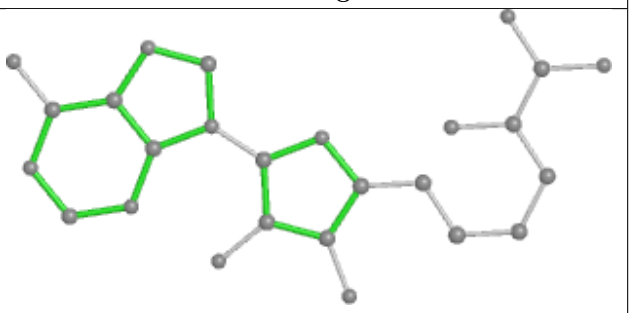
Ligand SAH A 1001



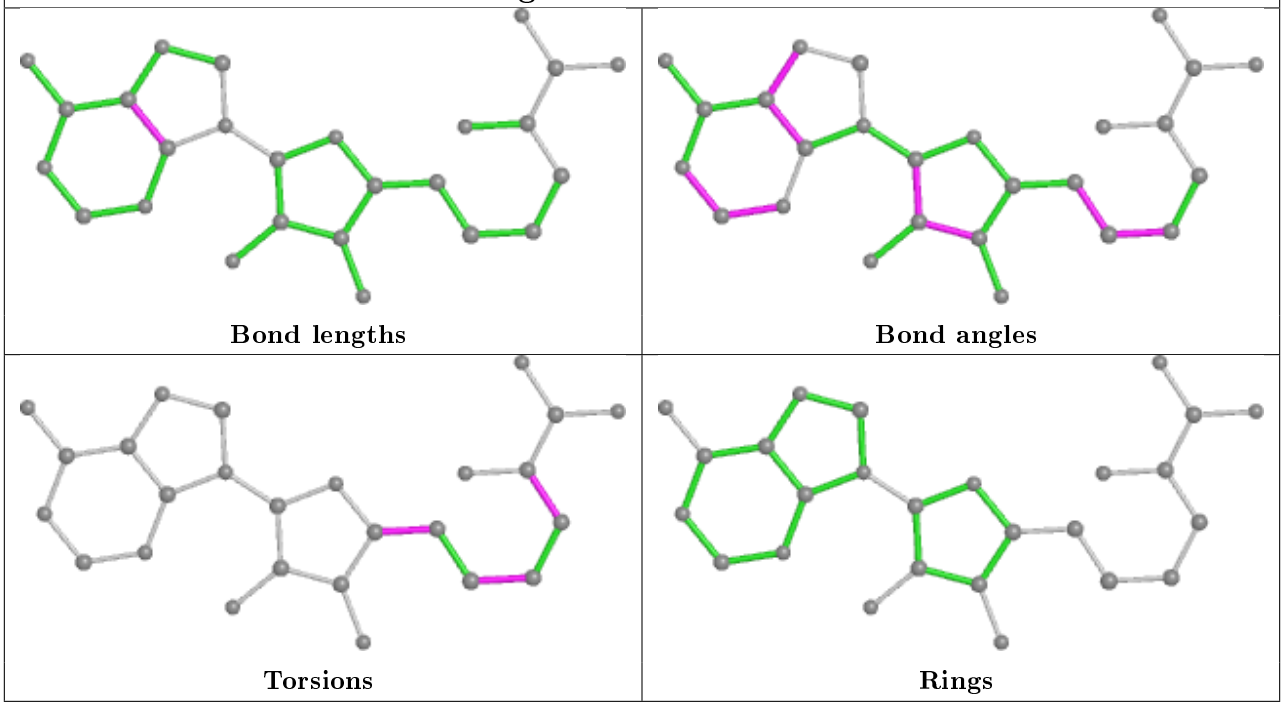
Ligand SAH C 1001



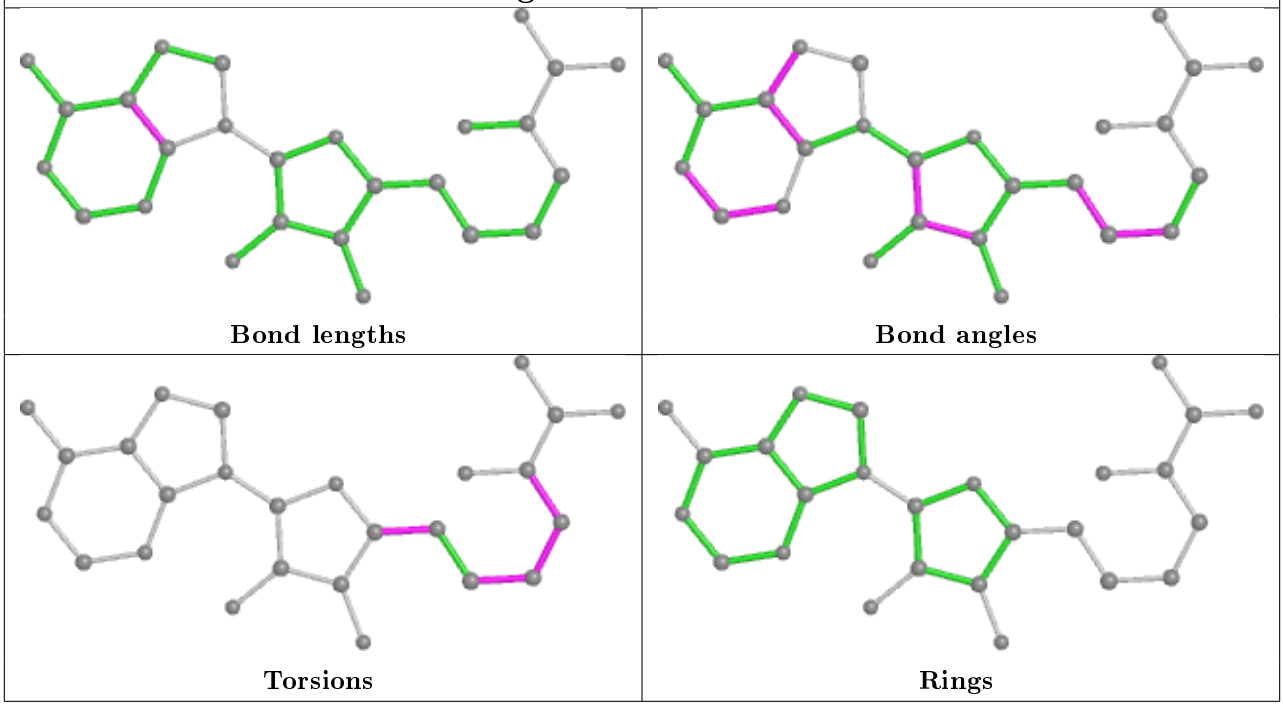
Ligand SAH D 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SAH B 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SAH F 1001



Ligand SAH E 1001



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	883/914 (96%)	0.45	47 (5%)	26	23	69, 163, 243, 327	0
1	B	882/914 (96%)	0.51	58 (6%)	18	15	73, 172, 263, 355	0
1	C	883/914 (96%)	0.50	58 (6%)	18	15	73, 159, 231, 295	0
1	D	883/914 (96%)	0.37	24 (2%)	54	45	73, 135, 197, 306	0
1	E	883/914 (96%)	0.37	30 (3%)	45	37	71, 142, 212, 266	0
1	F	883/914 (96%)	0.39	34 (3%)	39	32	71, 152, 215, 274	0
All	All	5297/5484 (96%)	0.43	251 (4%)	31	27	69, 154, 236, 355	0

All (251) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	416	GLU	5.2
1	A	578	VAL	5.0
1	C	669	VAL	4.7
1	A	660	MET	4.5
1	D	415	GLU	4.4
1	B	804	GLU	4.3
1	C	578	VAL	4.2
1	F	578	VAL	4.1
1	C	577	LYS	4.1
1	A	416	GLU	4.1
1	C	804	GLU	4.1
1	B	17	ASN	4.0
1	C	659	ARG	4.0
1	C	660	MET	4.0
1	B	802	LYS	3.9
1	B	801	GLY	3.9
1	A	661	ALA	3.8
1	A	723	GLY	3.7
1	A	804	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	436	VAL	3.6
1	B	533	ALA	3.6
1	E	459	ARG	3.6
1	C	580	LYS	3.5
1	E	416	GLU	3.5
1	C	746	ALA	3.5
1	B	452	VAL	3.5
1	C	668	VAL	3.4
1	D	575	GLN	3.4
1	C	579	VAL	3.4
1	A	658	LYS	3.4
1	A	819	TRP	3.4
1	C	670	LYS	3.4
1	C	744	PRO	3.4
1	A	669	VAL	3.4
1	B	84	ARG	3.3
1	B	416	GLU	3.3
1	D	413	ILE	3.3
1	A	746	ALA	3.3
1	D	417	GLU	3.3
1	C	320	SER	3.2
1	C	705	TRP	3.2
1	C	658	LYS	3.2
1	A	577	LYS	3.2
1	B	793	GLY	3.1
1	E	704	ASN	3.1
1	B	578	VAL	3.1
1	A	668	VAL	3.1
1	F	795	THR	3.1
1	B	800	HIS	3.0
1	C	704	ASN	3.0
1	C	745	GLY	3.0
1	F	715	PHE	3.0
1	B	708	VAL	3.0
1	D	717	LYS	3.0
1	F	705	TRP	3.0
1	A	506	GLY	3.0
1	D	301	TYR	2.9
1	C	661	ALA	2.9
1	F	577	LYS	2.9
1	B	707	GLU	2.9
1	A	722	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	579	VAL	2.9
1	B	547	ASP	2.9
1	A	461	LYS	2.9
1	A	670	LYS	2.8
1	E	586	GLU	2.8
1	C	631	LEU	2.8
1	B	16	LEU	2.8
1	F	669	VAL	2.8
1	A	745	GLY	2.8
1	E	577	LYS	2.8
1	F	593	ASP	2.8
1	F	668	VAL	2.8
1	C	478	MET	2.8
1	F	461	LYS	2.8
1	B	669	VAL	2.8
1	E	804	GLU	2.8
1	E	708	VAL	2.8
1	A	579	VAL	2.8
1	B	660	MET	2.8
1	A	300	PRO	2.7
1	B	668	VAL	2.7
1	B	566	ALA	2.7
1	A	10	GLU	2.7
1	D	586	GLU	2.7
1	B	386	LEU	2.7
1	C	768	TYR	2.7
1	D	206	LEU	2.7
1	B	704	ASN	2.7
1	F	583	ARG	2.7
1	A	452	VAL	2.7
1	C	484	PHE	2.7
1	B	536	THR	2.7
1	C	281	ARG	2.7
1	A	536	THR	2.6
1	B	583	ARG	2.6
1	C	707	GLU	2.6
1	D	601	ARG	2.6
1	D	414	PHE	2.6
1	E	89	TYR	2.6
1	E	514	GLN	2.6
1	A	523	MET	2.6
1	D	578	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	413	ILE	2.6
1	C	531	MET	2.6
1	A	301	TYR	2.6
1	A	535	ASP	2.6
1	C	506	GLY	2.6
1	D	89	TYR	2.6
1	E	461	LYS	2.6
1	E	802	LYS	2.6
1	C	17	ASN	2.6
1	F	34	GLU	2.6
1	B	414	PHE	2.6
1	B	206	LEU	2.6
1	C	657	LEU	2.5
1	E	34	GLU	2.5
1	F	716	ASN	2.5
1	C	413	ILE	2.5
1	D	577	LYS	2.5
1	E	709	PRO	2.5
1	A	386	LEU	2.5
1	B	441	GLU	2.5
1	C	793	GLY	2.5
1	C	474	ALA	2.5
1	B	534	ASP	2.5
1	C	461	LYS	2.5
1	D	587	LYS	2.5
1	F	688	LYS	2.5
1	E	669	VAL	2.5
1	A	667	CYS	2.5
1	B	447	GLU	2.5
1	D	412	ALA	2.5
1	F	84	ARG	2.4
1	B	702	TRP	2.4
1	E	215	SER	2.4
1	C	583	ARG	2.4
1	A	777	MET	2.4
1	B	417	GLU	2.4
1	B	353	GLN	2.4
1	E	531	MET	2.4
1	C	453	TYR	2.4
1	C	84	ARG	2.4
1	B	89	TYR	2.4
1	C	601	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	661	ALA	2.4
1	B	514	GLN	2.4
1	E	320	SER	2.4
1	B	310	TYR	2.4
1	C	89	TYR	2.3
1	F	654	TRP	2.3
1	B	803	GLY	2.3
1	E	794	ARG	2.3
1	E	414	PHE	2.3
1	F	211	LEU	2.3
1	A	413	ILE	2.3
1	A	744	PRO	2.3
1	A	720	LEU	2.3
1	B	532	TYR	2.3
1	A	878	ASP	2.3
1	F	804	GLU	2.3
1	B	215	SER	2.3
1	D	84	ARG	2.3
1	D	34	GLU	2.3
1	B	461	LYS	2.3
1	C	708	VAL	2.3
1	A	815	TRP	2.3
1	F	717	LYS	2.3
1	F	214	ASN	2.3
1	A	821	GLU	2.3
1	E	413	ILE	2.3
1	E	354	ARG	2.3
1	D	707	GLU	2.3
1	B	400	PHE	2.3
1	D	583	ARG	2.3
1	C	671	PRO	2.3
1	B	147	ILE	2.2
1	A	765	GLN	2.2
1	E	54	ALA	2.2
1	A	879	GLU	2.2
1	F	413	ILE	2.2
1	F	446	GLY	2.2
1	C	807	THR	2.2
1	E	297	GLU	2.2
1	F	710	PHE	2.2
1	A	657	LEU	2.2
1	B	794	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	243	ARG	2.2
1	F	800	HIS	2.2
1	C	473	ARG	2.2
1	E	707	GLU	2.2
1	A	143	LEU	2.2
1	F	206	LEU	2.2
1	B	382	LEU	2.2
1	B	114	VAL	2.2
1	E	458	LYS	2.2
1	E	705	TRP	2.2
1	C	13	LYS	2.1
1	A	526	ILE	2.1
1	B	601	ARG	2.1
1	A	417	GLU	2.1
1	A	640	ARG	2.1
1	B	584	PRO	2.1
1	A	717	LYS	2.1
1	F	796	THR	2.1
1	A	601	ARG	2.1
1	B	661	ALA	2.1
1	B	579	VAL	2.1
1	E	578	VAL	2.1
1	C	447	GLU	2.1
1	C	115	LEU	2.1
1	C	706	GLU	2.1
1	D	793	GLY	2.1
1	B	582	LEU	2.1
1	F	656	ARG	2.1
1	C	277	ILE	2.1
1	F	827	GLU	2.1
1	C	16	LEU	2.1
1	C	656	ARG	2.1
1	C	654	TRP	2.1
1	D	215	SER	2.1
1	B	709	PRO	2.1
1	F	580	LYS	2.1
1	A	533	ALA	2.1
1	B	490	LEU	2.1
1	C	321	LEU	2.1
1	C	762	GLN	2.1
1	F	452	VAL	2.1
1	B	385	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	29	LYS	2.1
1	B	688	LYS	2.1
1	B	705	TRP	2.0
1	B	13	LYS	2.0
1	C	319	SER	2.0
1	F	587	LYS	2.0
1	E	126	LEU	2.0
1	A	84	ARG	2.0
1	C	640	ARG	2.0
1	A	206	LEU	2.0
1	B	531	MET	2.0
1	C	455	MET	2.0
1	F	301	TYR	2.0
1	F	453	TYR	2.0
1	C	55	VAL	2.0
1	E	716	ASN	2.0
1	B	574	TYR	2.0
1	C	354	ARG	2.0
1	C	19	MET	2.0
1	D	716	ASN	2.0
1	E	301	TYR	2.0
1	C	452	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{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
3	PO4	D	1002	5/5	0.29	0.40	216,236,274,277	0

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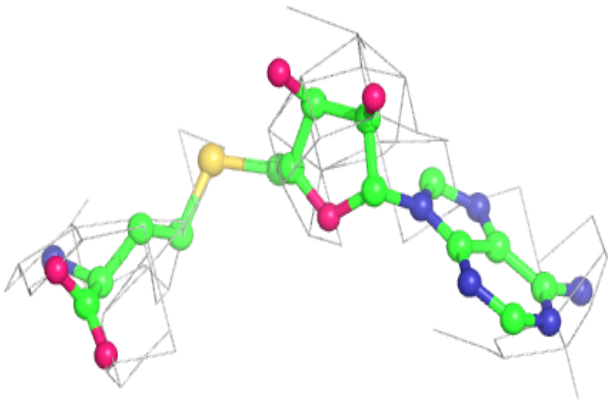
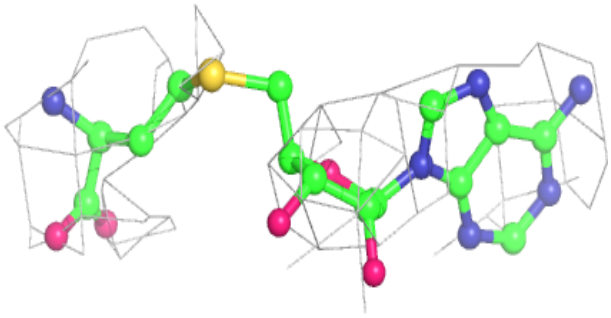
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PO4	E	1003	5/5	0.33	0.33	246,259,307,317	0
3	PO4	D	1004	5/5	0.34	0.33	206,229,255,258	0
3	PO4	C	1002	5/5	0.47	0.27	212,232,256,259	0
3	PO4	F	1004	5/5	0.56	0.29	189,200,254,283	0
3	PO4	F	1005	5/5	0.58	0.22	230,263,279,294	0
3	PO4	A	1003	5/5	0.63	0.19	221,228,263,270	0
3	PO4	D	1003	5/5	0.75	0.35	226,244,281,300	0
3	PO4	D	1005	5/5	0.76	0.32	184,191,205,218	0
3	PO4	F	1003	5/5	0.79	0.27	152,187,221,243	0
3	PO4	B	1002	5/5	0.79	0.17	190,205,223,231	0
3	PO4	A	1002	5/5	0.81	0.35	198,219,223,232	0
3	PO4	B	1003	5/5	0.81	0.32	242,270,298,299	0
2	SAH	F	1001	26/26	0.84	0.55	102,140,159,199	0
2	SAH	C	1001	26/26	0.84	0.60	106,137,166,188	0
3	PO4	F	1002	5/5	0.85	0.24	149,157,195,208	0
3	PO4	E	1002	5/5	0.87	0.29	167,192,199,201	0
2	SAH	B	1001	26/26	0.88	0.82	125,163,189,195	0
2	SAH	D	1001	26/26	0.89	0.59	99,154,179,197	0
2	SAH	A	1001	26/26	0.91	0.42	120,140,167,217	0
2	SAH	E	1001	26/26	0.92	0.57	103,133,172,202	0
4	ZN	A	1005	1/1	0.96	0.20	476,476,476,476	0
4	ZN	C	1003	1/1	0.96	0.19	161,161,161,161	0
4	ZN	F	1006	1/1	0.97	0.17	89,89,89,89	0
4	ZN	E	1004	1/1	0.98	0.17	188,188,188,188	0
4	ZN	B	1004	1/1	0.98	0.22	136,136,136,136	0
4	ZN	D	1006	1/1	0.98	0.18	135,135,135,135	0
4	ZN	E	1005	1/1	0.99	0.16	117,117,117,117	0
4	ZN	A	1004	1/1	0.99	0.18	139,139,139,139	0
4	ZN	D	1007	1/1	1.00	0.19	144,144,144,144	0
4	ZN	F	1007	1/1	1.00	0.18	173,173,173,173	0
4	ZN	C	1004	1/1	1.00	0.12	181,181,181,181	0

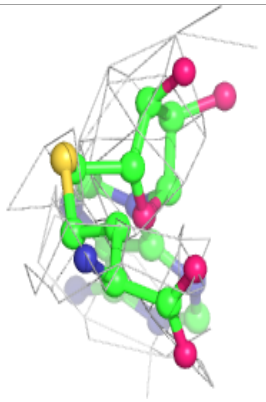
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SAH F 1001:

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

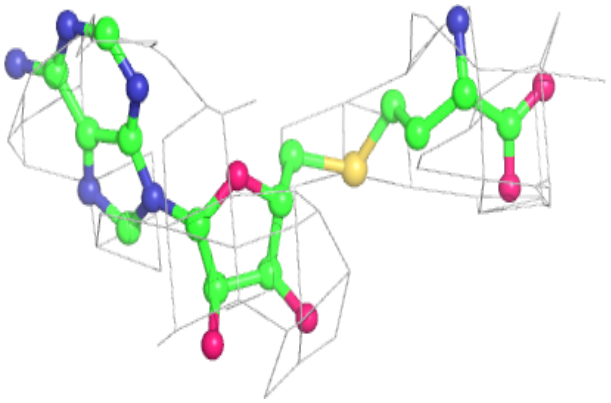


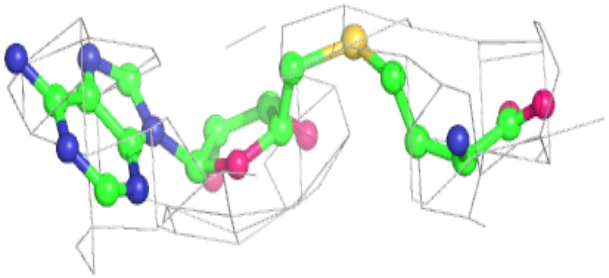


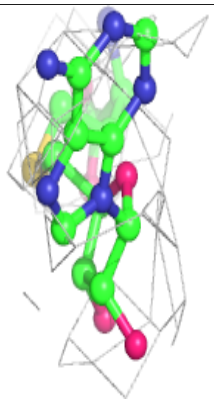


Electron density around SAH C 1001:

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

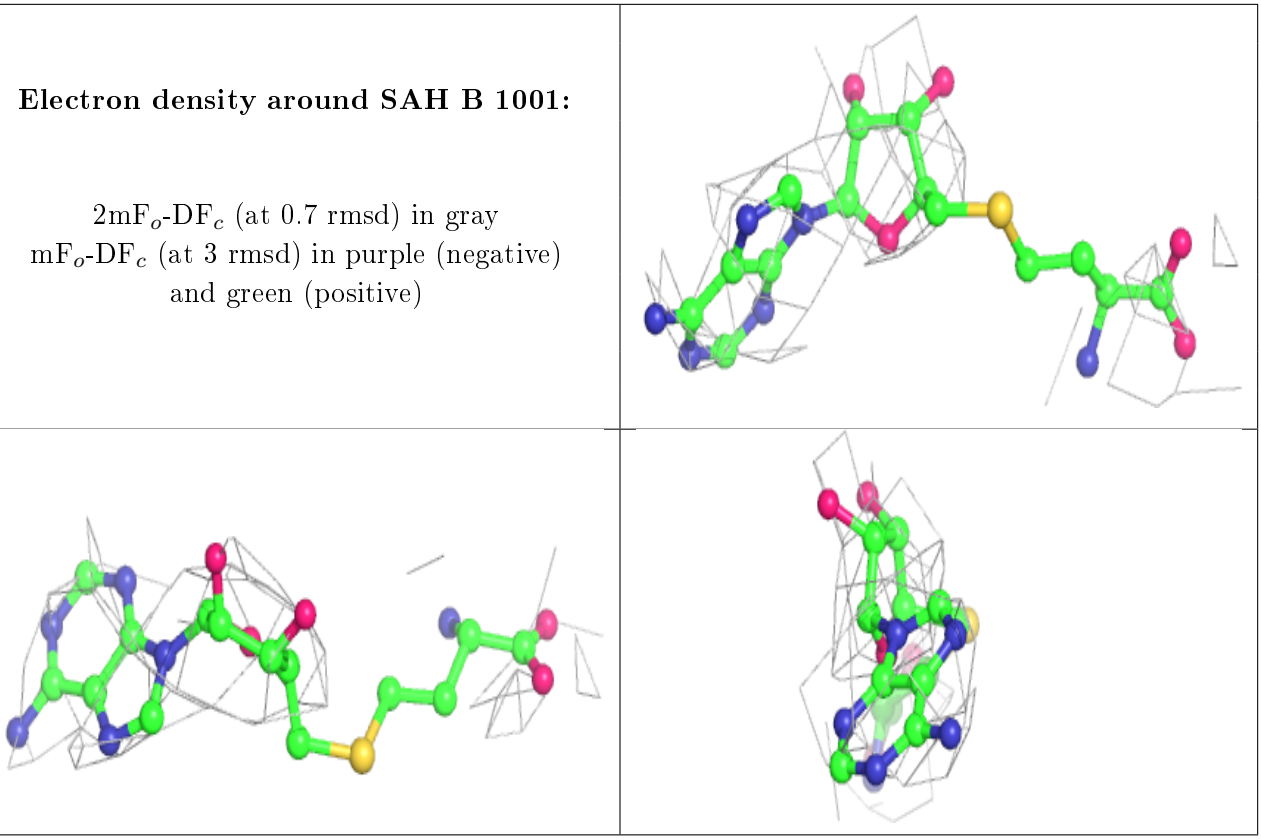






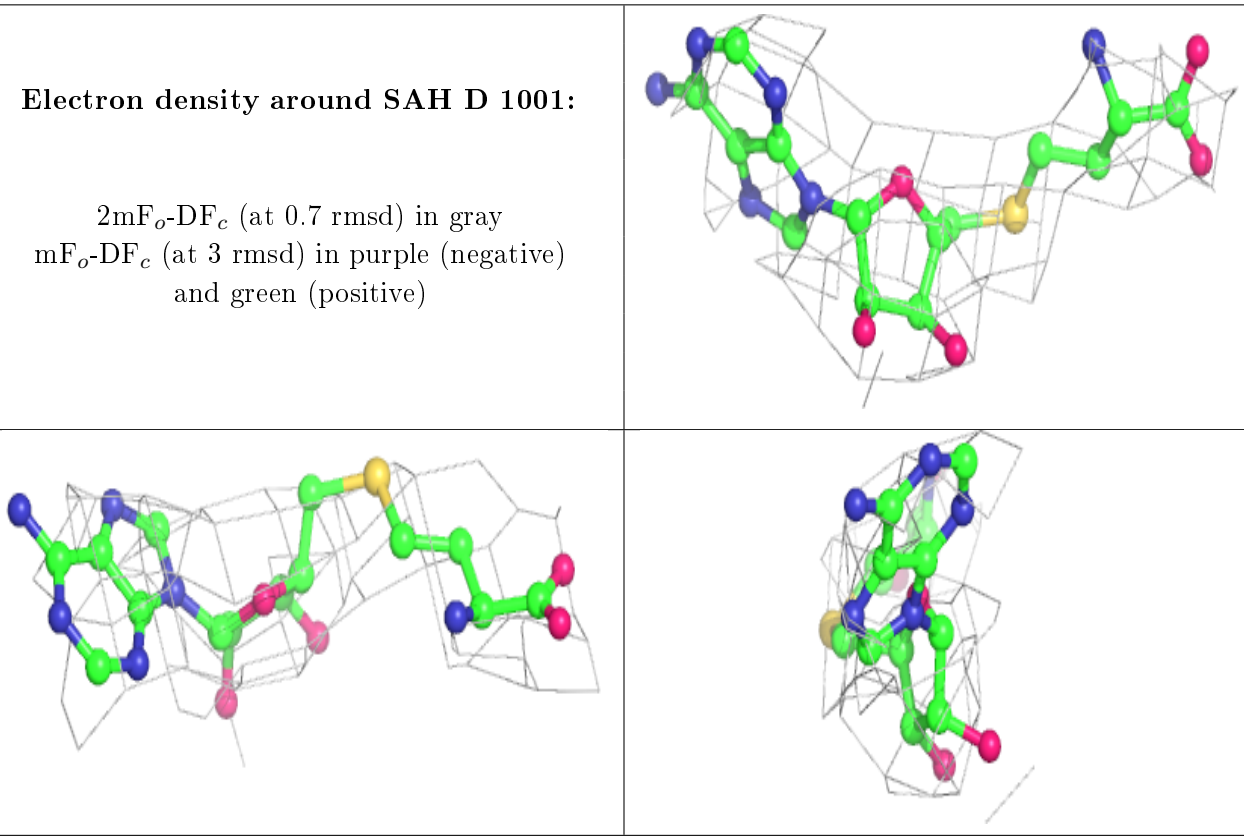
Electron density around SAH B 1001:

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



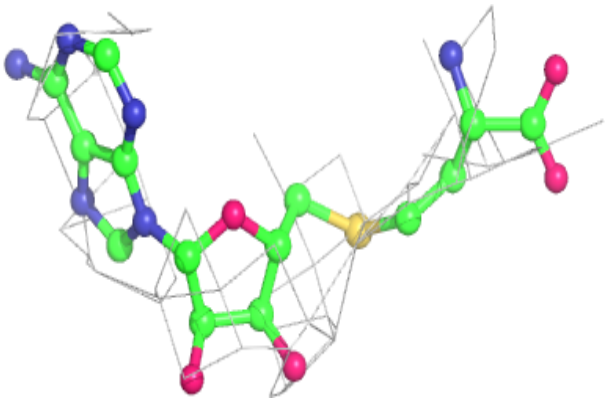
Electron density around SAH D 1001:

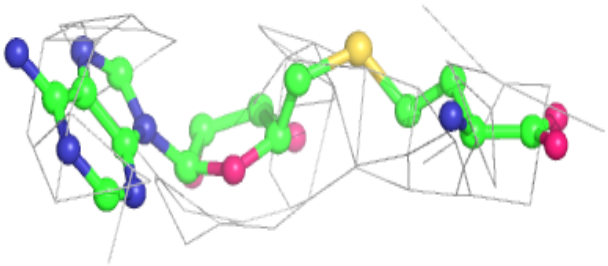
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

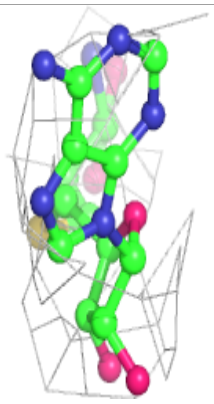


Electron density around SAH A 1001:

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

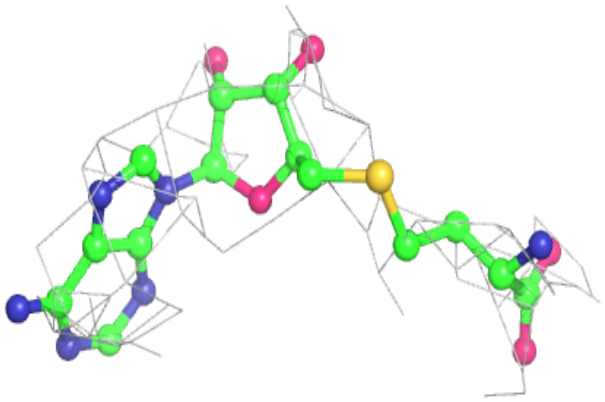


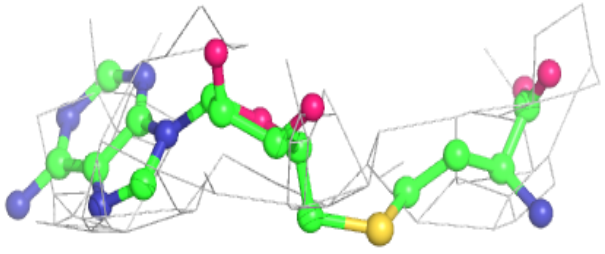


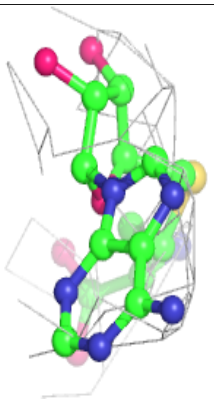


Electron density around SAH E 1001:

$2mF_o$-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.