



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 03:32 am BST

PDB ID : 1YFJ  
Title : T4Dam in Complex with AdoHcy and 15-mer Oligonucleotide Showing Semi-specific and Specific Contact  
Authors : Horton, J.R.; Liebert, K.; Hattman, S.; Jeltsch, A.; Cheng, X.  
Deposited on : 2005-01-02  
Resolution : 2.69 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](mailto: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.

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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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

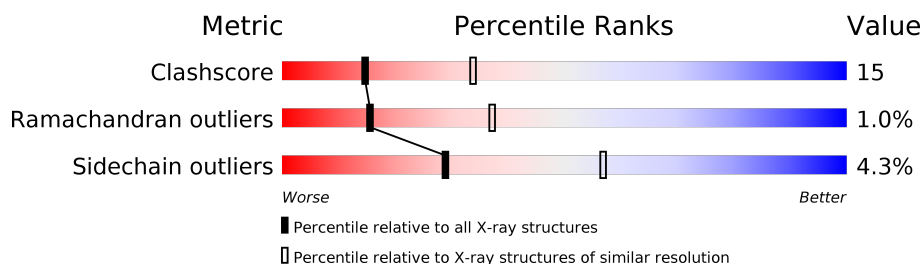
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.69 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))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	0	15	
1	1	15	
1	2	15	
1	3	15	
1	4	15	
1	5	15	
1	6	15	
1	7	15	

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Mol	Chain	Length	Quality of chain
1	8	15	<div><div></div><div>47%53%</div></div>
1	9	15	<div><div></div><div>40%60%</div></div>
2	A	259	<div><div></div><div>76%22%•</div></div>
2	B	259	<div><div></div><div>74%25%•</div></div>
2	C	259	<div><div></div><div>78%20%•</div></div>
2	D	259	<div><div></div><div>75%20%••</div></div>
2	E	259	<div><div></div><div>63%29%•6%</div></div>
2	F	259	<div><div></div><div>59%32%•6%</div></div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 15008 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 DNA chain called 5'-D(\*TP\*CP\*AP\*CP\*AP\*GP\*GP\*AP\*TP\*CP\*CP\*TP\*GP\*TP\*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	15	Total	C	N	O	P	0	0	0
			304	146	55	89	14			
1	2	15	Total	C	N	O	P	0	0	0
			308	146	55	92	15			
1	3	15	Total	C	N	O	P	0	0	0
			304	146	55	89	14			
1	4	15	Total	C	N	O	P	0	0	0
			304	146	55	89	14			
1	5	14	Total	C	N	O	P	0	0	0
			284	136	53	82	13			
1	6	15	Total	C	N	O	P	0	0	0
			290	136	50	89	15			
1	7	15	Total	C	N	O	P	0	0	0
			304	146	55	89	14			
1	8	15	Total	C	N	O	P	0	0	0
			304	146	55	89	14			
1	9	15	Total	C	N	O	P	0	0	0
			304	146	55	89	14			
1	0	15	Total	C	N	O	P	0	0	0
			304	146	55	89	14			

- Molecule 2 is a protein called DNA adenine methylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	259	Total	C	N	O	S	0	0	0
			2108	1362	355	386	5			
2	B	259	Total	C	N	O	S	0	0	0
			2112	1366	355	386	5			
2	C	259	Total	C	N	O	S	0	0	0
			2091	1351	353	382	5			
2	D	254	Total	C	N	O	S	0	0	0
			1981	1272	334	370	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	243	Total	C	N	O	S	0	0	0
			1833	1180	310	338	5			
2	F	243	Total	C	N	O	S	0	0	0
			1368	824	275	268	1			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	139	ARG	GLN	SEE REMARK 999	UNP P04392
A	140	PHE	TYR	SEE REMARK 999	UNP P04392
A	209	LEU	GLN	SEE REMARK 999	UNP P04392
B	139	ARG	GLN	SEE REMARK 999	UNP P04392
B	140	PHE	TYR	SEE REMARK 999	UNP P04392
B	209	LEU	GLN	SEE REMARK 999	UNP P04392
C	139	ARG	GLN	SEE REMARK 999	UNP P04392
C	140	PHE	TYR	SEE REMARK 999	UNP P04392
C	209	LEU	GLN	SEE REMARK 999	UNP P04392
D	139	ARG	GLN	SEE REMARK 999	UNP P04392
D	140	PHE	TYR	SEE REMARK 999	UNP P04392
D	209	LEU	GLN	SEE REMARK 999	UNP P04392
E	139	ARG	GLN	SEE REMARK 999	UNP P04392
E	140	PHE	TYR	SEE REMARK 999	UNP P04392
E	209	LEU	GLN	SEE REMARK 999	UNP P04392
F	139	ARG	GLN	SEE REMARK 999	UNP P04392
F	140	PHE	TYR	SEE REMARK 999	UNP P04392
F	209	LEU	GLN	SEE REMARK 999	UNP P04392

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	8	1	Total	Cl	0	0
			1	1		
3	2	2	Total	Cl	0	0
			2	2		
3	1	1	Total	Cl	0	0
			1	1		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

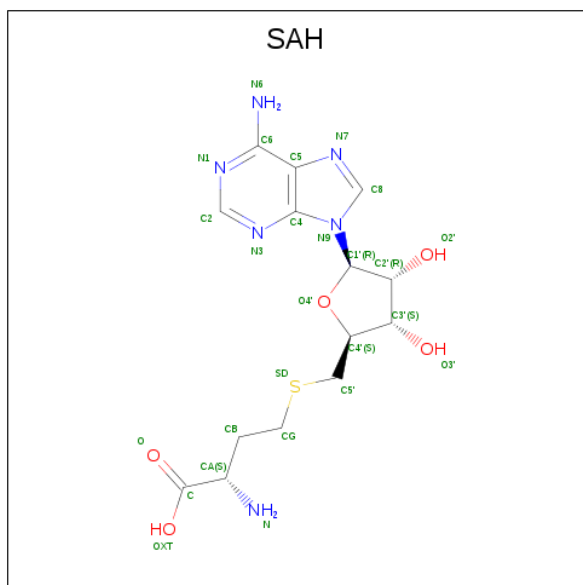
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	2	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	4	1	Total	Ca	0	0
			1	1		

- Molecule 5 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula:  $C_{14}H_{20}N_6O_5S$ ).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	1	8	Total	O	0	0
			8	8		
6	2	7	Total	O	0	0
			7	7		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	3	8	Total 8	O 8	0	0
6	4	13	Total 13	O 13	0	0
6	5	2	Total 2	O 2	0	0
6	6	1	Total 1	O 1	0	0
6	7	1	Total 1	O 1	0	0
6	8	2	Total 2	O 2	0	0
6	A	98	Total 98	O 98	0	0
6	B	102	Total 102	O 102	0	0
6	C	60	Total 60	O 60	0	0
6	D	29	Total 29	O 29	0	0
6	E	11	Total 11	O 11	0	0
6	F	1	Total 1	O 1	0	0

### 3 Residue-property plots [i](#)

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

Note EDS was not executed.

- Molecule 1: 5'-D(\*TP\*CP\*AP\*CP\*AP\*GP\*GP\*AP\*TP\*CP\*CP\*TP\*GP\*TP\*G)-3'

Chain 1: 



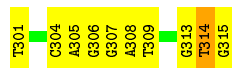
- Molecule 1: 5'-D(\*TP\*CP\*AP\*CP\*AP\*GP\*GP\*AP\*TP\*CP\*CP\*TP\*GP\*TP\*G)-3'

Chain 2: 



- Molecule 1: 5'-D(\*TP\*CP\*AP\*CP\*AP\*GP\*GP\*AP\*TP\*CP\*CP\*TP\*GP\*TP\*G)-3'

Chain 3: 



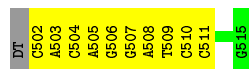
- Molecule 1: 5'-D(\*TP\*CP\*AP\*CP\*AP\*GP\*GP\*AP\*TP\*CP\*CP\*TP\*GP\*TP\*G)-3'

Chain 4: 



- Molecule 1: 5'-D(\*TP\*CP\*AP\*CP\*AP\*GP\*GP\*AP\*TP\*CP\*CP\*TP\*GP\*TP\*G)-3'

Chain 5: 



- Molecule 1: 5'-D(\*TP\*CP\*AP\*CP\*AP\*GP\*GP\*AP\*TP\*CP\*CP\*TP\*GP\*TP\*G)-3'



Chain 6: 



- Molecule 1: 5'-D(\*TP\*CP\*AP\*CP\*AP\*GP\*GP\*AP\*TP\*CP\*CP\*TP\*GP\*TP\*G)-3'

Chain 7: 



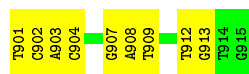
- Molecule 1: 5'-D(\*TP\*CP\*AP\*CP\*AP\*GP\*GP\*AP\*TP\*CP\*CP\*TP\*GP\*TP\*G)-3'

Chain 8: 



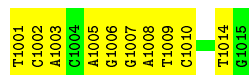
- Molecule 1: 5'-D(\*TP\*CP\*AP\*CP\*AP\*GP\*GP\*AP\*TP\*CP\*CP\*TP\*GP\*TP\*G)-3'

Chain 9: 



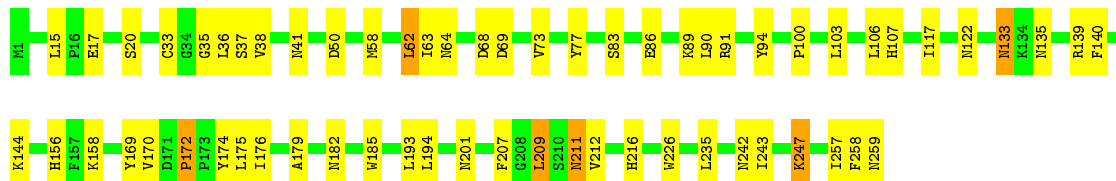
- Molecule 1: 5'-D(\*TP\*CP\*AP\*CP\*AP\*GP\*GP\*AP\*TP\*CP\*CP\*TP\*GP\*TP\*G)-3'

Chain 0: 



- Molecule 2: DNA adenine methylase

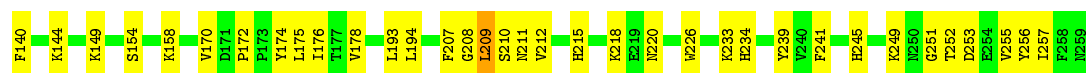
Chain A: 



- Molecule 2: DNA adenine methylase

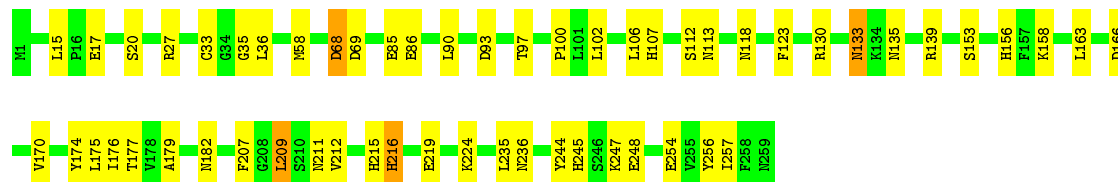
Chain B: 





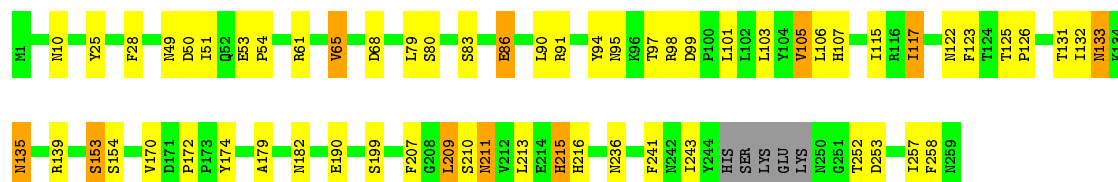
- Molecule 2: DNA adenine methylase

Chain C: 78% 20%



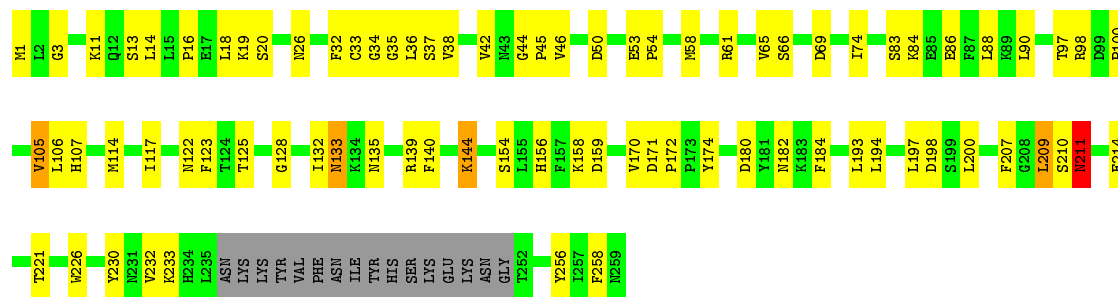
- Molecule 2: DNA adenine methylase

Chain D: 75% 20%



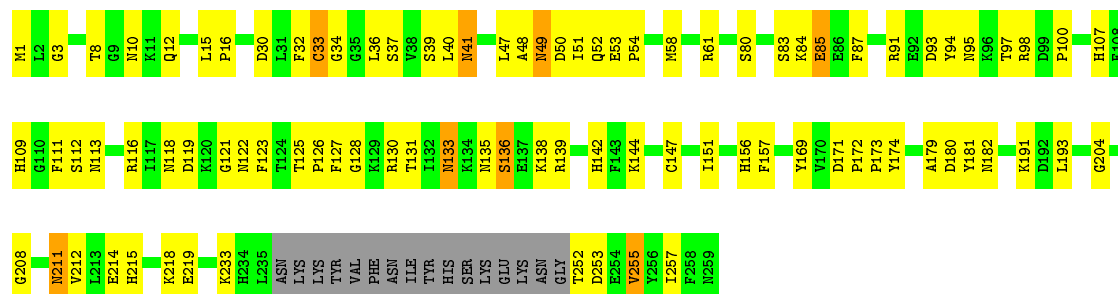
- Molecule 2: DNA adenine methylase

Chain E: 63% 29% 6%



- Molecule 2: DNA adenine methylase

Chain F: 59% 32% 6%



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.20Å 133.00Å 189.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.78 – 2.69	Depositor
% Data completeness (in resolution range)	96.8 (34.78-2.69)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.202 , 0.250	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15008	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

## 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: CA, SAH, CL

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	0	0.48	0/340	0.76	0/523
1	1	0.67	0/340	0.84	0/523
1	2	0.79	1/344 (0.3%)	0.92	1/527 (0.2%)
1	3	0.53	0/340	0.81	0/523
1	4	0.54	0/340	0.78	0/523
1	5	0.47	0/318	0.73	0/489
1	6	1.73	8/323 (2.5%)	1.67	11/495 (2.2%)
1	7	0.60	0/340	0.84	0/523
1	8	0.52	0/340	0.79	0/523
1	9	0.39	0/340	0.73	0/523
2	A	0.57	0/2159	0.80	2/2918 (0.1%)
2	B	0.58	0/2164	0.73	0/2923
2	C	0.54	0/2143	0.72	0/2898
2	D	0.48	0/2028	0.69	0/2757
2	E	0.45	0/1878	0.66	0/2560
2	F	0.42	0/1386	0.65	0/1917
All	All	0.58	9/15123 (0.1%)	0.77	14/21145 (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	1	0	2
1	3	0	1
1	4	0	1
1	7	0	1
1	8	0	1
All	All	0	6

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	6	601	DT	C3'-C2'	22.12	1.78	1.52
1	6	601	DT	C5-C7	7.93	1.54	1.50
1	6	601	DT	C3'-O3'	-7.89	1.33	1.44
1	6	601	DT	C4'-C3'	-6.95	1.45	1.52
1	2	201	DT	OP3-P	-6.48	1.53	1.61
1	6	602	DC	O3'-P	-6.15	1.53	1.61
1	6	602	DC	P-O5'	-5.97	1.53	1.59
1	6	602	DC	N1-C2	-5.87	1.34	1.40
1	6	601	DT	OP3-P	-5.30	1.54	1.61

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	601	DT	C4'-C3'-O3'	14.94	147.04	109.70
1	6	601	DT	O4'-C4'-C3'	13.13	113.88	106.00
1	6	601	DT	C4'-C3'-C2'	-9.29	94.74	103.10
1	6	602	DC	P-O3'-C3'	-8.89	109.03	119.70
1	6	601	DT	C2'-C3'-O3'	-8.76	83.70	112.60
1	6	601	DT	OP1-P-OP2	-8.17	107.35	119.60
1	6	602	DC	P-O5'-C5'	-7.57	108.79	120.90
1	6	603	DA	OP1-P-OP2	-6.96	109.16	119.60
2	A	77	TYR	CB-CG-CD2	6.39	124.83	121.00
1	6	602	DC	OP1-P-OP2	-6.06	110.51	119.60
1	6	601	DT	C6-C5-C7	-5.81	119.41	122.90
1	2	201	DT	OP1-P-OP2	-5.48	111.38	119.60
1	6	601	DT	C6-N1-C2	5.35	123.97	121.30
2	A	77	TYR	CB-CG-CD1	-5.03	117.98	121.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	107	DG	Sidechain
1	1	112	DT	Sidechain
1	3	314	DT	Sidechain
1	4	407	DG	Sidechain
1	7	713	DG	Sidechain
1	8	807	DG	Sidechain

## 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	0	304	0	171	17	0
1	1	304	0	171	2	0
1	2	308	0	170	6	0
1	3	304	0	171	11	0
1	4	304	0	171	6	0
1	5	284	0	159	9	0
1	6	290	0	158	11	0
1	7	304	0	171	12	0
1	8	304	0	171	7	0
1	9	304	0	171	14	0
2	A	2108	0	2058	42	0
2	B	2112	0	2063	47	0
2	C	2091	0	2021	41	0
2	D	1981	0	1830	37	0
2	E	1833	0	1618	76	0
2	F	1368	0	745	86	0
3	1	1	0	0	0	0
3	2	2	0	0	0	0
3	8	1	0	0	0	0
4	2	1	0	0	0	0
4	4	1	0	0	0	0
5	A	26	0	19	0	0
5	B	26	0	19	1	0
5	C	26	0	19	0	0
5	D	26	0	19	1	0
5	E	26	0	19	0	0
5	F	26	0	19	7	0
6	1	8	0	0	0	0
6	2	7	0	0	0	0
6	3	8	0	0	0	0
6	4	13	0	0	0	0
6	5	2	0	0	0	0
6	6	1	0	0	0	0
6	7	1	0	0	0	0
6	8	2	0	0	0	0
6	A	98	0	0	2	0
6	B	102	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	60	0	0	2	0
6	D	29	0	0	0	0
6	E	11	0	0	1	0
6	F	1	0	0	0	0
All	All	15008	0	12133	410	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 15.

All (410) 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)
1:6:601:DT:C3'	1:6:601:DT:C2'	1.78	1.32
1:6:602:DC:H2''	1:6:603:DA:OP2	1.33	1.14
1:7:703:DA:C2'	1:7:704:DC:H5''	1.75	1.14
2:D:83:SER:HB2	2:D:86:GLU:HG3	1.32	1.10
2:C:209:LEU:HD23	2:C:257:ILE:HB	1.44	0.99
1:6:601:DT:O3'	1:6:601:DT:C2'	2.11	0.99
1:7:703:DA:H2''	1:7:704:DC:H5''	1.00	0.99
1:7:703:DA:H2''	1:7:704:DC:C5'	1.94	0.95
2:E:133:ASN:HD22	2:E:135:ASN:H	1.14	0.95
2:E:170:VAL:HG12	2:E:172:PRO:HD3	1.49	0.94
1:9:903:DA:H2''	1:9:904:DC:O5'	1.69	0.93
2:F:214:GLU:HA	2:F:218:LYS:O	1.70	0.92
2:F:118:ASN:O	2:F:121:GLY:HA2	1.72	0.89
1:9:907:DG:H8	1:9:907:DG:H5'	1.37	0.89
2:F:95:ASN:HD21	2:F:122:ASN:CB	1.85	0.88
2:F:91:ARG:O	2:F:95:ASN:HB2	1.75	0.86
1:6:602:DC:C2'	1:6:603:DA:OP2	2.17	0.84
2:D:133:ASN:HD22	2:D:135:ASN:H	1.24	0.84
2:B:133:ASN:HD22	2:B:135:ASN:H	1.23	0.83
2:E:33:CYS:SG	2:E:50:ASP:HB2	2.19	0.82
2:E:232:VAL:HG12	2:E:233:LYS:H	1.43	0.82
2:D:83:SER:HB2	2:D:86:GLU:CG	2.09	0.82
2:F:135:ASN:O	2:F:138:LYS:CB	2.27	0.81
2:E:133:ASN:ND2	2:E:135:ASN:H	1.78	0.81
2:C:215:HIS:O	2:C:216:HIS:HB2	1.79	0.81
2:C:236:ASN:HB2	2:C:254:GLU:HG3	1.64	0.80
2:D:170:VAL:HG12	2:D:172:PRO:HD3	1.62	0.79
2:F:58:MET:HA	2:F:100:PRO:HB3	1.65	0.78
1:9:907:DG:C8	1:9:907:DG:H5'	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:232:VAL:HG12	2:E:233:LYS:N	2.00	0.76
2:E:133:ASN:HD21	2:E:135:ASN:HB3	1.51	0.76
2:A:201:ASN:HD22	2:A:259:ASN:HD22	1.33	0.76
2:F:118:ASN:HB3	2:F:122:ASN:H	1.51	0.75
2:F:95:ASN:ND2	2:F:122:ASN:CB	2.50	0.74
2:E:11:LYS:HE2	2:E:171:ASP:OD2	1.87	0.74
2:E:209:LEU:HG	2:E:210:SER:N	2.01	0.74
1:5:508:DA:H2''	1:5:509:DT:O5'	1.88	0.74
2:C:17:GLU:O	2:C:20:SER:HB3	1.87	0.73
1:5:504:DC:H2''	1:5:505:DA:C8	2.22	0.73
1:7:704:DC:H2''	1:7:705:DA:C8	2.24	0.73
2:C:156:HIS:ND1	2:C:158:LYS:HG2	2.03	0.73
2:F:95:ASN:OD1	2:F:122:ASN:CB	2.36	0.73
2:F:80:SER:H	2:F:83:SER:CB	2.01	0.73
2:E:156:HIS:CD2	2:E:158:LYS:H	2.06	0.73
2:E:133:ASN:C	2:E:133:ASN:HD22	1.93	0.72
2:E:156:HIS:HD2	2:E:158:LYS:H	1.37	0.72
2:E:230:TYR:HB3	2:E:258:PHE:O	1.90	0.71
2:A:139:ARG:HG2	2:A:139:ARG:HH11	1.55	0.70
2:B:15:LEU:HG	2:B:19:LYS:HE3	1.73	0.70
2:C:139:ARG:HG2	2:C:139:ARG:HH11	1.54	0.70
2:F:118:ASN:O	2:F:121:GLY:CA	2.40	0.70
2:F:32:PHE:CZ	2:F:172:PRO:HB3	2.28	0.69
1:0:1007:DG:H5'	2:F:8:THR:HA	1.75	0.69
2:B:79:LEU:HD11	2:B:90:LEU:HD22	1.73	0.69
2:F:32:PHE:HB2	2:F:171:ASP:O	1.93	0.69
2:A:133:ASN:HD22	2:A:133:ASN:C	1.95	0.69
2:D:174:TYR:CE1	2:D:211:ASN:HA	2.27	0.69
2:A:176:ILE:HD11	2:A:212:VAL:HG23	1.75	0.69
2:E:133:ASN:ND2	2:E:135:ASN:N	2.40	0.69
2:C:133:ASN:HD22	2:C:135:ASN:H	1.39	0.68
1:6:604:DC:H2''	1:6:605:DA:C8	2.29	0.67
2:F:94:TYR:O	2:F:98:ARG:N	2.28	0.67
1:8:809:DT:H1'	1:8:810:DC:H5''	1.77	0.67
2:B:170:VAL:HG12	2:B:172:PRO:HD3	1.76	0.67
2:E:133:ASN:HD22	2:E:135:ASN:N	1.88	0.67
2:B:176:ILE:HD11	2:B:212:VAL:HG23	1.77	0.67
2:F:10:ASN:OD1	2:F:12:GLN:HG3	1.95	0.67
2:B:42:VAL:O	2:B:149:LYS:NZ	2.28	0.66
2:F:233:LYS:O	2:F:255:VAL:CB	2.43	0.66
2:E:117:ILE:HA	2:E:122:ASN:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:504:DC:H2''	1:5:505:DA:N7	2.12	0.65
2:A:58:MET:HA	2:A:100:PRO:HB3	1.79	0.64
2:F:49:ASN:HD22	2:F:50:ASP:N	1.94	0.64
1:0:1009:DT:H1'	1:0:1010:DC:H5''	1.79	0.63
2:A:17:GLU:O	2:A:20:SER:HB2	1.98	0.63
1:7:703:DA:C3'	1:7:704:DC:H5''	2.28	0.63
2:E:44:GLY:HA2	2:E:46:VAL:HG23	1.80	0.63
2:B:135:ASN:HD22	2:B:138:LYS:HD2	1.63	0.62
2:C:33:CYS:HB2	2:C:36:LEU:HD23	1.81	0.62
1:4:410:DC:H6	1:4:410:DC:H5'	1.64	0.62
2:E:170:VAL:HG11	2:E:193:LEU:HD21	1.80	0.62
2:F:133:ASN:O	2:F:136:SER:CB	2.48	0.62
2:A:209:LEU:HD23	2:A:257:ILE:HB	1.81	0.62
2:C:139:ARG:NH1	2:C:139:ARG:HG2	2.15	0.62
2:A:17:GLU:HG2	2:A:235:LEU:HD22	1.80	0.62
2:E:13:SER:O	2:E:16:PRO:HD2	1.99	0.62
2:E:50:ASP:O	2:E:154:SER:HA	2.00	0.61
2:F:169:TYR:HA	2:F:208:GLY:O	2.01	0.61
2:F:32:PHE:CE1	2:F:172:PRO:HB3	2.36	0.61
1:0:1006:DG:OP2	2:F:133:ASN:ND2	2.34	0.61
2:F:15:LEU:CB	2:F:16:PRO:HD3	2.31	0.60
2:C:174:TYR:HB2	2:C:177:THR:OG1	2.02	0.60
2:E:232:VAL:CG1	2:E:233:LYS:H	2.14	0.60
2:E:174:TYR:CE1	2:E:211:ASN:HA	2.37	0.60
1:3:315:DG:C8	2:B:126:PRO:HG3	2.37	0.60
2:C:86:GLU:OE1	2:C:86:GLU:N	2.34	0.60
2:C:176:ILE:HD11	2:C:212:VAL:HG23	1.84	0.59
2:D:133:ASN:HD22	2:D:135:ASN:N	1.99	0.59
2:F:113:ASN:ND2	2:F:130:ARG:HH11	2.00	0.59
2:C:163:LEU:O	2:C:166:ASP:HB2	2.03	0.59
2:A:15:LEU:HD21	2:A:41:ASN:HB2	1.84	0.59
1:5:505:DA:H2'	1:5:506:DG:C8	2.38	0.59
2:A:139:ARG:HG2	2:A:139:ARG:NH1	2.18	0.59
1:6:605:DA:H2''	1:6:606:DG:C8	2.39	0.58
2:B:140:PHE:CZ	2:B:144:LYS:HD2	2.38	0.58
2:C:133:ASN:ND2	2:C:135:ASN:H	2.00	0.58
2:D:139:ARG:HG2	2:D:139:ARG:HH11	1.68	0.58
1:0:1001:DT:HO5'	1:0:1001:DT:H6	1.52	0.58
1:4:409:DT:H2''	1:4:410:DC:H5''	1.85	0.58
2:F:3:GLY:HA2	2:F:37:SER:HA	1.86	0.58
2:C:156:HIS:CE1	2:C:158:LYS:HG2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:208:DA:H1'	1:2:209:DT:H5''	1.86	0.57
2:E:61:ARG:O	2:E:65:VAL:HG13	2.03	0.57
1:3:308:DA:H2''	1:3:309:DT:C5'	2.35	0.57
2:A:174:TYR:CE1	2:A:211:ASN:HA	2.39	0.57
2:B:58:MET:HA	2:B:100:PRO:HB3	1.87	0.57
2:A:242:ASN:OD1	2:A:247:LYS:HE3	2.05	0.57
2:C:106:LEU:HD13	2:C:123:PHE:CD2	2.40	0.57
2:A:91:ARG:HA	2:A:106:LEU:HD11	1.86	0.56
2:C:118:ASN:HB2	6:C:433:HOH:O	2.04	0.56
2:D:210:SER:O	2:D:211:ASN:HB2	2.05	0.56
2:F:118:ASN:O	2:F:121:GLY:N	2.38	0.56
2:A:156:HIS:CE1	2:A:158:LYS:HG2	2.40	0.56
1:6:603:DA:OP2	1:6:603:DA:C8	2.59	0.56
2:E:54:PRO:CG	2:E:117:ILE:HD13	2.36	0.56
1:0:1001:DT:H2''	1:0:1002:DC:O4'	2.06	0.56
2:B:35:GLY:O	2:B:36:LEU:HB2	2.06	0.56
2:B:83:SER:HB2	2:B:86:GLU:HB2	1.88	0.56
2:B:44:GLY:HA2	2:B:46:VAL:HG23	1.88	0.56
2:C:35:GLY:O	2:C:36:LEU:HB2	2.06	0.56
2:C:90:LEU:HD11	2:C:102:LEU:HD22	1.86	0.56
2:F:172:PRO:O	2:F:174:TYR:HD1	1.90	0.55
2:B:178:VAL:O	2:B:178:VAL:HG12	2.05	0.55
2:F:15:LEU:CB	2:F:16:PRO:CD	2.83	0.55
2:F:97:THR:O	2:F:98:ARG:HB2	2.06	0.55
2:E:170:VAL:CG1	2:E:172:PRO:HD3	2.30	0.55
2:B:50:ASP:O	2:B:154:SER:HA	2.07	0.55
2:E:194:LEU:HD13	2:E:226:TRP:CG	2.42	0.55
2:C:58:MET:HA	2:C:100:PRO:HB3	1.90	0.54
2:D:50:ASP:O	2:D:154:SER:HA	2.07	0.54
1:9:902:DC:H2''	1:9:903:DA:C8	2.43	0.54
1:0:1008:DA:H2'	1:0:1008:DA:N3	2.23	0.54
2:F:91:ARG:CD	2:F:123:PHE:O	2.56	0.54
2:F:32:PHE:CB	2:F:171:ASP:O	2.55	0.54
2:B:133:ASN:HD22	2:B:135:ASN:N	2.01	0.54
2:D:117:ILE:HA	2:D:122:ASN:O	2.07	0.54
2:E:232:VAL:CG1	2:E:233:LYS:N	2.70	0.53
1:2:208:DA:C2'	1:2:209:DT:H5''	2.38	0.53
2:F:95:ASN:CG	2:F:122:ASN:CB	2.76	0.53
1:7:708:DA:H1'	1:7:709:DT:H5''	1.90	0.53
2:B:28:PHE:HB3	2:B:46:VAL:HG22	1.90	0.53
2:E:58:MET:HA	2:E:100:PRO:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:10:ASN:HA	5:F:406:SAH:O	2.08	0.53
1:2:208:DA:H2''	1:2:209:DT:C5'	2.37	0.53
1:8:815:DG:OP1	1:8:815:DG:H4'	2.08	0.53
2:A:15:LEU:CD2	2:A:41:ASN:HB2	2.39	0.53
2:F:33:CYS:HA	2:F:48:ALA:HB1	1.90	0.53
2:A:69:ASP:O	2:A:73:VAL:HG23	2.09	0.53
2:F:208:GLY:HA2	2:F:257:ILE:O	2.09	0.53
2:F:83:SER:C	2:F:85:GLU:N	2.61	0.53
1:7:702:DC:H2''	1:7:703:DA:C8	2.44	0.53
2:F:1:MET:CB	2:F:41:ASN:OD1	2.57	0.52
2:F:91:ARG:HD3	2:F:123:PHE:O	2.09	0.52
2:A:83:SER:HB2	2:A:86:GLU:HB2	1.91	0.52
2:B:209:LEU:HD23	2:B:257:ILE:HB	1.90	0.52
2:E:32:PHE:CE1	2:E:170:VAL:HG13	2.44	0.52
2:F:98:ARG:O	2:F:100:PRO:HD3	2.09	0.52
2:F:157:PHE:H	5:F:406:SAH:HN62	1.57	0.52
2:A:63:ILE:HG22	2:A:64:ASN:ND2	2.24	0.52
2:B:174:TYR:CE1	2:B:211:ASN:HA	2.45	0.52
2:C:170:VAL:CG2	2:C:209:LEU:HB2	2.39	0.52
2:E:174:TYR:CZ	2:E:211:ASN:HA	2.44	0.52
1:9:908:DA:N7	2:F:126:PRO:HG2	2.24	0.52
1:9:903:DA:H2''	1:9:904:DC:C5'	2.39	0.52
2:E:133:ASN:ND2	2:E:135:ASN:HB3	2.23	0.52
1:9:912:DT:H2''	1:9:913:DG:C8	2.45	0.52
2:B:54:PRO:HG2	2:B:117:ILE:HD13	1.92	0.52
2:B:33:CYS:O	2:B:34:GLY:C	2.49	0.52
2:F:172:PRO:O	2:F:174:TYR:CD1	2.63	0.52
2:E:90:LEU:HD23	2:E:106:LEU:HG	1.92	0.52
1:9:903:DA:OP1	1:9:903:DA:H4'	2.09	0.51
1:9:903:DA:C2'	1:9:904:DC:O5'	2.52	0.51
2:F:36:LEU:O	2:F:40:LEU:CB	2.59	0.51
2:A:117:ILE:HA	2:A:122:ASN:O	2.11	0.51
2:A:94:TYR:CE1	2:A:103:LEU:HB2	2.45	0.51
1:0:1014:DT:OP1	2:E:135:ASN:ND2	2.43	0.51
2:F:157:PHE:N	5:F:406:SAH:HN62	2.09	0.51
2:F:49:ASN:HD22	2:F:49:ASN:C	2.13	0.51
2:E:83:SER:HB2	2:E:86:GLU:OE1	2.11	0.51
1:1:106:DG:H2''	1:1:107:DG:OP2	2.12	0.50
1:5:505:DA:C2'	1:5:506:DG:C8	2.94	0.50
2:A:35:GLY:O	2:A:36:LEU:HB2	2.11	0.50
2:C:235:LEU:HD11	2:C:256:TYR:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:83:SER:O	2:F:85:GLU:N	2.44	0.50
2:A:156:HIS:ND1	2:A:158:LYS:HG2	2.26	0.50
2:A:38:VAL:HG21	2:A:169:TYR:CE2	2.47	0.50
1:3:308:DA:H1'	1:3:309:DT:H5''	1.93	0.50
1:6:603:DA:OP2	1:6:603:DA:H8	1.94	0.50
2:D:79:LEU:HD11	2:D:90:LEU:HD22	1.93	0.50
1:0:1001:DT:H2'	1:0:1002:DC:C6	2.46	0.50
1:0:1002:DC:H2''	1:0:1003:DA:OP2	2.12	0.50
2:E:3:GLY:O	2:E:139:ARG:HG2	2.11	0.50
2:F:30:ASP:HB3	2:F:48:ALA:HA	1.93	0.50
2:F:3:GLY:CA	2:F:37:SER:HA	2.42	0.50
2:E:170:VAL:HG21	2:E:197:LEU:HD21	1.94	0.49
2:A:17:GLU:HG2	2:A:235:LEU:CD2	2.43	0.49
2:B:17:GLU:O	2:B:20:SER:HB3	2.12	0.49
2:D:49:ASN:HA	2:D:153:SER:O	2.12	0.49
1:7:708:DA:C2'	1:7:709:DT:H5''	2.42	0.49
2:D:91:ARG:HB3	2:D:106:LEU:HD21	1.94	0.49
2:D:236:ASN:ND2	2:D:252:THR:HB	2.27	0.49
2:D:80:SER:OG	2:D:83:SER:HB3	2.12	0.49
2:D:106:LEU:HD13	2:D:123:PHE:CD2	2.47	0.49
2:E:170:VAL:HG12	2:E:209:LEU:HD12	1.95	0.49
2:D:179:ALA:O	2:D:182:ASN:HB2	2.12	0.49
2:F:49:ASN:ND2	2:F:49:ASN:C	2.66	0.49
2:F:173:PRO:HB3	2:F:182:ASN:HA	1.94	0.49
1:4:410:DC:H2''	1:4:411:DC:O5'	2.12	0.48
1:8:808:DA:H1'	1:8:809:DT:H5'	1.94	0.48
2:E:54:PRO:HG3	2:E:117:ILE:HD13	1.94	0.48
2:E:210:SER:O	2:E:211:ASN:HB2	2.13	0.48
1:6:601:DT:O3'	1:6:601:DT:H2''	2.06	0.48
2:A:170:VAL:HG11	2:A:193:LEU:HD11	1.95	0.48
1:9:903:DA:H2'	1:9:904:DC:C6	2.49	0.48
2:D:131:THR:HG23	2:D:132:ILE:N	2.27	0.48
2:E:66:SER:O	2:E:69:ASP:HB2	2.13	0.48
1:5:510:DC:H1'	1:5:511:DC:H5''	1.96	0.48
2:D:95:ASN:HB3	2:D:122:ASN:OD1	2.13	0.48
2:E:53:GLU:N	2:E:54:PRO:HD2	2.29	0.48
2:F:144:LYS:HA	2:F:147:CYS:CB	2.44	0.48
2:F:53:GLU:N	2:F:54:PRO:HD2	2.29	0.48
2:C:170:VAL:HG23	2:C:209:LEU:HB2	1.95	0.48
2:F:174:TYR:CD1	2:F:174:TYR:N	2.81	0.48
1:0:1009:DT:OP2	1:0:1009:DT:H3'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:308:DA:C2'	1:3:309:DT:H5''	2.44	0.47
2:F:174:TYR:N	2:F:174:TYR:HD1	2.11	0.47
2:E:90:LEU:CD2	2:E:106:LEU:HG	2.44	0.47
2:B:233:LYS:HE3	2:B:234:HIS:O	2.13	0.47
2:A:133:ASN:ND2	2:A:135:ASN:H	2.12	0.47
2:C:219:GLU:OE1	2:C:224:LYS:NZ	2.44	0.47
2:E:133:ASN:C	2:E:133:ASN:ND2	2.65	0.47
2:F:212:VAL:CB	2:F:253:ASP:O	2.63	0.47
2:C:179:ALA:O	2:C:182:ASN:HB2	2.15	0.47
2:E:38:VAL:O	2:E:42:VAL:HG13	2.15	0.47
1:8:804:DC:H2''	1:8:805:DA:N7	2.29	0.47
2:F:61:ARG:CB	2:F:100:PRO:HB2	2.45	0.47
2:F:119:ASP:C	2:F:121:GLY:H	2.16	0.47
2:C:244:TYR:O	2:C:245:HIS:CD2	2.68	0.47
1:4:409:DT:C2'	1:4:410:DC:H5''	2.44	0.47
2:D:207:PHE:CD1	2:D:207:PHE:C	2.88	0.47
2:E:35:GLY:O	2:E:36:LEU:HB2	2.15	0.47
1:7:708:DA:H2''	1:7:709:DT:C5'	2.44	0.47
2:D:99:ASP:C	2:D:99:ASP:OD1	2.54	0.47
2:F:118:ASN:CB	2:F:122:ASN:H	2.26	0.47
2:C:27:ARG:HB3	2:C:166:ASP:OD1	2.15	0.47
2:E:37:SER:HB3	6:E:408:HOH:O	2.14	0.47
2:F:95:ASN:ND2	2:F:123:PHE:H	2.12	0.47
1:4:410:DC:C6	1:4:410:DC:H5'	2.49	0.46
1:3:301:DT:O4	2:C:112:SER:N	2.43	0.46
1:3:304:DC:H2''	1:3:305:DA:C8	2.50	0.46
2:B:170:VAL:HG11	2:B:193:LEU:HD21	1.96	0.46
2:F:10:ASN:CG	2:F:12:GLN:HG3	2.36	0.46
1:9:901:DT:H73	2:E:128:GLY:HA2	1.97	0.46
2:B:170:VAL:CG1	2:B:172:PRO:HD3	2.43	0.46
2:D:213:LEU:HD12	2:D:253:ASP:OD2	2.15	0.46
1:0:1014:DT:OP1	2:E:139:ARG:NH1	2.49	0.46
1:2:208:DA:H2''	1:2:209:DT:H5''	1.98	0.46
2:C:93:ASP:O	2:C:97:THR:HG23	2.15	0.46
2:F:41:ASN:OD1	2:F:142:HIS:CE1	2.69	0.46
1:0:1001:DT:H2'	1:0:1002:DC:C5	2.51	0.46
2:A:33:CYS:SG	2:A:50:ASP:HB2	2.56	0.46
2:C:133:ASN:C	2:C:133:ASN:HD22	2.18	0.46
1:5:502:DC:H2''	1:5:503:DA:C8	2.51	0.46
2:B:90:LEU:HG	2:B:106:LEU:HG	1.98	0.46
2:E:14:LEU:O	2:E:18:LEU:HG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:179:ALA:O	2:A:182:ASN:HB2	2.16	0.45
2:B:249:LYS:C	2:B:251:GLY:H	2.20	0.45
2:C:133:ASN:HD22	2:C:135:ASN:N	2.10	0.45
2:F:111:PHE:HA	2:F:128:GLY:HA2	1.98	0.45
2:A:133:ASN:ND2	2:A:133:ASN:C	2.67	0.45
2:F:174:TYR:CE2	2:F:211:ASN:HA	2.51	0.45
2:C:207:PHE:CD1	2:C:207:PHE:C	2.89	0.45
2:E:133:ASN:HD21	2:E:135:ASN:CB	2.24	0.45
2:C:133:ASN:HD21	2:C:135:ASN:HB2	1.82	0.45
2:D:101:LEU:O	2:D:105:VAL:HG13	2.16	0.45
2:D:25:TYR:CE1	2:D:28:PHE:HB2	2.52	0.45
2:E:26:ASN:O	2:E:45:PRO:HD2	2.15	0.45
1:3:307:DG:H2'	1:3:308:DA:C8	2.52	0.45
2:B:178:VAL:CG1	2:B:178:VAL:O	2.65	0.45
2:A:37:SER:HB3	6:A:489:HOH:O	2.16	0.45
2:B:175:LEU:HD12	2:B:220:ASN:ND2	2.32	0.45
2:C:175:LEU:HA	6:C:436:HOH:O	2.17	0.45
2:F:34:GLY:HA3	5:F:406:SAH:HB1	1.99	0.44
2:F:125:THR:HA	2:F:126:PRO:HD3	1.88	0.44
2:F:32:PHE:CD2	2:F:172:PRO:HA	2.53	0.44
1:1:107:DG:H2''	1:1:108:DA:H5'	1.99	0.44
2:B:12:GLN:HA	6:B:482:HOH:O	2.17	0.44
1:8:810:DC:H5'	1:8:810:DC:H6	1.82	0.44
2:C:247:LYS:O	2:C:248:GLU:C	2.56	0.44
1:7:708:DA:H2''	1:7:709:DT:H5''	1.98	0.44
2:A:175:LEU:HD23	2:A:185:TRP:HD1	1.81	0.44
2:B:61:ARG:HG2	2:B:61:ARG:HH11	1.83	0.44
2:E:74:ILE:CD1	2:E:132:ILE:HD13	2.47	0.44
2:F:87:PHE:CE2	2:F:127:PHE:HA	2.53	0.44
2:F:47:LEU:HA	2:F:151:ILE:O	2.17	0.44
1:4:415:DG:O6	2:C:130:ARG:NH2	2.46	0.44
2:C:112:SER:O	2:C:113:ASN:HB2	2.18	0.44
2:D:241:PHE:C	2:D:243:ILE:H	2.21	0.44
2:F:116:ARG:HG3	2:F:180:ASP:CG	2.38	0.44
2:B:37:SER:HB3	6:B:437:HOH:O	2.17	0.44
2:E:209:LEU:O	2:E:256:TYR:HA	2.18	0.44
2:B:158:LYS:NZ	6:B:483:HOH:O	2.49	0.43
2:D:53:GLU:N	2:D:54:PRO:HD2	2.33	0.43
2:E:156:HIS:HD2	2:E:158:LYS:N	2.11	0.43
2:E:197:LEU:HA	2:E:200:LEU:HD12	1.99	0.43
1:3:308:DA:H2''	1:3:309:DT:H5'	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:314:DT:OP1	2:B:118:ASN:ND2	2.45	0.43
1:6:614:DT:H4'	1:6:614:DT:OP1	2.18	0.43
2:A:62:LEU:HD23	2:A:62:LEU:HA	1.83	0.43
2:F:181:TYR:CE1	5:F:406:SAH:H5'1	2.53	0.43
2:B:233:LYS:O	2:B:255:VAL:HA	2.18	0.43
2:E:182:ASN:C	2:E:184:PHE:H	2.22	0.43
1:9:909:DT:O4	2:F:112:SER:N	2.48	0.43
2:C:90:LEU:CD1	2:C:102:LEU:HD22	2.48	0.43
1:7:701:DT:H2'	1:7:701:DT:H6	1.46	0.43
1:9:902:DC:H2''	1:9:903:DA:H8	1.81	0.43
2:B:239:TYR:CZ	2:B:253:ASP:HB2	2.53	0.43
2:E:123:PHE:CZ	2:E:125:THR:HB	2.54	0.43
1:0:1008:DA:H8	2:F:179:ALA:HB2	1.82	0.43
1:0:1008:DA:N7	2:F:181:TYR:OH	2.41	0.43
2:A:140:PHE:CZ	2:A:144:LYS:HD2	2.54	0.43
2:E:90:LEU:HD23	2:E:106:LEU:CD2	2.48	0.43
1:0:1009:DT:H2''	1:0:1010:DC:C5'	2.49	0.43
2:B:84:LYS:NZ	6:B:468:HOH:O	2.46	0.43
2:F:135:ASN:O	2:F:138:LYS:N	2.52	0.43
2:B:207:PHE:C	2:B:207:PHE:CD1	2.91	0.43
2:D:10:ASN:HA	5:D:404:SAH:O	2.18	0.43
2:E:197:LEU:HD22	2:E:207:PHE:CD2	2.54	0.43
2:E:170:VAL:CG1	2:E:209:LEU:HD12	2.48	0.43
2:F:109:HIS:CE1	2:F:131:THR:HA	2.53	0.43
1:3:306:DG:H1'	1:3:307:DG:C8	2.54	0.43
2:C:212:VAL:HG23	2:C:212:VAL:O	2.18	0.43
1:5:506:DG:H1'	1:5:507:DG:C8	2.53	0.42
2:E:33:CYS:O	2:E:34:GLY:C	2.57	0.42
2:E:1:MET:HE2	2:E:1:MET:HA	2.01	0.42
2:E:11:LYS:CE	2:E:171:ASP:OD2	2.63	0.42
2:F:214:GLU:HA	2:F:219:GLU:HA	2.01	0.42
2:B:210:SER:O	2:B:211:ASN:HB2	2.19	0.42
2:D:215:HIS:O	2:D:216:HIS:HB2	2.19	0.42
2:E:170:VAL:CG1	2:E:193:LEU:HD21	2.49	0.42
1:5:510:DC:H2''	1:5:511:DC:C5'	2.50	0.42
2:B:10:ASN:HA	5:B:402:SAH:C	2.49	0.42
2:D:115:ILE:HG22	2:D:117:ILE:HD12	2.01	0.42
1:0:1001:DT:C2'	1:0:1002:DC:C6	3.02	0.42
2:C:15:LEU:HD12	2:C:15:LEU:HA	1.76	0.42
2:F:191:LYS:C	2:F:193:LEU:H	2.22	0.42
2:A:207:PHE:CD1	2:A:207:PHE:C	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:209:LEU:HG	2:E:210:SER:O	2.19	0.42
2:F:34:GLY:HA2	5:F:406:SAH:O3'	2.20	0.42
2:F:51:ILE:O	2:F:53:GLU:N	2.53	0.42
1:2:208:DA:C1'	1:2:209:DT:H5''	2.49	0.42
1:9:903:DA:C4'	1:9:903:DA:OP1	2.68	0.42
2:A:175:LEU:HA	6:A:418:HOH:O	2.20	0.42
2:E:106:LEU:HD22	2:E:123:PHE:CE2	2.54	0.42
2:F:118:ASN:N	2:F:122:ASN:O	2.51	0.42
2:B:218:LYS:HE3	2:B:218:LYS:HB2	1.69	0.42
2:A:139:ARG:CG	2:A:139:ARG:HH11	2.23	0.42
2:A:194:LEU:HD22	2:A:226:TRP:CD2	2.55	0.42
2:D:83:SER:CB	2:D:86:GLU:HG3	2.23	0.42
1:8:810:DC:H2''	1:8:811:DC:O5'	2.20	0.41
1:3:313:DG:C8	1:3:314:DT:H72	2.55	0.41
1:6:601:DT:H4'	1:6:601:DT:OP3	2.20	0.41
2:F:181:TYR:CZ	5:F:406:SAH:H5'1	2.56	0.41
1:7:709:DT:H2''	1:7:710:DC:O5'	2.21	0.41
2:D:125:THR:HA	2:D:126:PRO:HD3	1.79	0.41
2:D:97:THR:O	2:D:98:ARG:HB2	2.19	0.41
2:E:209:LEU:HD21	2:E:211:ASN:HB2	2.02	0.41
2:A:86:GLU:N	2:A:86:GLU:OE1	2.47	0.41
2:B:194:LEU:HD22	2:B:226:TRP:CE3	2.56	0.41
2:E:156:HIS:HB3	2:E:159:ASP:OD2	2.21	0.41
2:E:90:LEU:HD21	2:E:105:VAL:HG22	2.01	0.41
2:F:215:HIS:HA	2:F:252:THR:CB	2.50	0.41
2:D:209:LEU:HD23	2:D:257:ILE:HB	2.03	0.41
2:A:258:PHE:CD1	2:A:258:PHE:N	2.88	0.41
2:E:140:PHE:CZ	2:E:144:LYS:HD2	2.55	0.41
2:E:74:ILE:HD12	2:E:132:ILE:HD13	2.03	0.41
2:E:84:LYS:O	2:E:88:LEU:HG	2.20	0.41
2:B:208:GLY:HA3	2:B:256:TYR:OH	2.21	0.41
2:E:90:LEU:HD21	2:E:105:VAL:CG2	2.50	0.41
2:E:18:LEU:C	2:E:20:SER:H	2.24	0.41
1:0:1005:DA:H3'	2:F:133:ASN:ND2	2.36	0.41
2:C:68:ASP:O	2:C:69:ASP:C	2.58	0.41
2:A:139:ARG:CG	2:A:139:ARG:NH1	2.80	0.41
2:F:83:SER:O	2:F:84:LYS:C	2.57	0.41
2:B:215:HIS:ND1	2:B:252:THR:OG1	2.45	0.41
2:B:241:PHE:O	2:B:245:HIS:HD2	2.04	0.41
2:E:97:THR:O	2:E:98:ARG:HB2	2.21	0.41
2:A:170:VAL:HG12	2:A:172:PRO:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:258:PHE:N	2:D:258:PHE:CD1	2.89	0.40
2:E:114:MET:CE	2:E:180:ASP:HB2	2.50	0.40
2:D:61:ARG:O	2:D:65:VAL:HG13	2.21	0.40
2:F:113:ASN:ND2	2:F:130:ARG:NH1	2.67	0.40
2:A:90:LEU:HG	2:A:106:LEU:HG	2.04	0.40
2:B:15:LEU:O	2:B:19:LYS:HG3	2.21	0.40
2:B:61:ARG:HG2	2:B:61:ARG:NH1	2.37	0.40
2:D:94:TYR:CE1	2:D:103:LEU:HB2	2.56	0.40
1:2:214:DT:H2''	1:2:215:DG:C8	2.56	0.40
2:D:210:SER:O	2:D:211:ASN:CB	2.68	0.40
2:F:12:GLN:HE22	2:F:139:ARG:NH1	2.20	0.40
1:8:810:DC:H5'	1:8:810:DC:C6	2.57	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	
2	A	257/259 (99%)	244 (95%)	12 (5%)	1 (0%)	34	60
2	B	257/259 (99%)	246 (96%)	11 (4%)	0	100	100
2	C	257/259 (99%)	244 (95%)	13 (5%)	0	100	100
2	D	250/259 (96%)	229 (92%)	20 (8%)	1 (0%)	34	60
2	E	239/259 (92%)	206 (86%)	29 (12%)	4 (2%)	9	23
2	F	239/259 (92%)	188 (79%)	42 (18%)	9 (4%)	3	7
All	All	1499/1554 (96%)	1357 (90%)	127 (8%)	15 (1%)	15	37

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	52	GLN

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Mol	Chain	Res	Type
2	E	221	THR
2	F	33	CYS
2	F	136	SER
2	F	204	GLY
2	F	211	ASN
2	F	93	ASP
2	F	156	HIS
2	D	215	HIS
2	F	85	GLU
2	E	19	LYS
2	E	211	ASN
2	E	214	GLU
2	F	255	VAL
2	A	216	HIS

### 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	
2	A	230/242 (95%)	220 (96%)	10 (4%)	29	57
2	B	231/242 (96%)	227 (98%)	4 (2%)	60	84
2	C	226/242 (93%)	218 (96%)	8 (4%)	36	65
2	D	205/242 (85%)	191 (93%)	14 (7%)	16	36
2	E	175/242 (72%)	168 (96%)	7 (4%)	31	60
2	F	42/242 (17%)	37 (88%)	5 (12%)	5	12
All	All	1109/1452 (76%)	1061 (96%)	48 (4%)	29	57

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	62	LEU
2	A	68	ASP
2	A	89	LYS
2	A	107	HIS

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Mol	Chain	Res	Type
2	A	133	ASN
2	A	172	PRO
2	A	209	LEU
2	A	211	ASN
2	A	243	ILE
2	A	247	LYS
2	B	107	HIS
2	B	133	ASN
2	B	135	ASN
2	B	209	LEU
2	C	68	ASP
2	C	85	GLU
2	C	107	HIS
2	C	133	ASN
2	C	153	SER
2	C	209	LEU
2	C	211	ASN
2	C	216	HIS
2	D	51	ILE
2	D	65	VAL
2	D	68	ASP
2	D	86	GLU
2	D	105	VAL
2	D	107	HIS
2	D	117	ILE
2	D	133	ASN
2	D	135	ASN
2	D	153	SER
2	D	190	GLU
2	D	199	SER
2	D	209	LEU
2	D	211	ASN
2	E	105	VAL
2	E	107	HIS
2	E	133	ASN
2	E	144	LYS
2	E	198	ASP
2	E	209	LEU
2	E	211	ASN
2	F	39	SER
2	F	41	ASN
2	F	49	ASN

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Mol	Chain	Res	Type
2	F	107	HIS
2	F	133	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	26	ASN
2	A	64	ASN
2	A	76	GLN
2	A	133	ASN
2	A	135	ASN
2	A	201	ASN
2	B	76	GLN
2	B	133	ASN
2	B	135	ASN
2	B	146	ASN
2	B	245	HIS
2	C	21	HIS
2	C	26	ASN
2	C	76	GLN
2	C	113	ASN
2	C	133	ASN
2	C	135	ASN
2	C	145	GLN
2	C	146	ASN
2	D	76	GLN
2	D	133	ASN
2	D	135	ASN
2	D	145	GLN
2	D	201	ASN
2	E	43	ASN
2	E	133	ASN
2	E	156	HIS
2	E	231	ASN
2	F	12	GLN
2	F	49	ASN
2	F	113	ASN
2	F	142	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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$
5	SAH	A	401	-	21,28,28	2.02	7 (33%)	20,40,40	2.43	7 (35%)
5	SAH	E	405	-	21,28,28	1.81	5 (23%)	20,40,40	2.19	7 (35%)
5	SAH	D	404	-	21,28,28	1.85	6 (28%)	20,40,40	2.35	8 (40%)
5	SAH	C	403	-	21,28,28	1.96	6 (28%)	20,40,40	2.28	7 (35%)
5	SAH	B	402	-	21,28,28	1.83	4 (19%)	20,40,40	2.29	7 (35%)
5	SAH	F	406	-	21,28,28	1.69	4 (19%)	20,40,40	2.34	7 (35%)

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
5	SAH	A	401	-	-	0/7/31/31	0/3/3/3
5	SAH	E	405	-	-	1/7/31/31	0/3/3/3
5	SAH	D	404	-	-	0/7/31/31	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SAH	C	403	-	-	0/7/31/31	0/3/3/3
5	SAH	B	402	-	-	0/7/31/31	0/3/3/3
5	SAH	F	406	-	-	0/7/31/31	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	401	SAH	O4'-C1'	5.56	1.48	1.41
5	C	403	SAH	O4'-C1'	5.49	1.48	1.41
5	E	405	SAH	O4'-C1'	4.97	1.48	1.41
5	D	404	SAH	O4'-C1'	4.93	1.48	1.41
5	B	402	SAH	O4'-C1'	4.34	1.47	1.41
5	A	401	SAH	C2-N3	4.27	1.39	1.32
5	F	406	SAH	O4'-C1'	3.84	1.46	1.41
5	C	403	SAH	C8-N7	-3.70	1.28	1.34
5	F	406	SAH	C2-N3	3.58	1.37	1.32
5	B	402	SAH	C8-N7	-3.52	1.28	1.34
5	B	402	SAH	C2-N3	3.49	1.37	1.32
5	E	405	SAH	C2-N3	3.46	1.37	1.32
5	A	401	SAH	C8-N7	-3.31	1.28	1.34
5	D	404	SAH	C2-N3	3.31	1.37	1.32
5	C	403	SAH	C2-N3	3.27	1.37	1.32
5	F	406	SAH	CA-N	2.87	1.53	1.47
5	D	404	SAH	CA-N	2.81	1.53	1.47
5	E	405	SAH	CA-N	2.79	1.53	1.47
5	E	405	SAH	C8-N7	-2.76	1.29	1.34
5	C	403	SAH	CA-N	2.67	1.53	1.47
5	D	404	SAH	C8-N7	-2.60	1.30	1.34
5	B	402	SAH	CA-N	2.48	1.52	1.47
5	F	406	SAH	C8-N7	-2.38	1.30	1.34
5	D	404	SAH	C5'-C4'	2.34	1.61	1.52
5	E	405	SAH	C5'-C4'	2.33	1.61	1.52
5	D	404	SAH	C2'-C3'	2.30	1.59	1.53
5	A	401	SAH	O4'-C4'	-2.26	1.40	1.45
5	C	403	SAH	C2'-C3'	2.24	1.59	1.53
5	A	401	SAH	C5'-C4'	2.13	1.61	1.52
5	A	401	SAH	CA-N	2.12	1.51	1.47
5	C	403	SAH	C5'-C4'	2.10	1.60	1.52
5	A	401	SAH	C2'-C3'	2.08	1.59	1.53

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	401	SAH	O4'-C1'-C2'	-7.98	95.27	106.93
5	B	402	SAH	O4'-C1'-C2'	-7.15	96.47	106.93
5	D	404	SAH	O4'-C1'-C2'	-6.90	96.84	106.93
5	C	403	SAH	O4'-C1'-C2'	-6.74	97.08	106.93
5	F	406	SAH	O4'-C1'-C2'	-6.58	97.31	106.93
5	E	405	SAH	O4'-C1'-C2'	-6.23	97.82	106.93
5	F	406	SAH	CB-CG-SD	-3.55	105.34	113.31
5	C	403	SAH	N3-C2-N1	-3.44	123.30	128.68
5	F	406	SAH	N3-C2-N1	-3.44	123.31	128.68
5	A	401	SAH	CB-CG-SD	-3.43	105.62	113.31
5	E	405	SAH	N3-C2-N1	-3.41	123.35	128.68
5	D	404	SAH	N3-C2-N1	-3.36	123.42	128.68
5	D	404	SAH	CB-CG-SD	-3.35	105.79	113.31
5	E	405	SAH	CB-CG-SD	-3.33	105.84	113.31
5	F	406	SAH	C1'-N9-C4	-3.18	121.05	126.64
5	A	401	SAH	N3-C2-N1	-3.04	123.93	128.68
5	B	402	SAH	N3-C2-N1	-3.02	123.95	128.68
5	C	403	SAH	CB-CG-SD	-2.96	106.67	113.31
5	D	404	SAH	C2-N1-C6	2.86	123.64	118.75
5	F	406	SAH	C2-N1-C6	2.84	123.61	118.75
5	C	403	SAH	C2-N1-C6	2.83	123.60	118.75
5	B	402	SAH	C5-C6-N1	-2.81	113.98	120.35
5	E	405	SAH	C1'-N9-C4	-2.71	121.87	126.64
5	D	404	SAH	O4'-C4'-C5'	-2.69	101.91	108.83
5	B	402	SAH	O4'-C4'-C5'	-2.67	101.96	108.83
5	A	401	SAH	C5-C6-N1	-2.67	114.30	120.35
5	D	404	SAH	C5-C6-N6	2.64	124.36	120.35
5	B	402	SAH	C2-N1-C6	2.64	123.26	118.75
5	E	405	SAH	C2-N1-C6	2.63	123.25	118.75
5	C	403	SAH	O4'-C4'-C5'	-2.56	102.23	108.83
5	D	404	SAH	C5-C6-N1	-2.53	114.61	120.35
5	C	403	SAH	C5-C6-N1	-2.49	114.70	120.35
5	F	406	SAH	C5-C6-N1	-2.46	114.78	120.35
5	B	402	SAH	CB-CG-SD	-2.45	107.82	113.31
5	E	405	SAH	C5-C6-N6	2.40	124.00	120.35
5	A	401	SAH	C2-N1-C6	2.38	122.83	118.75
5	B	402	SAH	C5-C6-N6	2.38	123.97	120.35
5	D	404	SAH	C1'-N9-C4	-2.34	122.53	126.64
5	E	405	SAH	C5-C6-N1	-2.34	115.05	120.35
5	F	406	SAH	C5-C6-N6	2.31	123.86	120.35
5	A	401	SAH	O4'-C4'-C5'	-2.29	102.93	108.83
5	C	403	SAH	C1'-N9-C4	-2.28	122.63	126.64
5	A	401	SAH	N6-C6-N1	2.10	122.94	118.57

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	405	SAH	CA-CB-CG-SD

There are no ring outliers.

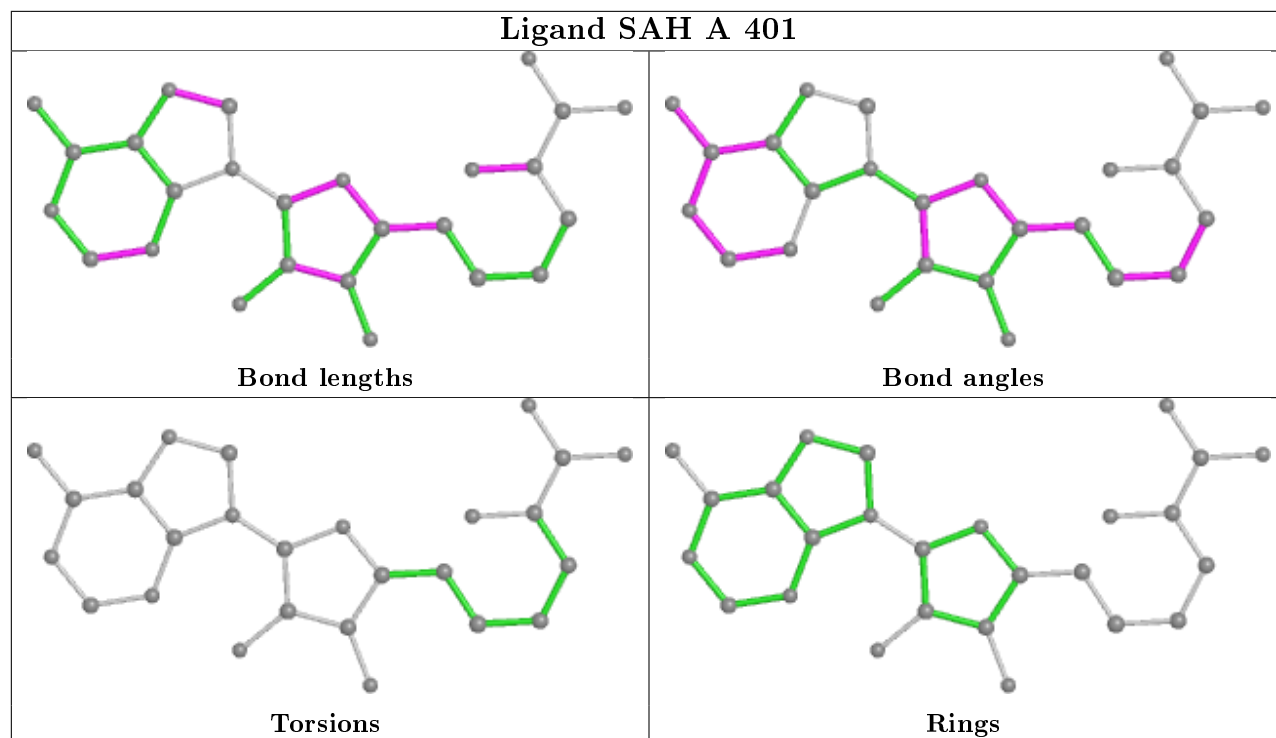
3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	404	SAH	1	0
5	B	402	SAH	1	0
5	F	406	SAH	7	0

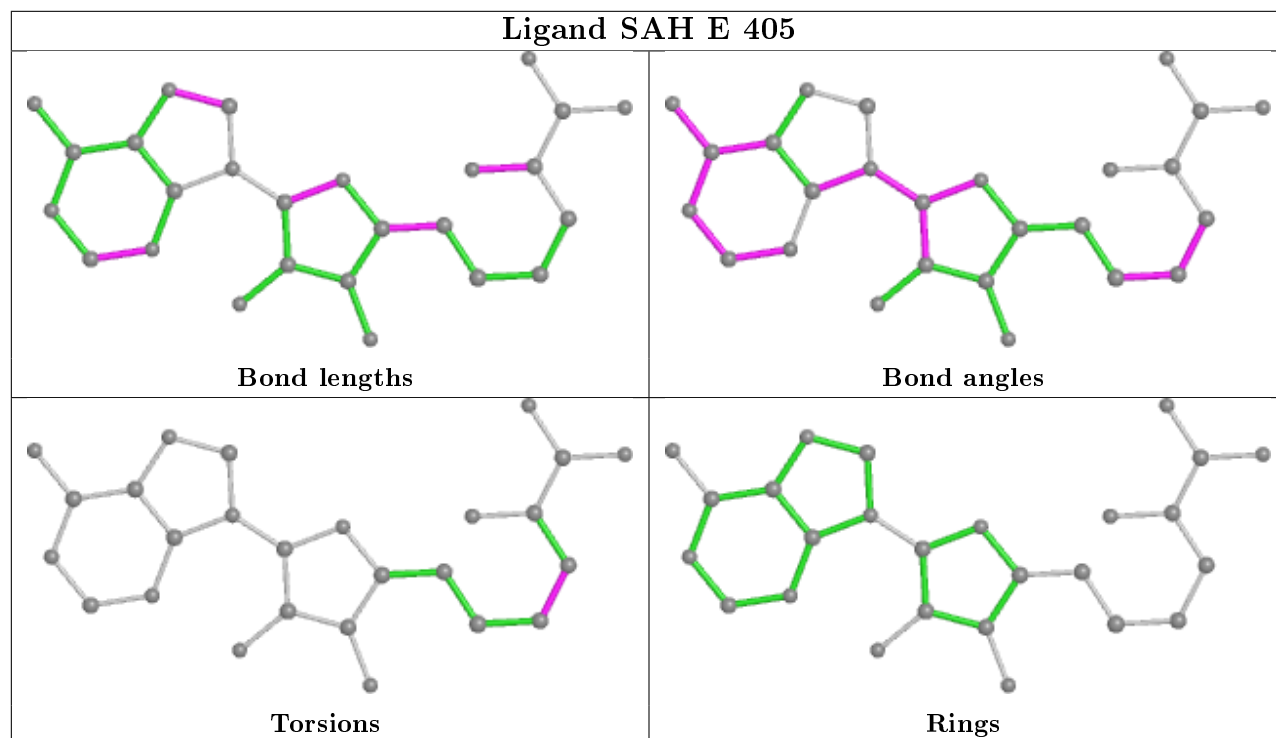
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



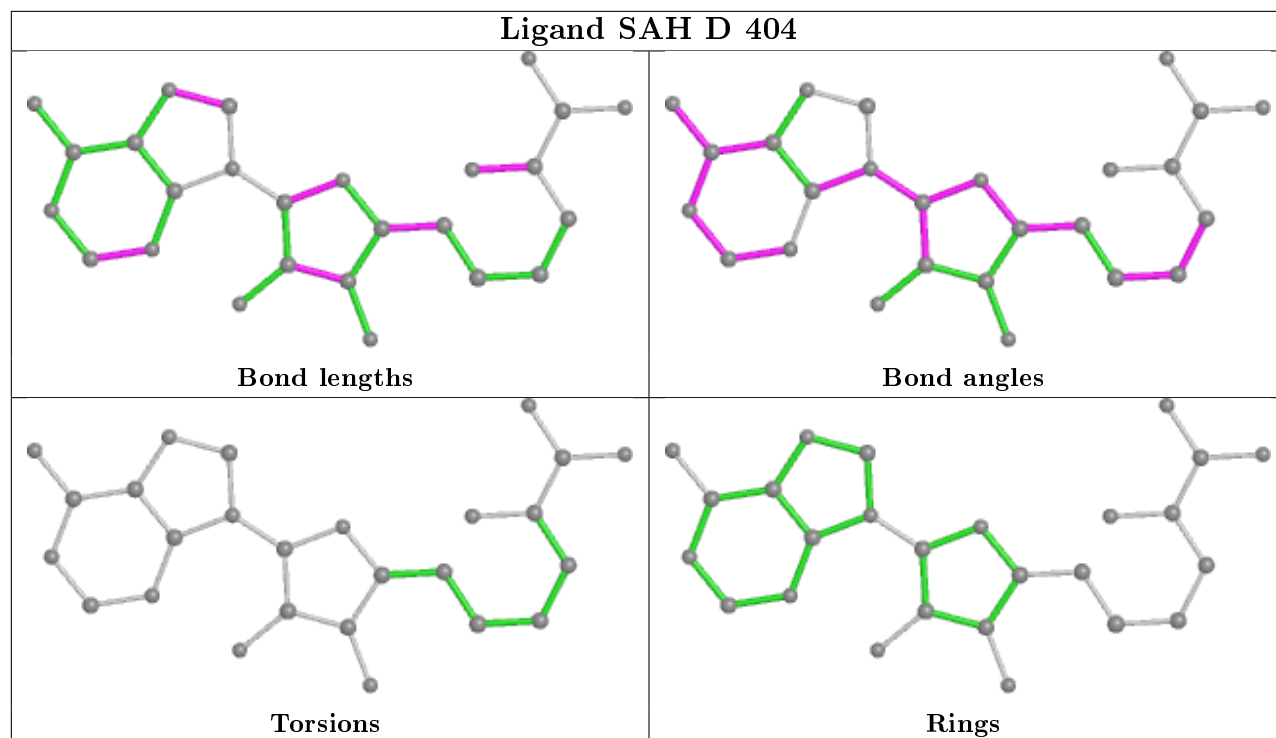
## Ligand SAH A 401



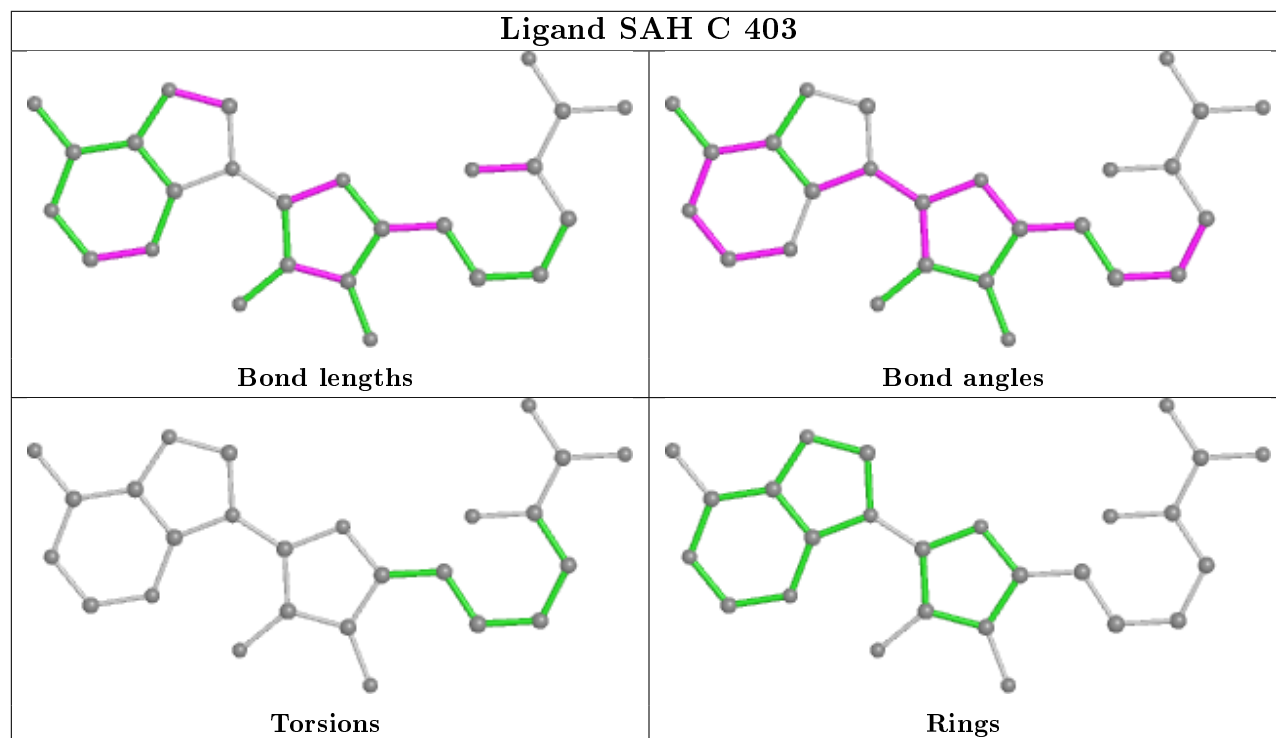
## Ligand SAH E 405

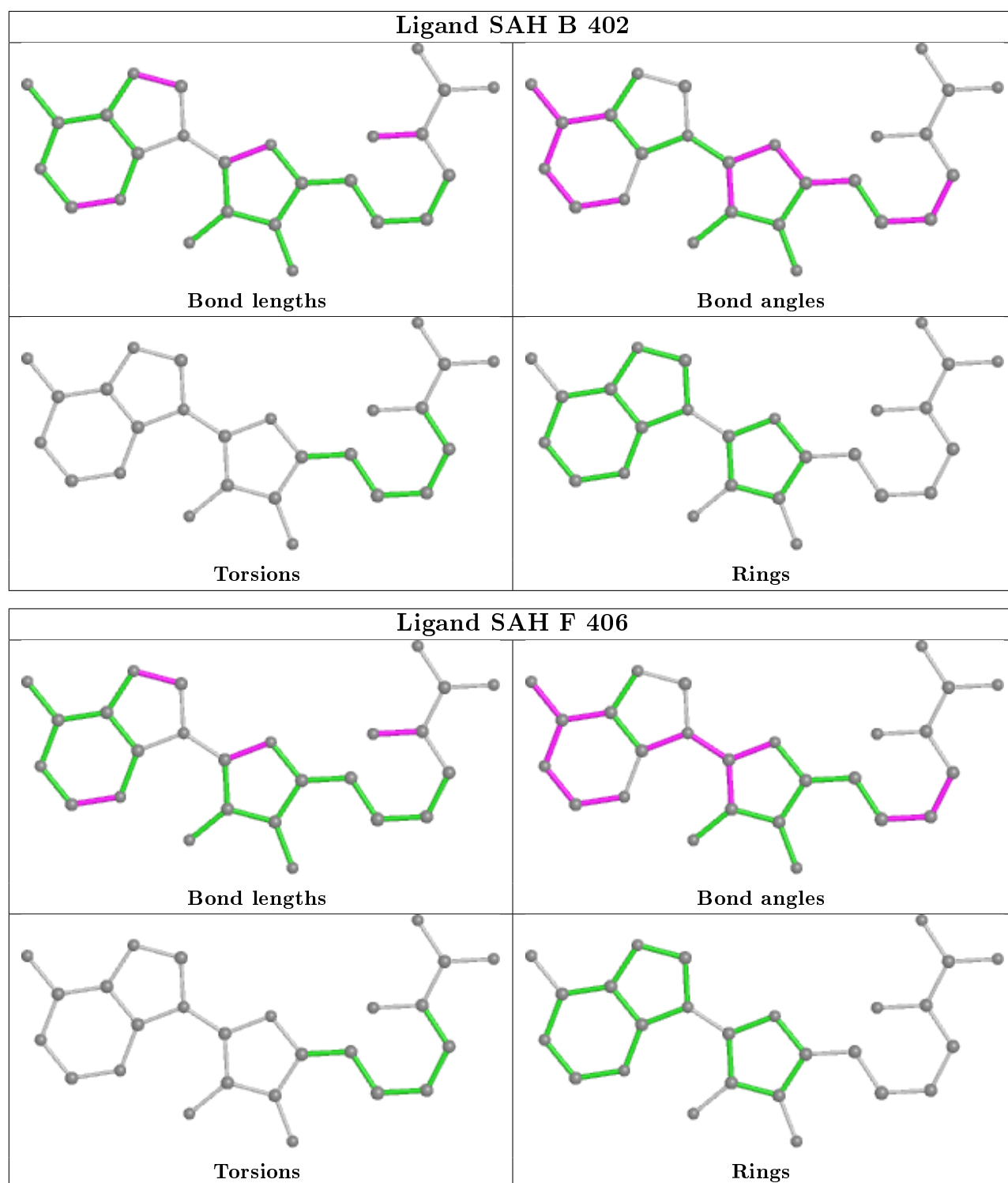


## Ligand SAH D 404



## Ligand SAH C 403





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.