



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 01:40 PM EDT

PDB ID : 6I7P / pdb_00006i7p
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 : 2018-11-16
Resolution : 3.98 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

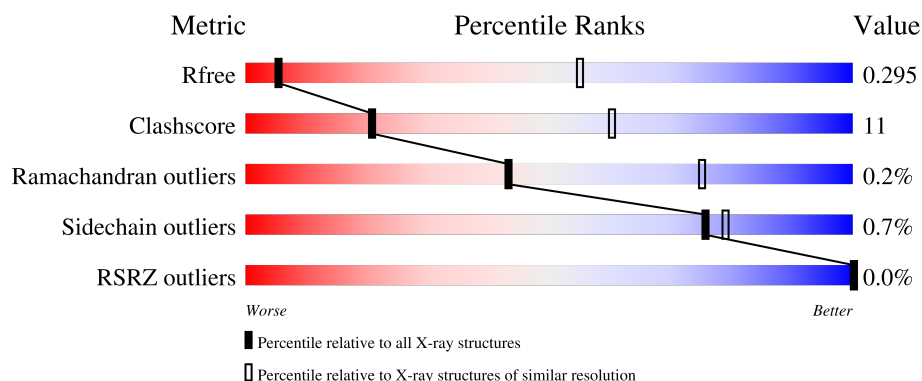
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.98 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1016 (4.18-3.78)
Clashscore	190562	1007 (4.16-3.80)
Ramachandran outliers	187476	1000 (4.18-3.78)
Sidechain outliers	187428	1131 (4.20-3.76)
RSRZ outliers	180081	1016 (4.18-3.78)

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

Mol	Chain	Length	Quality of chain
1	A	914	72% 24% .
1	B	914	75% 21% .
1	C	914	75% 21% .
1	D	914	71% 25% .
1	E	914	72% 25% .

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Mol	Chain	Length	Quality of chain
1	F	914	

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	1003	-	-	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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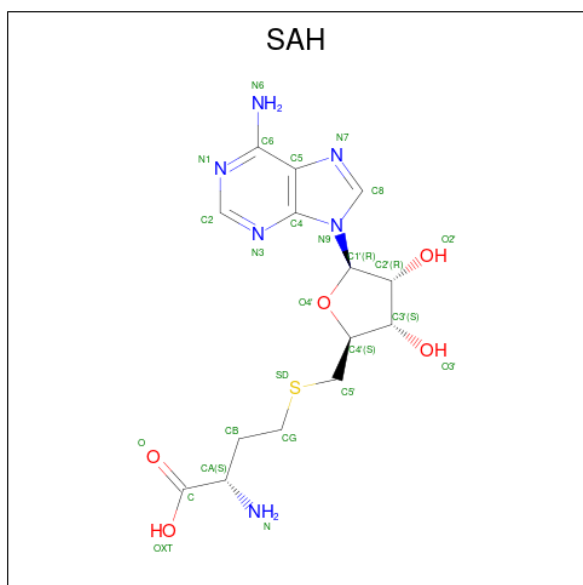
Chain	Residue	Modelled	Actual	Comment	Reference
B	909	HIS	-	expression tag	UNP A0A1B2ZC85
B	910	HIS	-	expression tag	UNP A0A1B2ZC85
B	911	HIS	-	expression tag	UNP A0A1B2ZC85
B	912	HIS	-	expression tag	UNP A0A1B2ZC85
B	913	HIS	-	expression tag	UNP A0A1B2ZC85
C	0	MET	-	initiating methionine	UNP A0A1B2ZC85
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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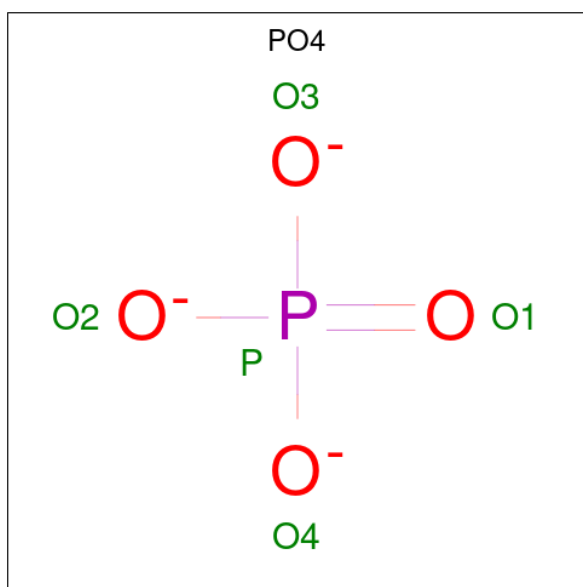
Chain	Residue	Modelled	Actual	Comment	Reference
F	907	SER	-	expression tag	UNP A0A1B2ZC85
F	908	HIS	-	expression tag	UNP A0A1B2ZC85
F	909	HIS	-	expression tag	UNP A0A1B2ZC85
F	910	HIS	-	expression tag	UNP A0A1B2ZC85
F	911	HIS	-	expression tag	UNP A0A1B2ZC85
F	912	HIS	-	expression tag	UNP A0A1B2ZC85
F	913	HIS	-	expression tag	UNP A0A1B2ZC85

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: 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 (CCD ID: PO4) (formula: O_4P).



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

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

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

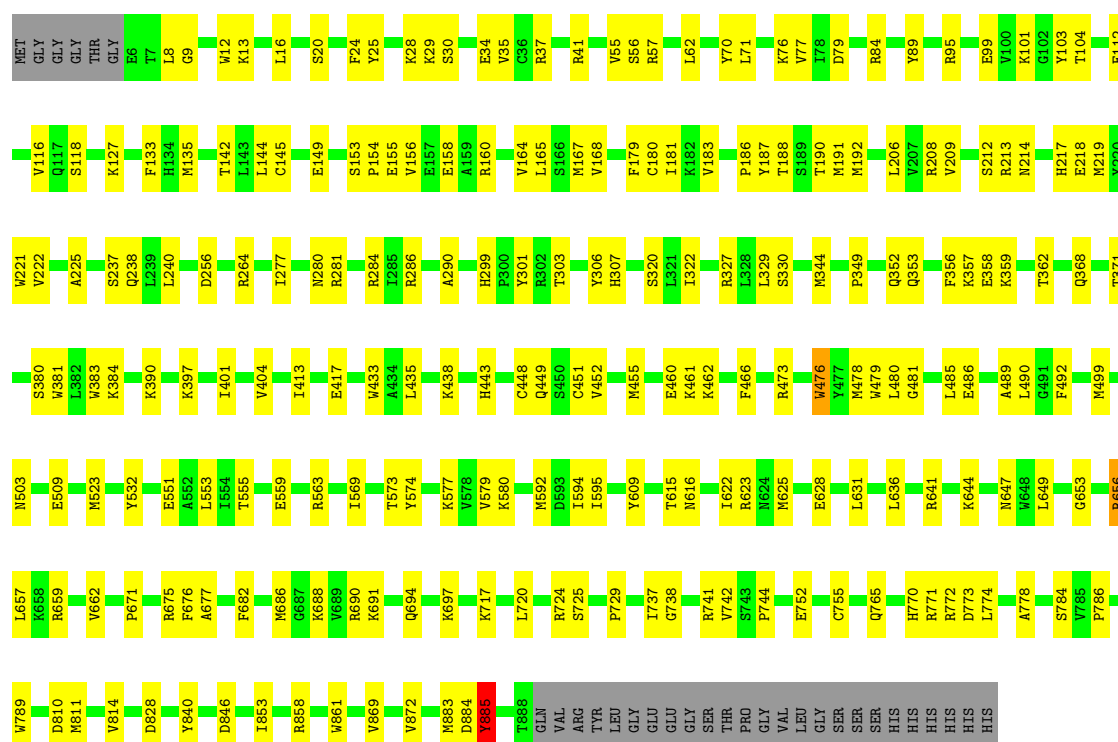
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Zn	0	0
			2	2		
4	B	1	Total	Zn	0	0
			1	1		
4	C	2	Total	Zn	0	0
			2	2		
4	D	2	Total	Zn	0	0
			2	2		
4	E	2	Total	Zn	0	0
			2	2		
4	F	2	Total	Zn	0	0
			2	2		

3 Residue-property plots

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.

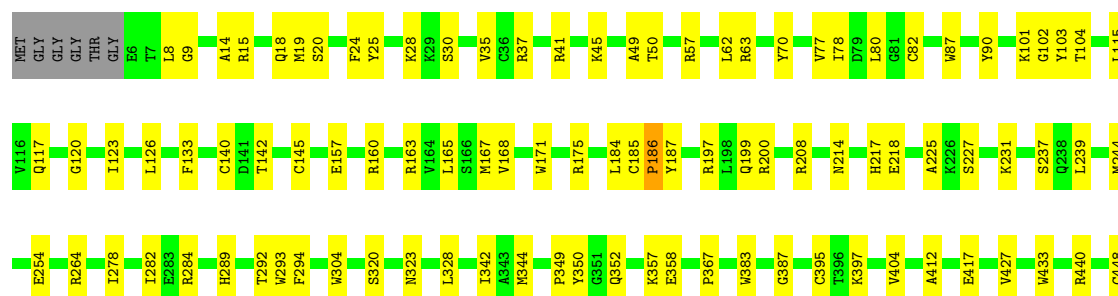
• Molecule 1: NS5

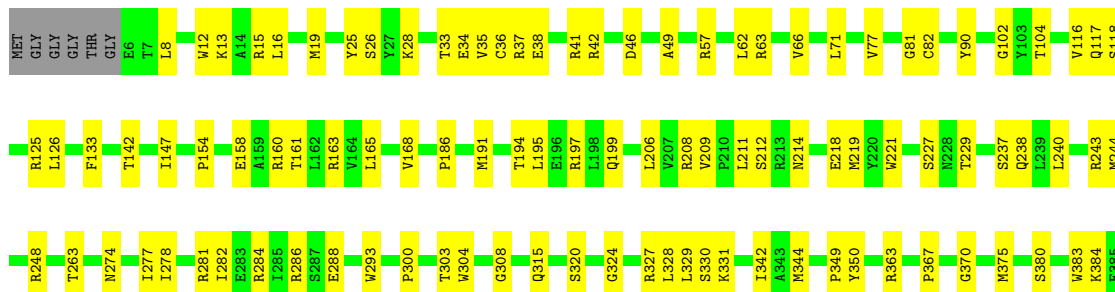
Chain A: 

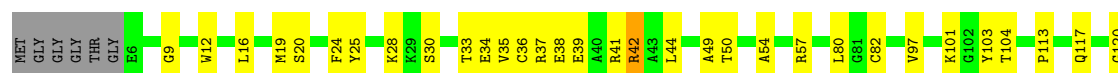


• Molecule 1: NS5

Chain B: 







C782	S783	S784	W805	W819	E827	D828	L841	S851	L852	L853	R858	V869	R873	R874	I875	I876	G877	Y882	M883	D884	Y885	I886	S887	T888	GLN	VAL	ARG	TVR	LEU	LEU	GLY	GLU	GLU	GLY	SER	THR	PRO	GLY	VAL	LEU	GLY	SER	SER	SER	HIS	HIS	HIS	HIS		
A677	F682	M686	R690	K691	Q694	K697	G698	S699	E706	S712	H713	N716	K717	L718	H719	L720	S603	R724	S725	I726	R731	H732	Q733	L736	I737	G738	R741	P744	G747	Q762	Q765	L766	L767	Y768	F769	H770	R771	R772	D773	L774	A778	I781	F676	R675						
Y574	K577	V578	K580	V581	L582	E586	K587	G588	K589	T590	V591	M592	D593	I594	I595	S596	R597	Q598	D599	Q600		S603	T608	L611	M612	T613	Q620	N624	E628	W637	L638	K644	V645	T646	N647	L649	R656	A661	V662	V669	K670	P671								
A412	I413	E416	E417	V424	V427	R440	C448	Q449	N454	M455	M456	E460	K461	K462	F466	R473	W476	W479	E488	Q514	E521	E522	M523	S524	R525	Y532	W539	I543	E551	I554	T555	M556	Q557	R563	I569	Y572	T573													
K252	Y253	E254	L259	G262	T263	R264	K276	I277	I278	G279	N280	R281	I282	E283	R284	H289	P300	Y301	Y306	L329	S330	T342	A343	M344	T345	D346	T347	T348	P349	Q353	R354	V355	P367	T371	W383	G387	C395	E398	I401	N402	K403	V404	G411							
F133	L143	E157	E158	T161	L165	S166	M167	V168	L172	F179	C180	C185	P186	Y187	M191	M192	E193	T194	L195	E196	R197	L198	Q199	R200		G204	G205	L206	V207	R208	V209	P210	L211	S212	R213	N214	W221	L230	L240	L241	G242	R243	P247	R248	R249					

4 Data and refinement statistics

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 – 3.98 49.52 – 3.98	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.52-3.98) 98.2 (49.52-3.98)	Depositor EDS
R_{merge}	0.96	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 4.00Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.280 , 0.280 0.283 , 0.295	Depositor DCC
R_{free} test set	6430 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	77.2	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 93.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.28$, $\langle L^2 \rangle = 0.11$	Xtriage
Estimated twinning fraction	0.217 for k,h,-l	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	42817	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SAH, PO4, ZN

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	0.37	2/7262 (0.0%)	0.58	3/9813 (0.0%)
1	B	0.29	0/7255	0.53	2/9803 (0.0%)
1	C	0.31	0/7262	0.52	0/9813
1	D	0.51	3/7262 (0.0%)	0.58	4/9813 (0.0%)
1	E	0.36	1/7262 (0.0%)	0.58	1/9813 (0.0%)
1	F	0.46	6/7262 (0.1%)	0.66	7/9813 (0.1%)
All	All	0.39	12/43565 (0.0%)	0.58	17/58868 (0.0%)

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	A	0	1
1	F	0	1
All	All	0	2

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	886	LEU	C-N	22.94	1.65	1.33
1	D	663	SER	C-N	-18.65	1.06	1.33
1	F	875	ILE	C-N	17.67	1.56	1.33
1	A	884	ASP	C-N	14.48	1.53	1.33
1	D	887	SER	C-N	14.25	1.53	1.33

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	599	ASP	O-C-N	-16.87	100.35	122.78
1	F	599	ASP	CA-C-N	14.79	149.80	121.54
1	F	599	ASP	C-N-CA	14.79	149.80	121.54
1	A	885	TYR	O-C-N	-14.44	103.39	122.59
1	E	663	SER	O-C-N	10.23	136.44	123.14

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	885	TYR	Mainchain
1	F	600	GLN	Mainchain

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	184	0
1	B	7090	0	6993	144	0
1	C	7097	0	6998	138	0
1	D	7097	0	6997	156	0
1	E	7097	0	6998	158	0
1	F	7097	0	6998	168	0
2	A	26	0	19	1	0
2	B	26	0	19	1	0
2	C	26	0	19	3	0
2	D	26	0	19	1	0
2	E	26	0	19	1	0
2	F	26	0	19	0	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
3	C	5	0	0	0	0
3	D	20	0	0	3	0
3	E	10	0	0	0	0
3	F	20	0	0	2	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	42095	938	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 11.

The worst 5 of 938 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:GLU:HB2	1:A:479:TRP:CH2	1.45	1.50
1:A:479:TRP:CD1	1:A:481:GLY:H	1.45	1.34
1:B:633:MET:HE1	1:B:681:ARG:CD	1.63	1.26
1:D:633:MET:HE1	1:D:681:ARG:CD	1.64	1.25
1:B:479:TRP:CD1	1:B:481:GLY:H	1.56	1.23

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%)	836 (95%)	45 (5%)	0	100	100
1	B	880/914 (96%)	837 (95%)	42 (5%)	1 (0%)	48	80
1	C	881/914 (96%)	832 (94%)	47 (5%)	2 (0%)	43	75
1	D	881/914 (96%)	829 (94%)	49 (6%)	3 (0%)	36	70
1	E	881/914 (96%)	834 (95%)	45 (5%)	2 (0%)	43	75
1	F	881/914 (96%)	835 (95%)	45 (5%)	1 (0%)	48	80
All	All	5285/5484 (96%)	5003 (95%)	273 (5%)	9 (0%)	43	75

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	36	CYS
1	D	451	CYS
1	B	186	PRO
1	C	186	PRO
1	E	186	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	756/779 (97%)	754 (100%)	2 (0%)	86	85
1	B	755/779 (97%)	752 (100%)	3 (0%)	84	84
1	C	756/779 (97%)	751 (99%)	5 (1%)	76	79
1	D	756/779 (97%)	747 (99%)	9 (1%)	63	73
1	E	756/779 (97%)	749 (99%)	7 (1%)	70	76
1	F	756/779 (97%)	750 (99%)	6 (1%)	73	77
All	All	4535/4674 (97%)	4503 (99%)	32 (1%)	76	79

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	476	TRP
1	F	479	TRP
1	D	281	ARG
1	D	42	ARG
1	F	514	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	289	HIS
1	F	463	GLN

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Mol	Chain	Res	Type
1	D	503	ASN
1	F	442	HIS
1	F	716	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
3	PO4	F	1004	-	4,4,4	0.91	0	6,6,6	0.50	0
2	SAH	F	1001	-	27,28,28	1.10	3 (11%)	36,40,40	2.07	11 (30%)
2	SAH	B	1001	-	27,28,28	1.18	4 (14%)	36,40,40	2.08	13 (36%)
3	PO4	F	1005	-	4,4,4	0.91	0	6,6,6	0.50	0
2	SAH	E	1001	-	27,28,28	1.17	5 (18%)	36,40,40	2.15	10 (27%)
3	PO4	A	1002	-	4,4,4	0.92	0	6,6,6	0.41	0
3	PO4	F	1002	-	4,4,4	0.94	0	6,6,6	0.47	0
2	SAH	C	1001	-	27,28,28	1.11	4 (14%)	36,40,40	1.93	12 (33%)
3	PO4	D	1003	-	4,4,4	0.98	0	6,6,6	0.51	0
3	PO4	B	1002	-	4,4,4	0.95	0	6,6,6	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PO4	A	1003	-	4,4,4	0.86	0	6,6,6	0.60	0
2	SAH	D	1001	-	27,28,28	1.20	5 (18%)	36,40,40	2.18	11 (30%)
2	SAH	A	1001	-	27,28,28	1.03	4 (14%)	36,40,40	2.16	11 (30%)
3	PO4	C	1002	-	4,4,4	0.93	0	6,6,6	0.50	0
3	PO4	E	1003	-	4,4,4	0.96	0	6,6,6	0.47	0
3	PO4	D	1005	-	4,4,4	0.85	0	6,6,6	0.54	0
3	PO4	E	1002	-	4,4,4	0.91	0	6,6,6	0.54	0
3	PO4	B	1003	-	4,4,4	0.97	0	6,6,6	0.45	0
3	PO4	F	1003	-	4,4,4	0.95	0	6,6,6	0.37	0
3	PO4	D	1004	-	4,4,4	0.92	0	6,6,6	0.52	0
3	PO4	D	1002	-	4,4,4	0.91	0	6,6,6	0.44	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	-	-	10/15/31/31	0/3/3/3
2	SAH	C	1001	-	-	7/15/31/31	0/3/3/3
2	SAH	F	1001	-	-	0/15/31/31	0/3/3/3
2	SAH	B	1001	-	-	10/15/31/31	0/3/3/3
2	SAH	E	1001	-	-	6/15/31/31	0/3/3/3
2	SAH	D	1001	-	-	7/15/31/31	0/3/3/3

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	SAH	C2-N1	2.94	1.39	1.33
2	E	1001	SAH	C2-N3	2.87	1.39	1.33
2	B	1001	SAH	C2-N3	2.84	1.39	1.33
2	D	1001	SAH	C2-N3	2.80	1.38	1.33
2	F	1001	SAH	C2-N3	2.79	1.38	1.33

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1001	SAH	C5-C4-N3	-5.56	119.06	126.72
2	E	1001	SAH	N3-C2-N1	-5.44	120.35	128.58
2	A	1001	SAH	N3-C2-N1	-5.44	120.35	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1001	SAH	N3-C2-N1	-5.33	120.52	128.58
2	A	1001	SAH	C5-C4-N3	-5.30	119.42	126.72

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

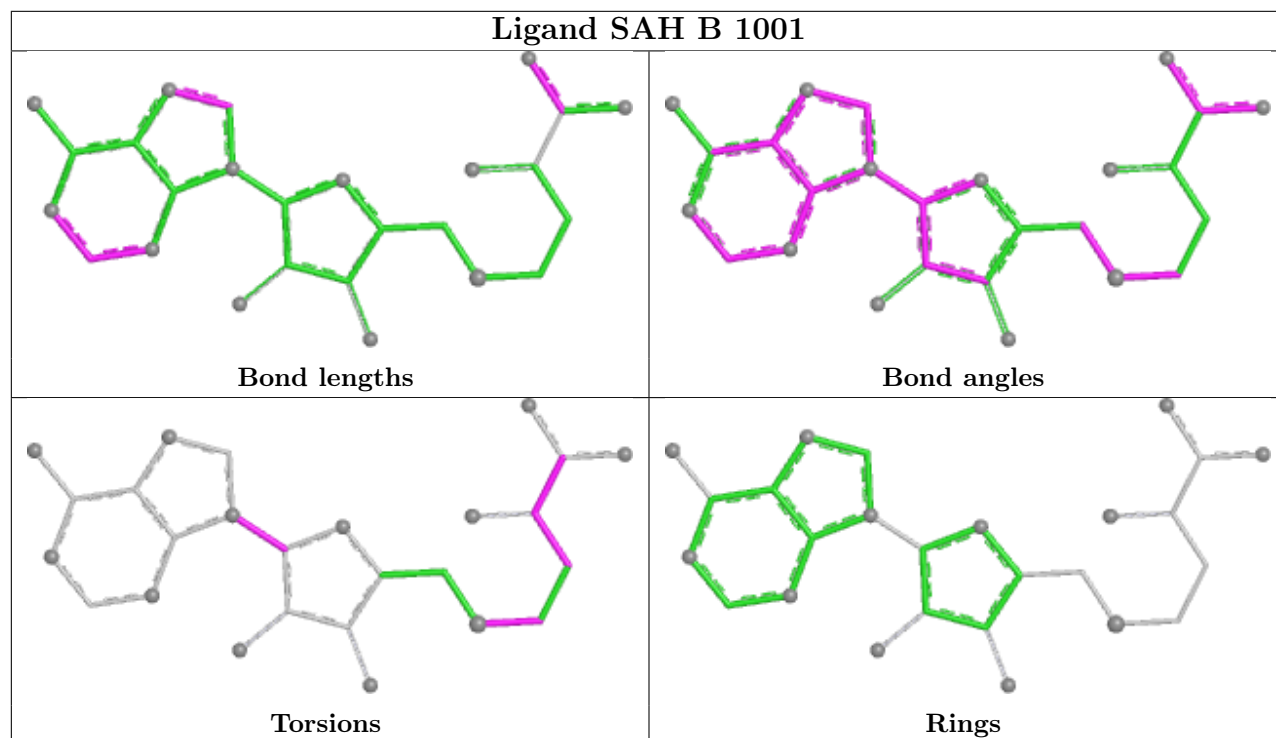
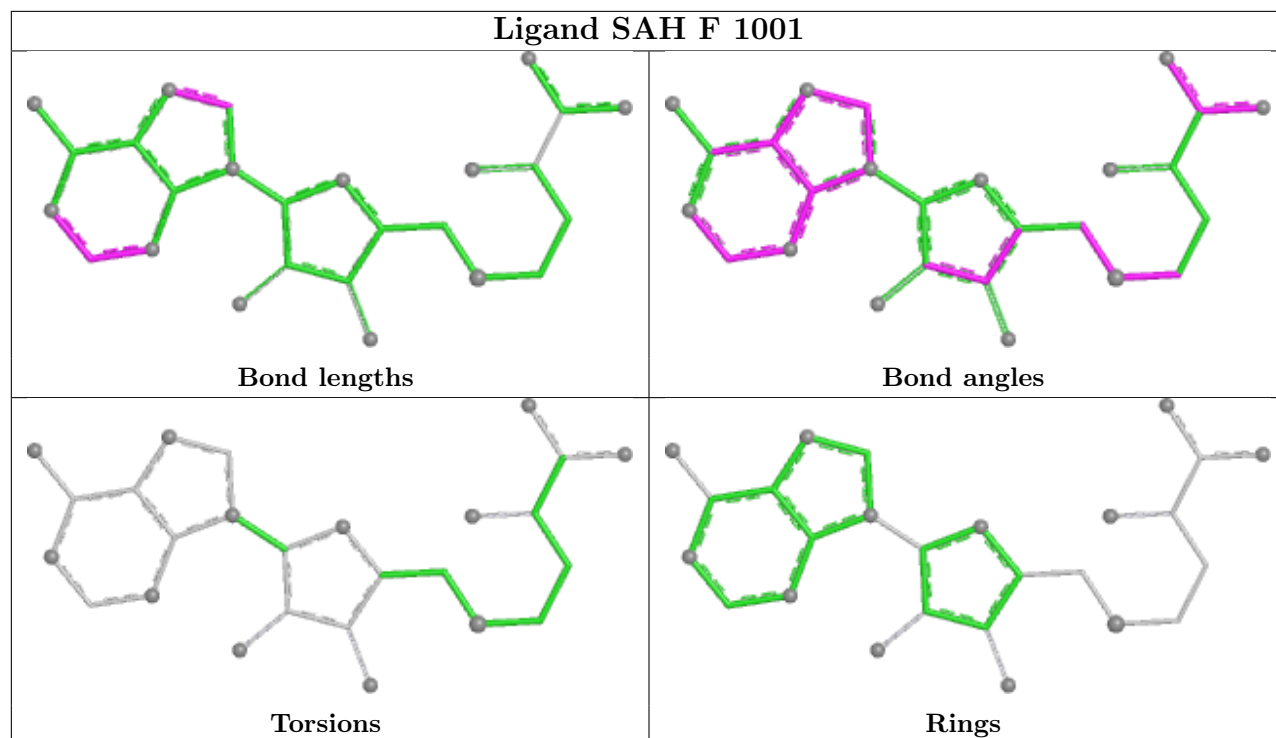
Mol	Chain	Res	Type	Atoms
2	B	1001	SAH	N-CA-CB-CG
2	B	1001	SAH	C-CA-CB-CG
2	B	1001	SAH	OXT-C-CA-N
2	E	1001	SAH	CA-CB-CG-SD
2	E	1001	SAH	C2'-C1'-N9-C8

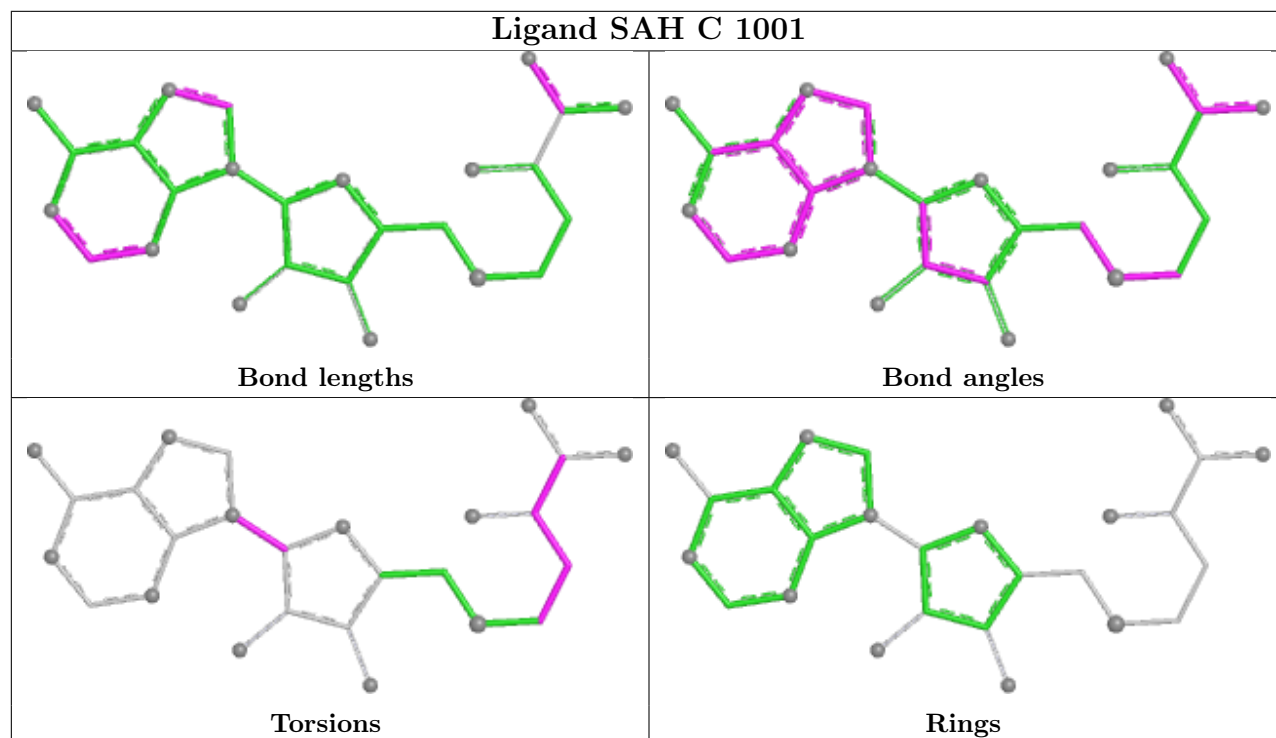
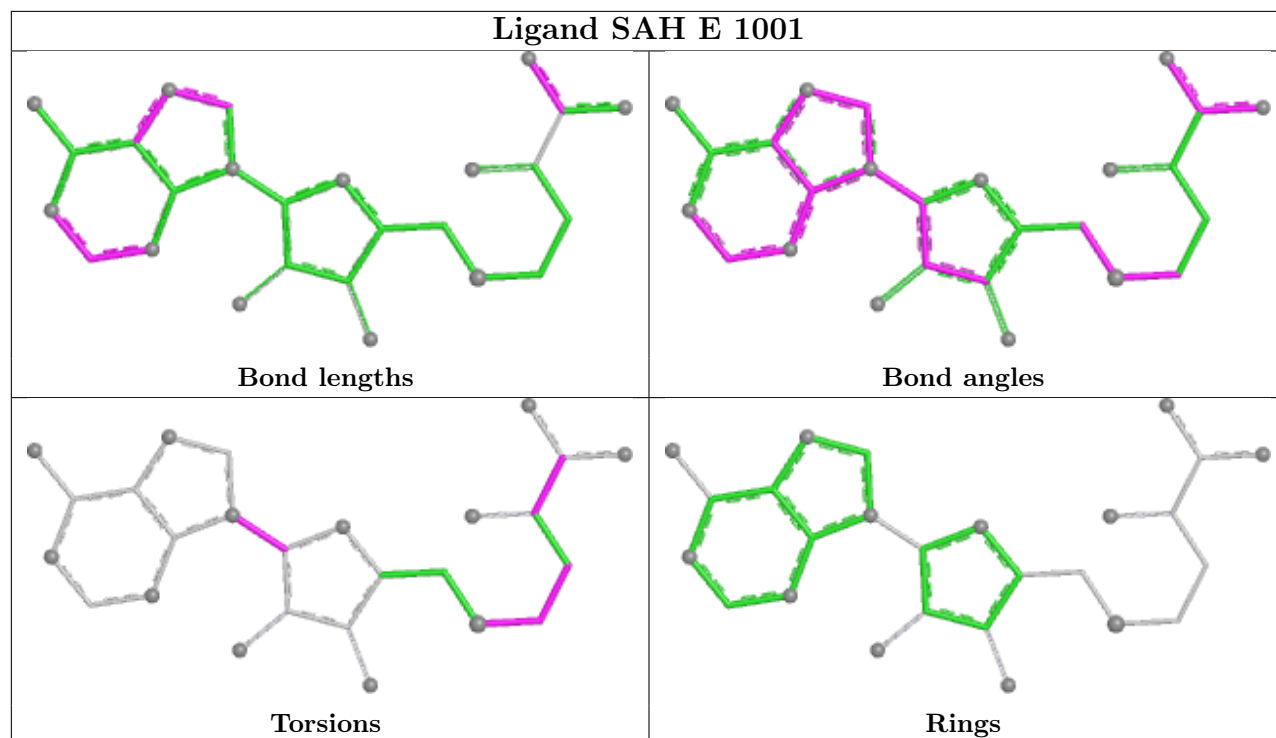
There are no ring outliers.

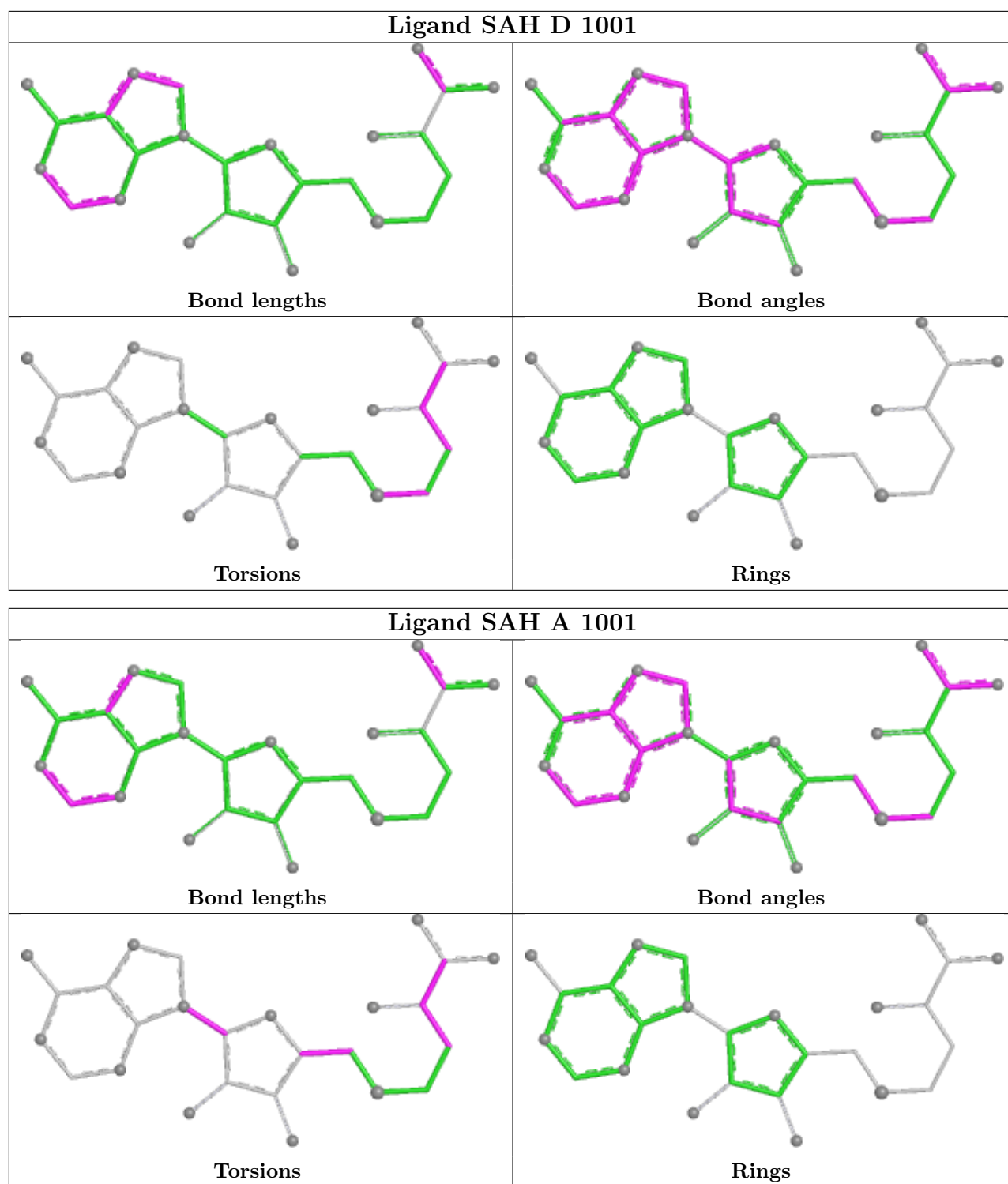
9 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	SAH	1	0
2	E	1001	SAH	1	0
3	F	1002	PO4	1	0
2	C	1001	SAH	3	0
3	D	1003	PO4	2	0
2	D	1001	SAH	1	0
2	A	1001	SAH	1	0
3	D	1005	PO4	1	0
3	F	1003	PO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	2
1	F	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	886:LEU	C	887:SER	N	1.65
1	F	876:ILE	C	877:GLY	N	1.18
1	F	599:ASP	C	600:GLN	N	1.16
1	D	663:SER	C	664:GLY	N	1.06

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(Å²)	Q<0.9	
1	A	883/914 (96%)	-1.20	0	100	100	20, 104, 182, 261	0
1	B	882/914 (96%)	-1.12	0	100	100	26, 111, 191, 253	0
1	C	883/914 (96%)	-1.17	0	100	100	18, 108, 166, 222	0
1	D	883/914 (96%)	-1.26	0	100	100	17, 77, 131, 187	0
1	E	883/914 (96%)	-1.20	0	100	100	19, 86, 156, 221	0
1	F	883/914 (96%)	-1.20	1 (0%)	92	87	27, 91, 149, 195	0
All	All	5297/5484 (96%)	-1.19	1 (0%)	100	100	17, 96, 171, 261	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	827	GLU	2.5

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

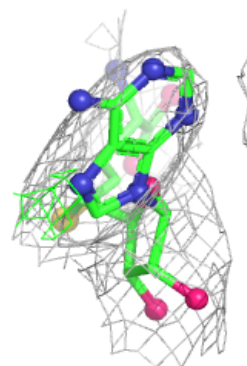
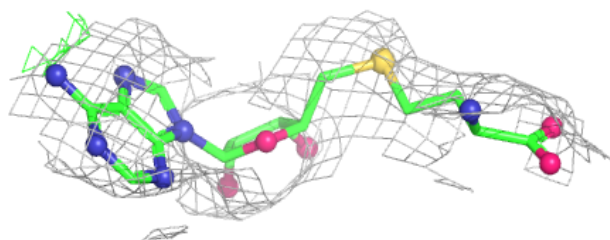
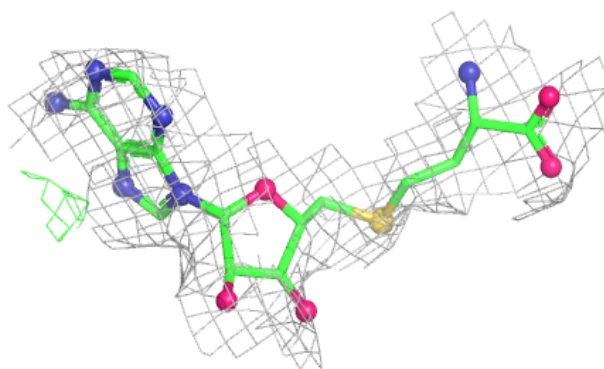
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PO4	E	1003	5/5	0.94	0.07	168,181,230,239	0
3	PO4	B	1003	5/5	0.97	0.09	157,184,212,213	0
3	PO4	B	1002	5/5	0.97	0.04	94,109,127,135	0
3	PO4	F	1003	5/5	0.97	0.06	103,138,171,194	0
3	PO4	F	1005	5/5	0.97	0.07	163,195,212,227	0
3	PO4	D	1005	5/5	0.98	0.07	119,125,139,152	0
3	PO4	A	1002	5/5	0.98	0.05	127,148,153,161	0
3	PO4	D	1002	5/5	0.98	0.08	123,143,182,184	0
3	PO4	F	1004	5/5	0.98	0.05	79,90,144,173	0
3	PO4	D	1004	5/5	0.98	0.10	156,179,206,209	0
3	PO4	D	1003	5/5	0.99	0.05	151,169,206,225	0
2	SAH	A	1001	26/26	0.99	0.04	44,65,92,141	0
3	PO4	A	1003	5/5	0.99	0.04	88,95,130,137	0
3	PO4	E	1002	5/5	0.99	0.04	78,104,111,113	0
2	SAH	C	1001	26/26	0.99	0.04	43,74,103,125	0
3	PO4	F	1002	5/5	0.99	0.05	70,78,116,131	0
2	SAH	D	1001	26/26	0.99	0.05	31,85,110,128	0
3	PO4	C	1002	5/5	0.99	0.03	110,129,154,157	0
2	SAH	F	1001	26/26	0.99	0.04	43,81,100,140	0
2	SAH	B	1001	26/26	1.00	0.03	68,105,131,138	0
2	SAH	E	1001	26/26	1.00	0.04	38,67,106,137	0
4	ZN	A	1004	1/1	1.00	0.01	73,73,73,73	0
4	ZN	A	1005	1/1	1.00	0.01	154,154,154,154	0
4	ZN	B	1004	1/1	1.00	0.01	32,32,32,32	0
4	ZN	C	1003	1/1	1.00	0.01	68,68,68,68	0
4	ZN	C	1004	1/1	1.00	0.02	142,142,142,142	0
4	ZN	D	1006	1/1	1.00	0.01	44,44,44,44	0
4	ZN	D	1007	1/1	1.00	0.01	51,51,51,51	0
4	ZN	E	1004	1/1	1.00	0.01	156,156,156,156	0
4	ZN	E	1005	1/1	1.00	0.02	10,10,10,10	0
4	ZN	F	1006	1/1	1.00	0.02	57,57,57,57	0
4	ZN	F	1007	1/1	1.00	0.01	118,118,118,118	0

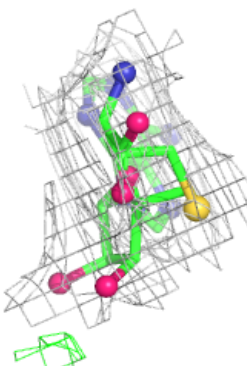
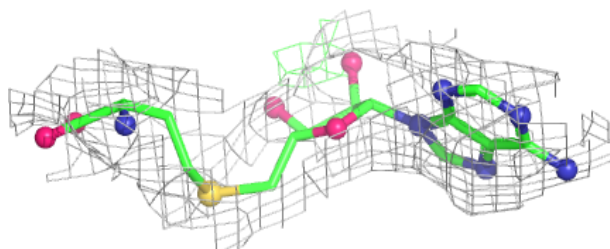
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SAH 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)

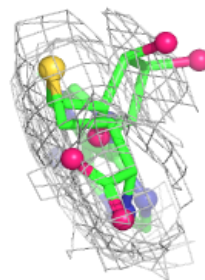
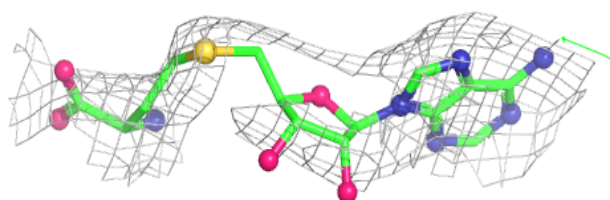
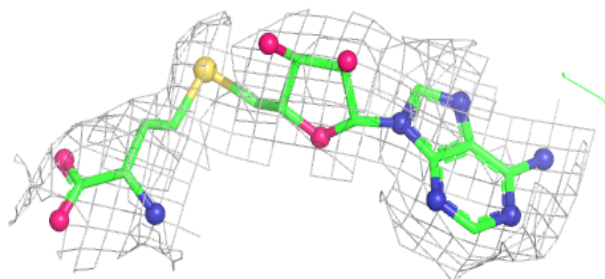
**Electron density around SAH C 1001:**

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

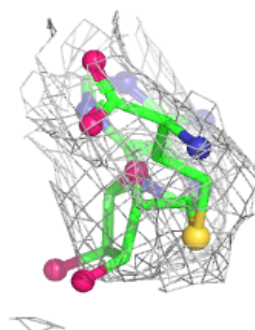
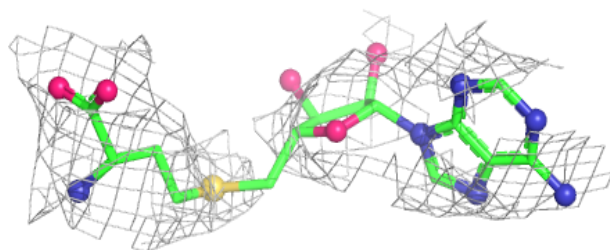
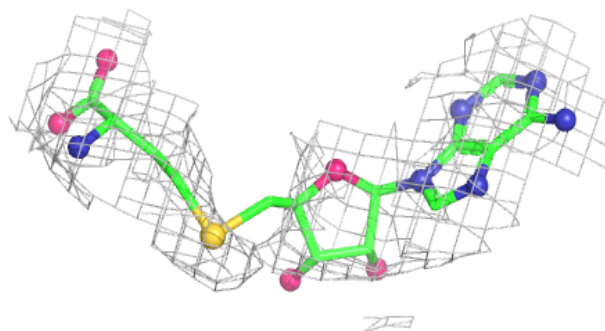


Electron density around SAH D 1001:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

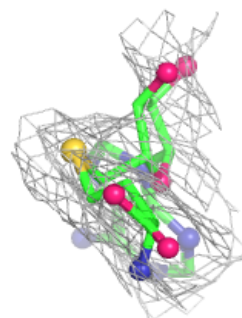
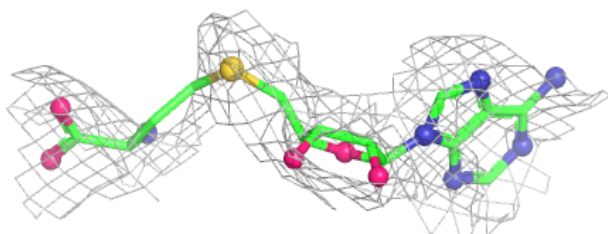
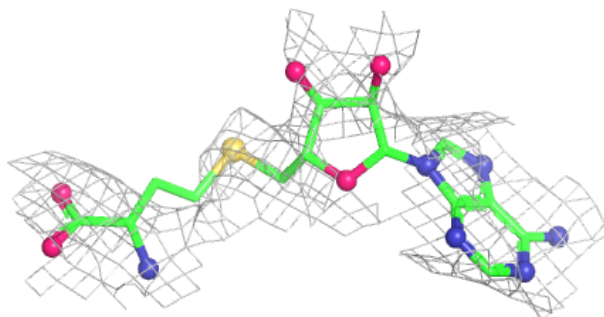
**Electron density around SAH F 1001:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

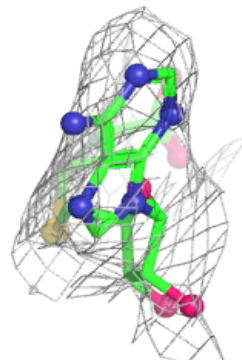
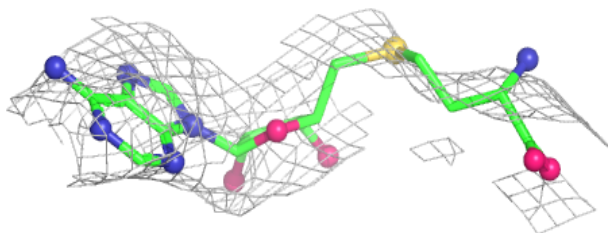
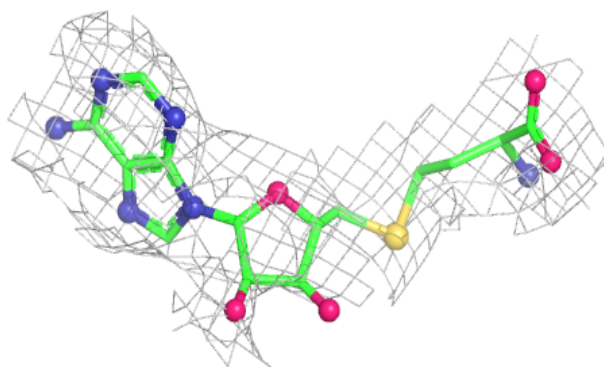


Electron density around SAH B 1001:

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

**Electron density around SAH 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.