Full wwPDB X-ray Structure Validation Report (i)

May 25, 2020 – 12:53 pm BST

PDB ID	:	6I7P
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

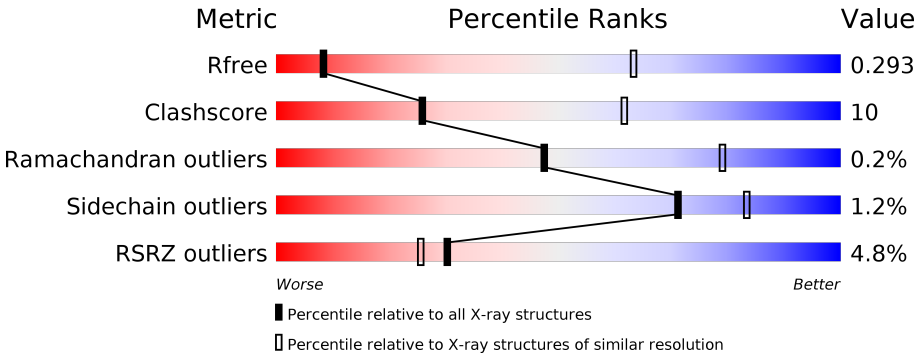
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance

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}	130704	1039 (4.26-3.70)
Clashscore	141614	1099 (4.26-3.70)
Ramachandran outliers	138981	1061 (4.26-3.70)
Sidechain outliers	138945	1053 (4.26-3.70)
RSRZ outliers	127900	1021 (4.30-3.66)

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	6% 73% 24%
1	B	914	7% 75% 21%
1	C	914	7% 76% 21%
1	D	914	2% 72% 25%
1	E	914	2% 72% 24%
1	F	914	4% 73% 23%

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

Continued on next page...

Continued from previous page...

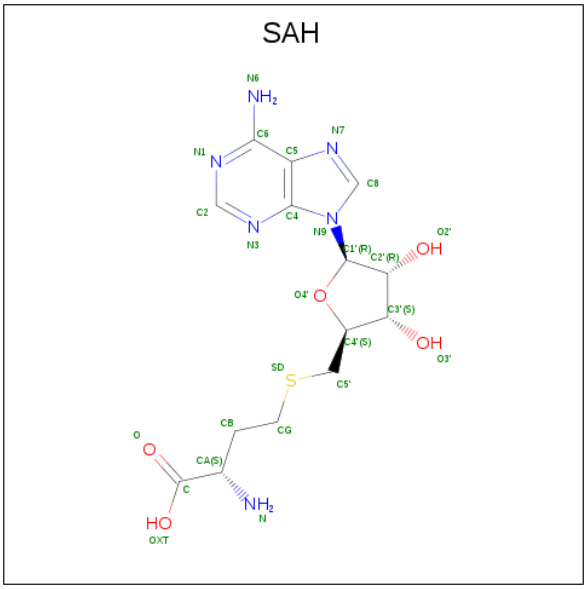
Chain	Residue	Modelled	Actual	Comment	Reference
B	909	HIS	-	expression tag	UNP A0A1B2ZC85
B	910	HIS	-	expression tag	UNP A0A1B2ZC85
B	911	HIS	-	expression tag	UNP A0A1B2ZC85
B	912	HIS	-	expression tag	UNP A0A1B2ZC85
B	913	HIS	-	expression tag	UNP A0A1B2ZC85
C	0	MET	-	initiating methionine	UNP A0A1B2ZC85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

Continued on next page...

Continued from previous page...

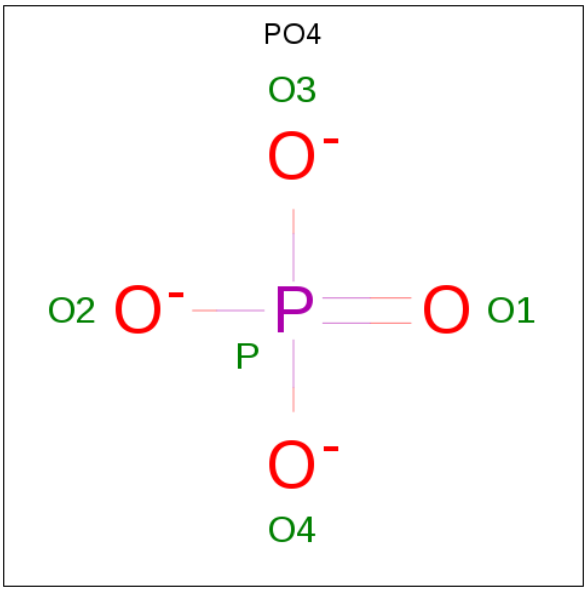
Chain	Residue	Modelled	Actual	Comment	Reference
F	907	SER	-	expression tag	UNP A0A1B2ZC85
F	908	HIS	-	expression tag	UNP A0A1B2ZC85
F	909	HIS	-	expression tag	UNP A0A1B2ZC85
F	910	HIS	-	expression tag	UNP A0A1B2ZC85
F	911	HIS	-	expression tag	UNP A0A1B2ZC85
F	912	HIS	-	expression tag	UNP A0A1B2ZC85
F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

Continued on next page...

Continued from previous page...

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).

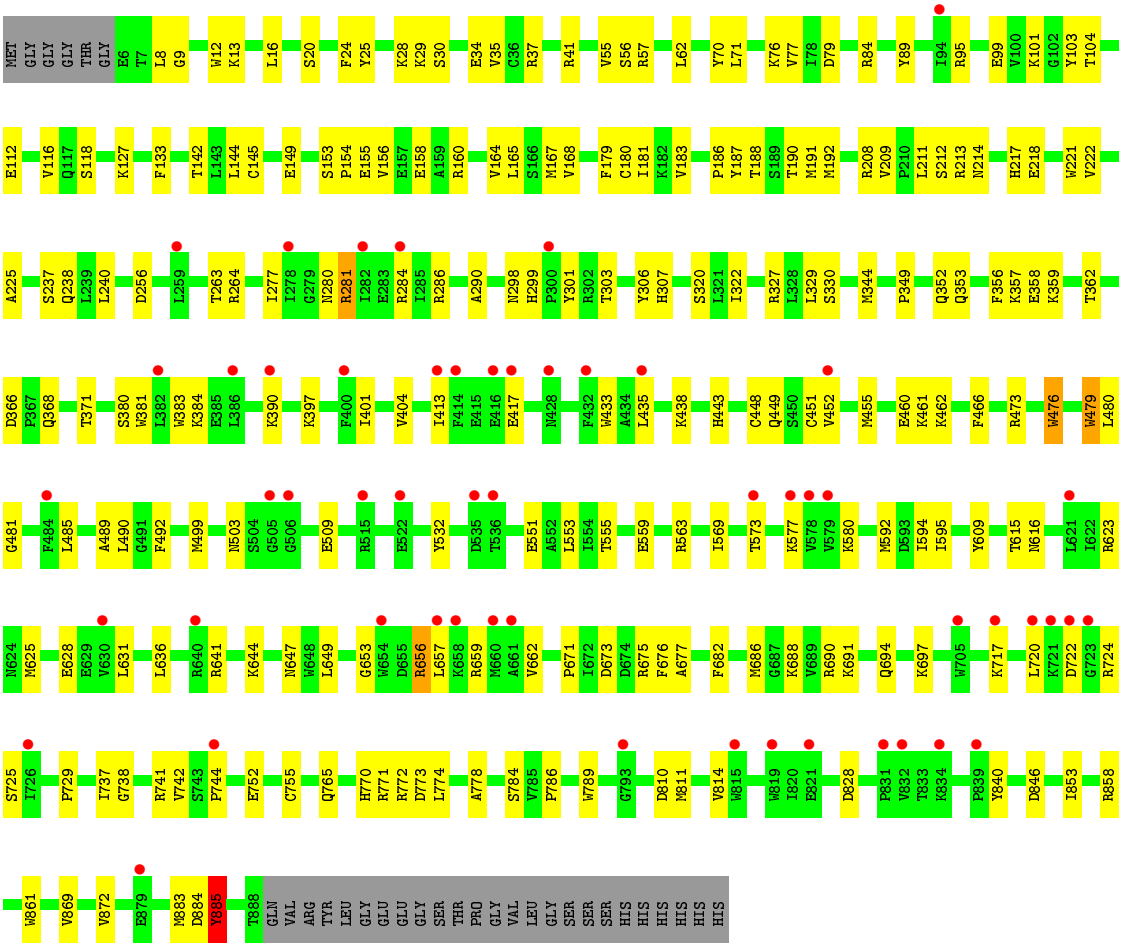
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	2	Total Zn 2 2	0	0
4	E	2	Total Zn 2 2	0	0
4	B	1	Total Zn 1 1	0	0
4	C	2	Total Zn 2 2	0	0
4	A	2	Total Zn 2 2	0	0
4	F	2	Total Zn 2 2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

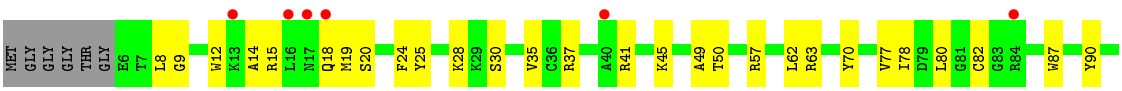
- Molecule 1: NS5

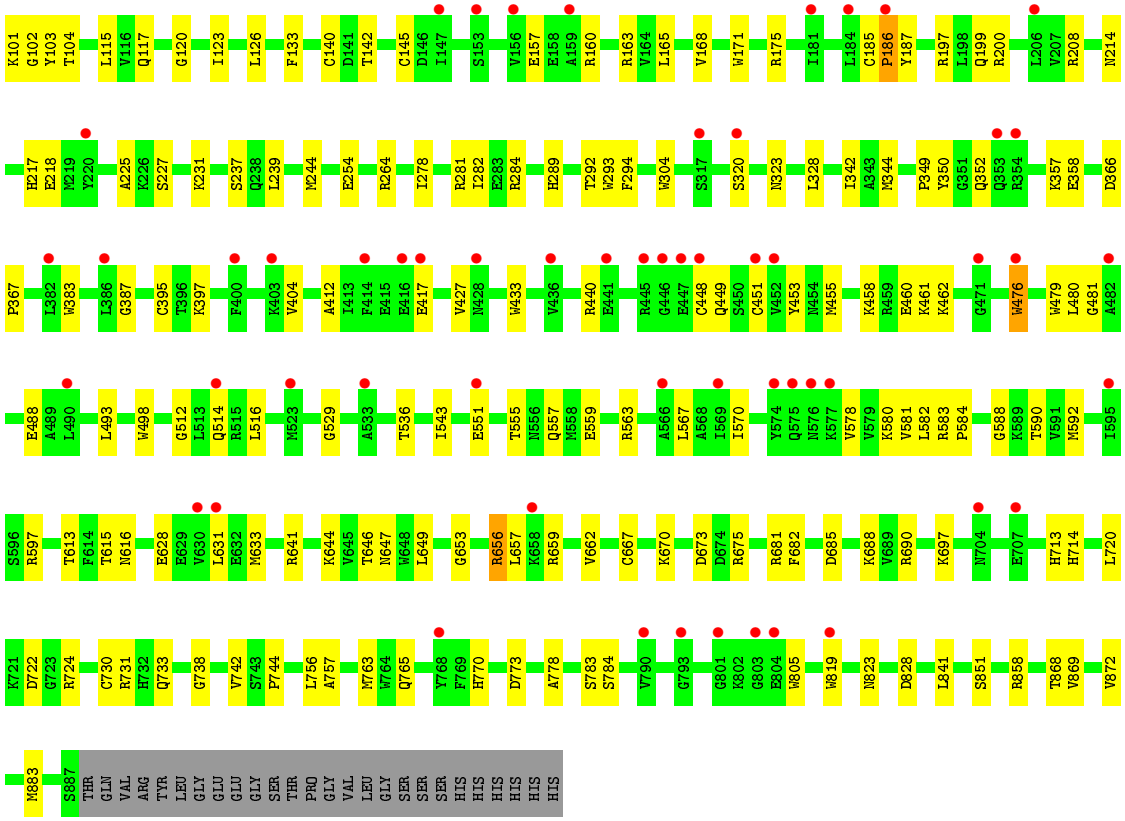
Chain A:



- Molecule 1: NS5

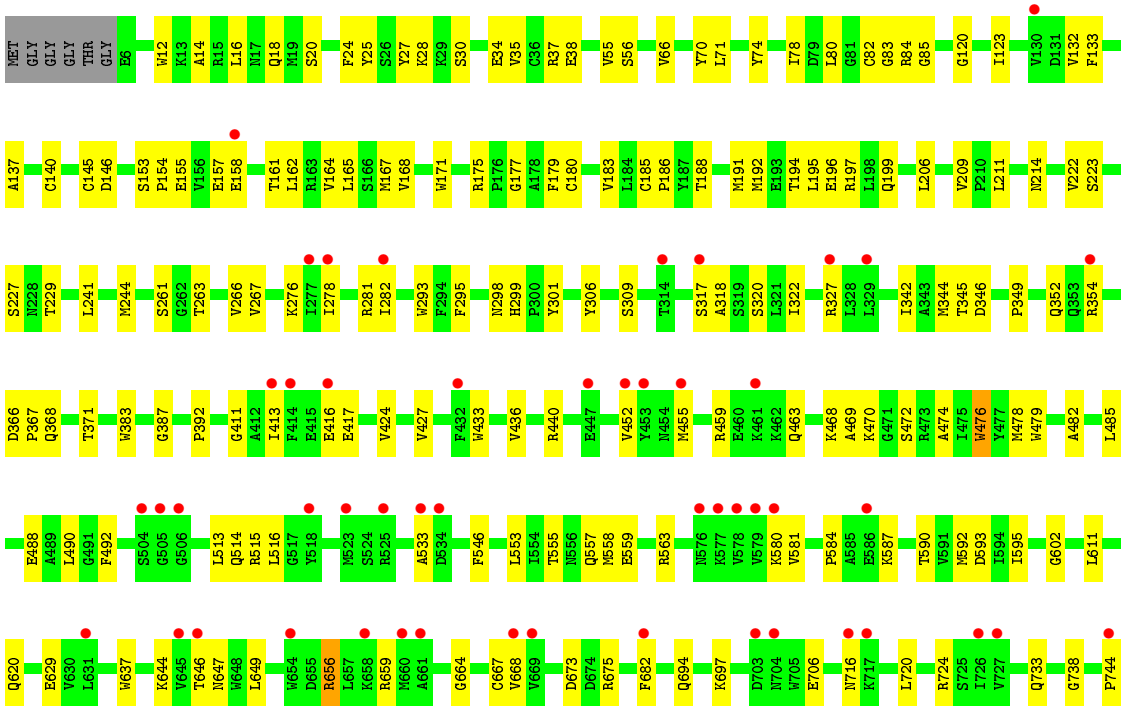
Chain B:

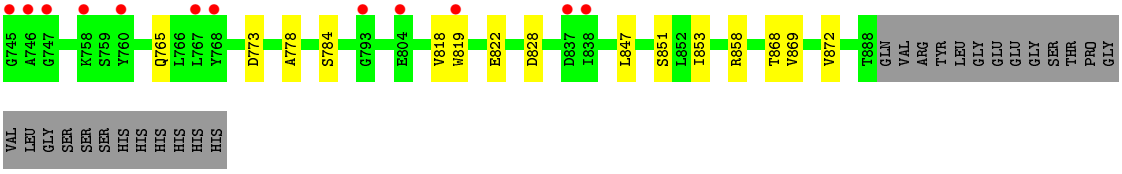




• Molecule 1: NS5

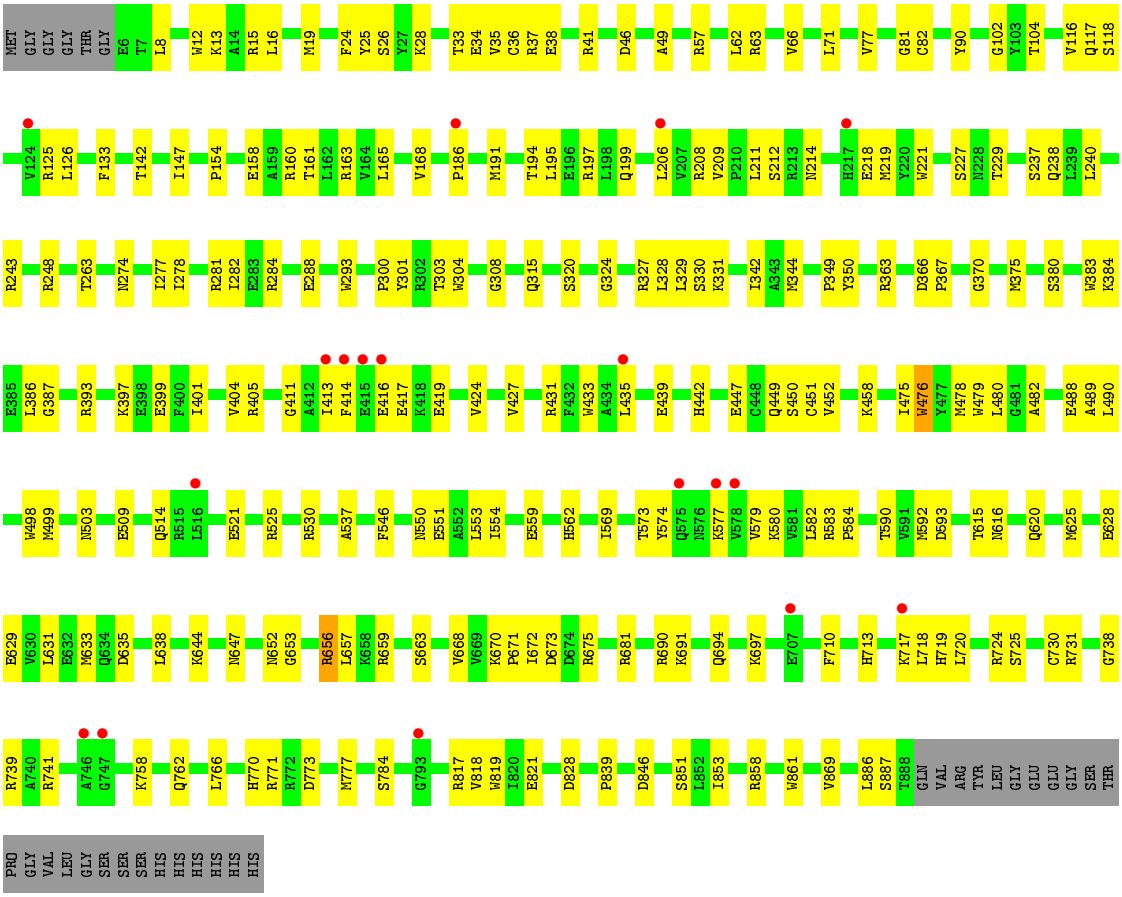
Chain C:





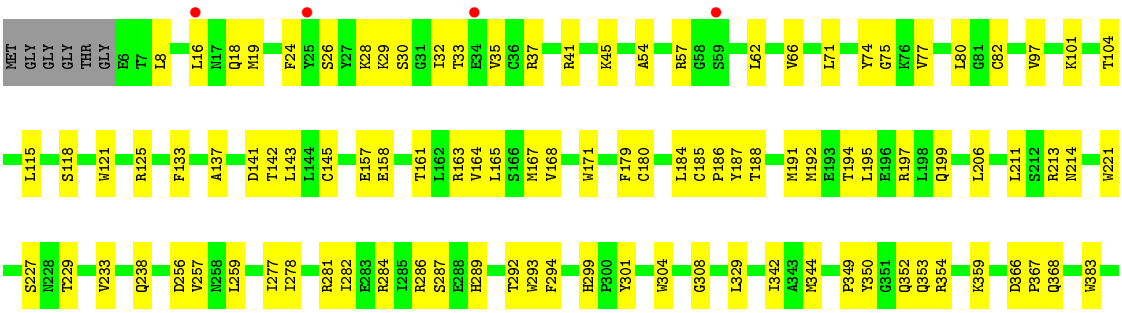
• Molecule 1: NS5

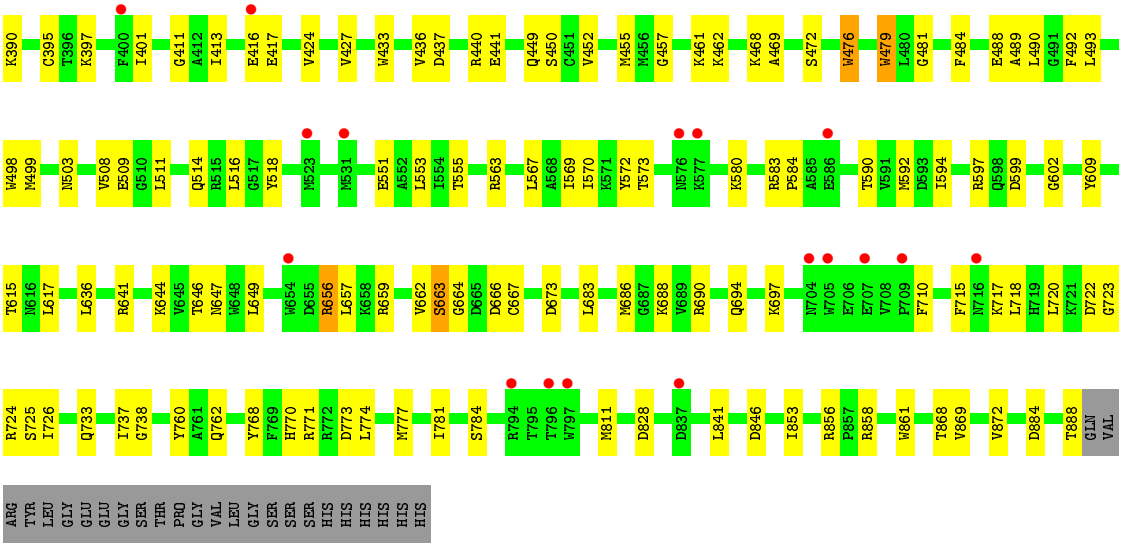
Chain D:



• Molecule 1: NS5

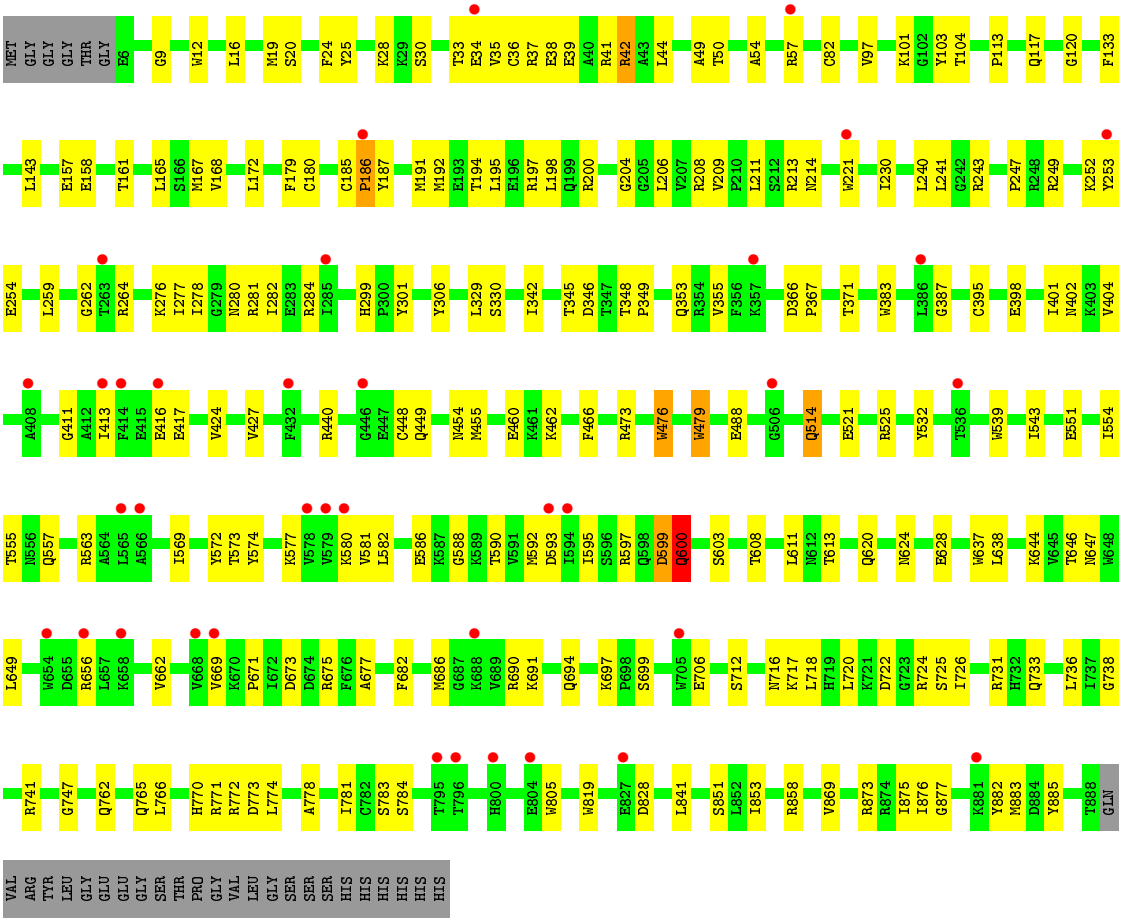
Chain E:





- Molecule 1: NS5

Chain F:



4 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 – 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
$< I/\sigma(I) >$ [1]	1.69 (at 4.00Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.280 , 0.280 0.279 , 0.293	Depositor DCC
R_{free} test set	6430 reflections (5.00%)	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 , 63.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.28$, $< L^2 > = 0.11$	Xtriage
Estimated twinning fraction	0.217 for k,h,-l	Xtriage
F_o,F_c correlation	0.77	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.*

[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	0.39	2/7262 (0.0%)	0.58	3/9813 (0.0%)
1	B	0.36	0/7255	0.54	0/9803
1	C	0.37	0/7262	0.55	0/9813
1	D	0.46	3/7262 (0.0%)	0.59	1/9813 (0.0%)
1	E	0.40	1/7262 (0.0%)	0.58	2/9813 (0.0%)
1	F	0.42	4/7262 (0.1%)	0.61	5/9813 (0.1%)
All	All	0.40	10/43565 (0.0%)	0.58	11/58868 (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

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	663	SER	C-N	-14.88	1.06	1.33
1	D	886	LEU	C-N	13.81	1.65	1.34
1	F	875	ILE	C-N	9.58	1.56	1.34
1	A	884	ASP	C-N	8.66	1.53	1.34
1	D	887	SER	C-N	8.37	1.53	1.34
1	F	876	ILE	C-N	-8.29	1.18	1.33
1	F	599	ASP	C-N	-7.59	1.16	1.34
1	E	662	VAL	C-N	7.29	1.50	1.34
1	F	877	GLY	C-N	6.06	1.48	1.34
1	A	885	TYR	C-N	5.87	1.47	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	599	ASP	O-C-N	-13.97	100.35	122.70
1	A	885	TYR	O-C-N	-12.07	103.39	122.70
1	F	599	ASP	C-N-CA	11.24	149.80	121.70
1	F	599	ASP	CA-C-N	9.71	138.57	117.20
1	E	663	SER	O-C-N	7.79	136.44	123.20
1	E	663	SER	CA-C-N	-7.50	101.20	116.20
1	A	885	TYR	CA-C-N	6.65	131.83	117.20
1	F	600	GLN	CA-C-N	-6.10	103.78	117.20
1	A	211	LEU	CA-CB-CG	5.38	127.68	115.30
1	F	600	GLN	C-N-CA	-5.22	108.66	121.70
1	D	887	SER	CA-C-N	-5.03	106.14	117.20

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7097	0	6997	179	0
1	B	7090	0	6993	139	0
1	C	7097	0	6998	131	0
1	D	7097	0	6997	147	0
1	E	7097	0	6998	147	0
1	F	7097	0	6998	159	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	891	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 10.

All (891) 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:F:143:LEU:HD23	1:F:172:LEU:HD21	1.27	1.17
1:B:412:ALA:HA	1:B:417:GLU:OE1	1.45	1.16
1:A:359:LYS:NZ	1:A:473:ARG:CD	2.10	1.15
1:A:417:GLU:CB	1:A:479:TRP:CH2	2.33	1.11
1:A:479:TRP:HD1	1:A:481:GLY:N	1.49	1.10
1:F:143:LEU:HD23	1:F:172:LEU:CD2	1.80	1.10
1:A:359:LYS:NZ	1:A:473:ARG:HD3	1.67	1.09
1:F:36:CYS:SG	1:F:253:TYR:HE2	1.78	1.06
1:B:479:TRP:HD1	1:B:481:GLY:N	1.54	1.05
1:D:35:VAL:HG23	1:D:37:ARG:HG2	1.33	1.05
1:A:417:GLU:OE1	1:A:479:TRP:CZ2	2.09	1.04
1:A:479:TRP:CD1	1:A:481:GLY:N	2.26	0.97
1:F:36:CYS:HG	1:F:253:TYR:HE2	1.14	0.95
1:F:460:GLU:OE1	1:F:462:LYS:HE3	1.64	0.95
1:C:78:ILE:HD12	1:C:140:CYS:HB3	1.49	0.93
1:A:417:GLU:HB2	1:A:479:TRP:HH2	1.23	0.93
1:F:460:GLU:OE1	1:F:462:LYS:CE	2.17	0.93
1:A:30:SER:O	1:A:214:ASN:ND2	2.05	0.89
1:B:35:VAL:HG23	1:B:37:ARG:HG2	1.54	0.88
1:B:724:ARG:HD3	1:B:828:ASP:HB3	1.55	0.87
1:B:633:MET:HE3	1:B:681:ARG:HD3	1.54	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:656:ARG:HA	1:D:659:ARG:HD2	1.54	0.87
1:A:417:GLU:OE1	1:A:479:TRP:HZ2	1.58	0.86
1:F:36:CYS:SG	1:F:253:TYR:CE2	2.68	0.86
1:A:359:LYS:HZ2	1:A:473:ARG:CD	1.89	0.85
1:D:35:VAL:HG23	1:D:37:ARG:CG	2.07	0.85
1:E:609:TYR:HE1	1:E:663:SER:HG	1.20	0.85
1:A:417:GLU:CD	1:A:479:TRP:CZ2	2.51	0.84
1:A:359:LYS:HZ1	1:A:473:ARG:HD3	1.41	0.84
1:F:460:GLU:OE1	1:F:462:LYS:NZ	2.10	0.84
1:B:412:ALA:CA	1:B:417:GLU:OE1	2.25	0.83
1:A:359:LYS:HZ2	1:A:473:ARG:NE	1.76	0.83
1:D:633:MET:CE	1:D:681:ARG:CD	2.57	0.83
1:E:666:ASP:OD1	1:E:667:CYS:N	2.10	0.83
1:F:37:ARG:NH1	1:F:57:ARG:HD2	1.94	0.82
1:E:609:TYR:CE1	1:E:663:SER:OG	2.30	0.82
1:E:35:VAL:HG23	1:E:37:ARG:HG2	1.60	0.82
1:D:633:MET:HE3	1:D:681:ARG:HD3	1.61	0.81
1:E:609:TYR:HE1	1:E:663:SER:OG	1.62	0.81
1:B:633:MET:CE	1:B:681:ARG:CD	2.59	0.81
1:D:633:MET:HE1	1:D:681:ARG:NE	1.97	0.80
1:F:214:ASN:OD1	1:F:243:ARG:NH2	2.14	0.80
1:A:479:TRP:HD1	1:A:481:GLY:H	0.82	0.80
1:B:479:TRP:HD1	1:B:481:GLY:H	0.83	0.79
1:F:613:THR:HG23	1:F:662:VAL:HG12	1.64	0.79
1:B:342:ILE:HD12	1:B:738:GLY:HA3	1.65	0.78
1:F:460:GLU:CD	1:F:462:LYS:HE3	2.03	0.78
1:F:143:LEU:CD2	1:F:172:LEU:CD2	2.60	0.78
1:A:299:HIS:HB2	1:A:301:TYR:HD2	1.48	0.77
1:B:633:MET:HE1	1:B:681:ARG:CD	2.15	0.77
1:B:479:TRP:CD1	1:B:481:GLY:N	2.38	0.77
1:E:694:GLN:HB3	1:E:697:LYS:HB2	1.65	0.76
1:F:644:LYS:HA	1:F:647:ASN:HB2	1.68	0.76
1:E:35:VAL:CG2	1:E:37:ARG:HD3	2.16	0.76
1:A:359:LYS:NZ	1:A:473:ARG:CG	2.48	0.76
1:A:417:GLU:HB2	1:A:479:TRP:CZ3	2.20	0.75
1:E:411:GLY:HA3	1:E:479:TRP:HA	1.67	0.75
1:F:784:SER:HB3	1:F:869:VAL:HG13	1.67	0.75
1:B:417:GLU:HG3	1:B:479:TRP:CE2	2.08	0.75
1:D:773:ASP:OD1	1:D:858:ARG:NE	2.19	0.74
1:B:633:MET:CE	1:B:681:ARG:HD3	2.16	0.74
1:C:35:VAL:HG23	1:C:37:ARG:HG2	1.68	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:395:CYS:HB2	1:E:488:GLU:HA	1.68	0.74
1:A:784:SER:HB3	1:A:869:VAL:HG13	1.68	0.74
1:A:359:LYS:NZ	1:A:473:ARG:NE	2.33	0.74
1:E:354:ARG:NH2	1:E:469:ALA:O	2.20	0.74
1:E:437:ASP:OD1	1:E:440:ARG:NH1	2.21	0.74
1:F:577:LYS:NZ	1:F:600:GLN:O	2.18	0.74
1:C:784:SER:HB3	1:C:869:VAL:HG13	1.69	0.73
1:B:395:CYS:HB2	1:B:488:GLU:HA	1.69	0.72
1:D:633:MET:HE1	1:D:681:ARG:CD	2.19	0.72
1:B:417:GLU:CD	1:B:417:GLU:O	2.27	0.72
1:B:175:ARG:NH1	1:C:175:ARG:O	2.23	0.72
1:E:35:VAL:HG23	1:E:37:ARG:CG	2.19	0.72
1:F:30:SER:O	1:F:214:ASN:ND2	2.23	0.72
1:E:194:THR:HG23	1:E:197:ARG:HH22	1.55	0.71
1:E:724:ARG:HD3	1:E:828:ASP:HB3	1.72	0.71
1:F:38:GLU:HA	1:F:41:ARG:HB2	1.70	0.71
1:B:417:GLU:HG3	1:B:479:TRP:CD2	2.24	0.71
1:B:417:GLU:HG3	1:B:479:TRP:CE3	2.16	0.70
1:D:419:GLU:OE2	1:D:431:ARG:NH2	2.23	0.70
1:A:299:HIS:HB2	1:A:301:TYR:CD2	2.27	0.70
1:D:574:TYR:O	1:D:577:LYS:NZ	2.20	0.70
1:C:165:LEU:HA	1:C:168:VAL:HG22	1.72	0.70
1:A:329:LEU:O	1:A:861:TRP:NE1	2.24	0.70
1:F:165:LEU:HA	1:F:168:VAL:HG22	1.74	0.70
1:F:773:ASP:OD1	1:F:858:ARG:NE	2.24	0.69
1:B:720:LEU:HD12	1:B:724:ARG:HB2	1.74	0.69
1:D:633:MET:CE	1:D:681:ARG:HD3	2.20	0.69
1:F:395:CYS:HB2	1:F:488:GLU:HA	1.75	0.69
1:F:301:TYR:OH	1:F:593:ASP:OD2	2.10	0.69
1:A:153:SER:HB2	1:A:155:GLU:OE1	1.92	0.69
1:A:359:LYS:HZ3	1:A:473:ARG:CD	2.03	0.68
1:C:694:GLN:HB3	1:C:697:LYS:HB2	1.75	0.68
1:E:35:VAL:HG23	1:E:37:ARG:CD	2.23	0.68
1:A:359:LYS:HZ3	1:A:473:ARG:HD3	1.53	0.68
1:E:784:SER:HB3	1:E:869:VAL:HG13	1.76	0.68
1:A:359:LYS:NZ	1:A:473:ARG:HG2	2.08	0.68
1:C:317:SER:O	1:C:459:ARG:NH1	2.27	0.68
1:A:79:ASP:HA	1:A:144:LEU:HB2	1.76	0.67
1:A:644:LYS:HA	1:A:647:ASN:HB2	1.77	0.67
1:F:143:LEU:CD2	1:F:172:LEU:HD23	2.24	0.66
1:F:342:ILE:HD12	1:F:738:GLY:HA3	1.76	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:35:VAL:HG21	1:E:37:ARG:HD3	1.77	0.66
1:C:773:ASP:OD1	1:C:858:ARG:NE	2.26	0.66
1:C:78:ILE:HD13	1:C:171:TRP:HZ3	1.61	0.66
1:C:195:LEU:HD22	1:C:206:LEU:HD21	1.77	0.66
1:D:208:ARG:NH1	1:D:218:GLU:O	2.29	0.66
1:E:165:LEU:HA	1:E:168:VAL:HG22	1.78	0.66
1:D:569:ILE:O	1:D:573:THR:HB	1.96	0.66
1:A:720:LEU:HD12	1:A:724:ARG:HB2	1.78	0.65
1:F:455:MET:HB2	1:F:476:TRP:HB3	1.79	0.65
1:F:209:VAL:HG12	1:F:211:LEU:H	1.62	0.65
1:A:359:LYS:HZ3	1:A:473:ARG:CG	2.08	0.65
1:C:158:GLU:HG3	1:C:191:MET:HG2	1.79	0.65
1:E:194:THR:HG23	1:E:197:ARG:NH2	2.10	0.65
1:E:342:ILE:HD12	1:E:738:GLY:HA3	1.79	0.65
1:D:329:LEU:O	1:D:861:TRP:NE1	2.30	0.65
1:D:380:SER:HB3	1:D:384:LYS:HE2	1.77	0.65
1:A:28:LYS:NZ	1:B:45:LYS:HE2	2.12	0.65
1:D:724:ARG:HD3	1:D:828:ASP:HB3	1.78	0.64
1:F:454:ASN:O	1:F:476:TRP:HA	1.97	0.64
1:F:569:ILE:O	1:F:573:THR:HB	1.96	0.64
1:F:34:GLU:HG2	1:F:35:VAL:H	1.63	0.64
1:E:644:LYS:HA	1:E:647:ASN:HB2	1.80	0.64
1:D:694:GLN:HB3	1:D:697:LYS:HB2	1.80	0.64
1:A:773:ASP:OD1	1:A:858:ARG:NE	2.26	0.63
1:F:440:ARG:NH2	1:F:488:GLU:OE1	2.30	0.63
1:A:694:GLN:HB3	1:A:697:LYS:HB2	1.80	0.63
1:C:306:TYR:HA	1:C:595:ILE:HG22	1.81	0.63
1:F:720:LEU:HD12	1:F:724:ARG:HB2	1.80	0.63
1:F:455:MET:HB3	1:F:581:VAL:HG12	1.78	0.63
1:B:412:ALA:HA	1:B:417:GLU:CD	2.18	0.63
1:D:499:MET:HB2	1:D:509:GLU:HG3	1.81	0.63
1:A:641:ARG:HB2	1:A:644:LYS:HE3	1.81	0.63
1:F:42:ARG:HG2	1:F:42:ARG:HH21	1.62	0.63
1:F:691:LYS:NZ	3:F:1003:PO4:O3	2.32	0.62
1:B:543:ILE:HD13	1:B:688:LYS:HE3	1.81	0.62
1:E:30:SER:O	1:E:214:ASN:ND2	2.33	0.62
1:E:286:ARG:HG3	1:E:293:TRP:CD1	2.34	0.62
1:D:401:ILE:O	1:D:404:VAL:HG12	1.99	0.62
1:D:713:HIS:NE2	1:D:731:ARG:HD2	2.15	0.61
1:A:165:LEU:HA	1:A:168:VAL:HG22	1.83	0.61
1:A:623:ARG:NH2	1:A:676:PHE:O	2.27	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:603:SER:HA	1:F:608:THR:HG21	1.81	0.61
1:E:690:ARG:NH2	1:E:697:LYS:O	2.30	0.61
1:B:49:ALA:HB1	1:B:117:GLN:N	2.16	0.61
1:F:12:TRP:HB2	1:F:241:LEU:HG	1.82	0.61
1:F:42:ARG:HH21	1:F:42:ARG:CG	2.14	0.60
1:F:284:ARG:HH11	1:F:449:GLN:HB3	1.65	0.60
1:A:479:TRP:CD1	1:A:480:LEU:N	2.69	0.60
1:C:706:GLU:OE1	1:C:716:ASN:ND2	2.31	0.60
1:D:580:LYS:HG2	1:D:592:MET:SD	2.41	0.60
1:E:888:THR:OG1	1:E:888:THR:O	2.16	0.60
1:F:186:PRO:HD2	1:F:187:TYR:HD1	1.66	0.60
1:C:327:ARG:HH22	1:D:160:ARG:HH22	1.49	0.60
1:B:455:MET:HB3	1:B:581:VAL:HG22	1.84	0.60
1:D:82:CYS:SG	1:D:104:THR:HB	2.41	0.60
1:E:293:TRP:CZ2	1:E:308:GLY:HA3	2.37	0.60
1:F:299:HIS:HB2	1:F:301:TYR:CD2	2.37	0.60
1:A:417:GLU:HG3	1:A:417:GLU:O	2.02	0.59
1:C:157:GLU:HB3	1:C:185:CYS:HB2	1.84	0.59
1:A:417:GLU:CB	1:A:479:TRP:CZ3	2.82	0.59
1:E:569:ILE:O	1:E:573:THR:HB	2.02	0.59
1:A:209:VAL:O	1:A:212:SER:OG	2.20	0.59
1:F:455:MET:SD	1:F:581:VAL:CG1	2.90	0.59
1:A:686:MET:O	1:A:688:LYS:NZ	2.35	0.59
1:D:628:GLU:HA	1:D:675:ARG:NH2	2.17	0.59
1:E:180:CYS:HA	1:E:221:TRP:O	2.02	0.59
1:E:720:LEU:HD12	1:E:724:ARG:HB2	1.84	0.59
1:C:209:VAL:HG12	1:C:211:LEU:H	1.68	0.59
1:A:417:GLU:CG	1:A:479:TRP:CH2	2.85	0.59
1:D:41:ARG:HH22	1:D:57:ARG:NH2	2.00	0.58
1:E:666:ASP:OD2	1:E:710:PHE:HA	2.03	0.58
1:D:209:VAL:HG23	1:D:212:SER:OG	2.04	0.58
1:E:33:THR:HB	1:E:211:LEU:HD23	1.84	0.58
1:A:70:TYR:HB3	1:A:222:VAL:HG21	1.86	0.58
1:A:417:GLU:CG	1:A:479:TRP:CZ2	2.86	0.58
1:C:724:ARG:HD3	1:C:828:ASP:HB3	1.85	0.58
1:F:731:ARG:HD3	1:F:736:LEU:HD21	1.85	0.58
1:F:770:HIS:O	1:F:841:LEU:N	2.27	0.58
1:B:633:MET:HE1	1:B:681:ARG:NE	2.19	0.58
1:C:383:TRP:CD1	1:C:553:LEU:HB2	2.39	0.58
1:E:455:MET:HB2	1:E:476:TRP:HB3	1.86	0.58
1:F:306:TYR:HA	1:F:595:ILE:HG22	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:730:CYS:HB2	1:B:770:HIS:HE1	1.68	0.58
1:B:784:SER:HB3	1:B:869:VAL:HG13	1.86	0.58
1:A:353:GLN:HA	1:A:356:PHE:HB3	1.85	0.57
1:E:188:THR:O	1:E:192:MET:HG2	2.03	0.57
1:A:352:GLN:HE22	1:A:455:MET:HG2	1.69	0.57
1:E:413:ILE:HD13	1:E:452:VAL:HB	1.86	0.57
1:A:209:VAL:HG23	1:A:212:SER:OG	2.05	0.57
1:A:70:TYR:CD1	1:A:225:ALA:HB2	2.40	0.57
1:B:529:GLY:O	1:B:670:LYS:NZ	2.28	0.57
1:D:644:LYS:HA	1:D:647:ASN:HB2	1.85	0.57
1:A:551:GLU:OE2	1:A:615:THR:OG1	2.23	0.57
1:A:180:CYS:HA	1:A:221:TRP:O	2.04	0.57
1:B:175:ARG:O	1:C:175:ARG:NH1	2.34	0.57
1:A:217:HIS:NE2	1:A:237:SER:OG	2.33	0.57
1:C:20:SER:O	1:C:24:PHE:HB2	2.05	0.57
1:D:77:VAL:HG22	1:D:142:THR:HB	1.87	0.57
1:E:476:TRP:N	1:E:476:TRP:CD1	2.72	0.56
1:A:76:LYS:HE3	1:A:99:GLU:OE1	2.06	0.56
1:B:82:CYS:SG	1:B:104:THR:HB	2.46	0.56
1:B:157:GLU:HB3	1:B:185:CYS:HB2	1.88	0.56
1:D:165:LEU:HA	1:D:168:VAL:HG22	1.86	0.56
1:E:289:HIS:O	1:E:293:TRP:HB2	2.05	0.56
1:C:206:LEU:HD13	1:C:229:THR:HG22	1.86	0.56
1:E:551:GLU:OE2	1:E:615:THR:OG1	2.23	0.56
1:C:349:PRO:HG2	1:C:590:THR:HG21	1.86	0.56
1:D:690:ARG:NH2	1:D:697:LYS:O	2.33	0.56
1:A:41:ARG:HH12	1:A:57:ARG:HH21	1.53	0.56
1:C:555:THR:O	1:C:563:ARG:HD3	2.05	0.56
1:D:161:THR:O	1:D:165:LEU:HG	2.06	0.56
1:A:77:VAL:HG22	1:A:142:THR:HB	1.88	0.56
1:D:439:GLU:OE1	1:D:449:GLN:HB2	2.06	0.56
1:F:35:VAL:HG12	1:F:254:GLU:O	2.05	0.56
1:F:353:GLN:NE2	1:F:582:LEU:O	2.38	0.56
1:D:327:ARG:HH12	1:D:331:LYS:NZ	2.04	0.56
1:F:383:TRP:CE3	1:F:554:ILE:HD13	2.40	0.56
1:B:773:ASP:OD1	1:B:858:ARG:NE	2.37	0.56
1:E:199:GLN:NE2	1:E:227:SER:O	2.39	0.56
1:C:196:GLU:HG3	1:C:229:THR:OG1	2.06	0.55
1:D:730:CYS:HB2	1:D:770:HIS:HE1	1.71	0.55
1:E:344:MET:HE2	1:E:461:LYS:HG2	1.87	0.55
1:C:161:THR:HG21	1:C:183:VAL:HG13	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:784:SER:HB3	1:D:869:VAL:HG13	1.88	0.55
1:E:868:THR:O	1:E:872:VAL:HG23	2.07	0.55
1:A:186:PRO:HD2	1:A:217:HIS:HB3	1.87	0.55
1:A:322:ILE:HG21	1:A:327:ARG:HD2	1.88	0.55
1:A:476:TRP:CD1	1:A:476:TRP:N	2.74	0.55
1:A:738:GLY:O	1:A:742:VAL:HG23	2.06	0.55
1:A:786:PRO:HG2	1:A:789:TRP:CH2	2.41	0.55
1:C:765:GLN:HG3	1:C:778:ALA:HB1	1.87	0.55
1:D:370:GLY:HA3	1:D:635:ASP:O	2.07	0.55
1:A:359:LYS:HZ2	1:A:473:ARG:HG2	1.70	0.55
1:B:551:GLU:OE2	1:B:615:THR:OG1	2.22	0.55
1:A:724:ARG:HD3	1:A:828:ASP:HB3	1.88	0.55
1:E:390:LYS:HE2	1:E:503:ASN:HB2	1.89	0.55
1:B:744:PRO:HD3	1:B:756:LEU:HD22	1.89	0.55
1:A:208:ARG:NH2	1:A:213:ARG:O	2.40	0.55
1:D:393:ARG:NH2	1:D:399:GLU:OE2	2.39	0.55
1:F:476:TRP:HZ3	1:F:577:LYS:HD2	1.71	0.55
1:D:633:MET:CE	1:D:681:ARG:NE	2.69	0.55
1:E:580:LYS:HE2	1:E:592:MET:HG2	1.89	0.55
1:C:322:ILE:HG21	1:C:327:ARG:HD2	1.88	0.55
1:C:656:ARG:HA	1:C:659:ARG:HD2	1.89	0.55
1:D:278:ILE:O	1:D:282:ILE:HG12	2.07	0.54
1:D:672:ILE:O	1:D:673:ASP:OD1	2.24	0.54
1:A:286:ARG:O	1:A:290:ALA:HB2	2.07	0.54
1:A:359:LYS:HZ2	1:A:473:ARG:CG	2.15	0.54
1:C:455:MET:HB3	1:C:581:VAL:HG12	1.88	0.54
1:C:533:ALA:HB2	1:C:668:VAL:HG22	1.88	0.54
1:C:387:GLY:HA3	1:C:557:GLN:OE1	2.07	0.54
1:D:342:ILE:HD12	1:D:738:GLY:HA3	1.89	0.54
1:A:344:MET:HE2	1:A:461:LYS:HG2	1.89	0.54
1:B:580:LYS:HG2	1:B:592:MET:SD	2.47	0.54
1:C:515:ARG:NH2	1:C:822:GLU:O	2.41	0.54
1:D:82:CYS:O	2:D:1001:SAH:N	2.41	0.54
1:F:299:HIS:HB2	1:F:301:TYR:HD2	1.70	0.54
1:B:412:ALA:CB	1:B:417:GLU:OE1	2.55	0.54
1:D:206:LEU:HB3	1:D:219:MET:HE2	1.90	0.54
1:D:771:ARG:HH21	1:D:851:SER:HB2	1.73	0.54
1:E:143:LEU:O	1:E:179:PHE:HA	2.08	0.54
1:B:165:LEU:HA	1:B:168:VAL:HG22	1.88	0.54
1:E:75:GLY:H	1:E:97:VAL:HA	1.72	0.54
1:C:263:THR:OG1	1:C:298:ASN:O	2.22	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:713:HIS:NE2	1:B:731:ARG:HD2	2.22	0.54
1:C:476:TRP:N	1:C:476:TRP:CD1	2.76	0.54
1:A:413:ILE:HD13	1:A:452:VAL:HB	1.90	0.54
1:E:133:PHE:CE1	1:E:163:ARG:HG2	2.43	0.53
1:E:66:VAL:HG22	1:E:71:LEU:HB3	1.90	0.53
1:D:424:VAL:HA	1:D:427:VAL:HG22	1.90	0.53
1:E:41:ARG:HH21	1:E:57:ARG:HH11	1.55	0.53
1:F:724:ARG:HD3	1:F:828:ASP:HB3	1.89	0.53
1:C:188:THR:O	1:C:192:MET:HG2	2.09	0.53
1:D:81:GLY:HA3	1:D:147:ILE:HG12	1.90	0.53
1:F:771:ARG:HB2	1:F:774:LEU:HB2	1.90	0.53
1:C:78:ILE:CD1	1:C:140:CYS:HB3	2.32	0.53
1:E:609:TYR:OH	1:E:663:SER:OG	2.27	0.53
1:B:9:GLY:HA3	1:B:187:TYR:HB2	1.91	0.53
1:C:78:ILE:HD13	1:C:171:TRP:CZ3	2.42	0.53
1:A:628:GLU:HA	1:A:675:ARG:NH2	2.23	0.53
1:F:694:GLN:HB3	1:F:697:LYS:HB2	1.89	0.53
1:E:157:GLU:HB3	1:E:185:CYS:HB2	1.90	0.53
1:F:37:ARG:HH11	1:F:57:ARG:HD2	1.71	0.53
1:E:299:HIS:HB2	1:E:301:TYR:CD2	2.44	0.53
1:C:468:LYS:HG2	1:C:469:ALA:H	1.74	0.53
1:F:346:ASP:OD1	1:F:348:THR:OG1	2.17	0.53
1:B:320:SER:HB2	1:B:344:MET:HB2	1.90	0.53
1:B:738:GLY:O	1:B:742:VAL:HG23	2.09	0.53
1:D:274:ASN:HB2	1:D:277:ILE:HD12	1.91	0.53
1:E:329:LEU:O	1:E:861:TRP:NE1	2.42	0.53
1:E:80:LEU:HD12	1:E:145:CYS:HB2	1.90	0.53
1:A:284:ARG:HH11	1:A:449:GLN:HB3	1.75	0.52
1:E:195:LEU:HD22	1:E:206:LEU:HD21	1.91	0.52
1:A:158:GLU:OE2	1:A:190:THR:HB	2.10	0.52
1:F:33:THR:HB	1:F:211:LEU:HD23	1.91	0.52
1:F:455:MET:SD	1:F:581:VAL:HG12	2.49	0.52
1:F:762:GLN:NE2	1:F:805:TRP:O	2.42	0.52
1:E:617:LEU:HD22	1:E:657:LEU:HD11	1.92	0.52
1:B:581:VAL:HG12	1:B:582:LEU:N	2.25	0.52
1:F:514:GLN:HB3	1:F:819:TRP:CH2	2.45	0.52
1:D:125:ARG:HH22	3:D:1003:PO4:P	2.32	0.52
1:B:514:GLN:HG2	1:B:819:TRP:CZ2	2.45	0.52
1:E:82:CYS:SG	1:E:104:THR:HB	2.50	0.52
1:D:327:ARG:HG3	1:D:741:ARG:NH1	2.25	0.52
1:E:284:ARG:HH11	1:E:449:GLN:HB3	1.73	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:304:TRP:HZ3	1:D:579:VAL:HG21	1.75	0.52
1:D:349:PRO:HG2	1:D:590:THR:HG21	1.91	0.52
1:F:455:MET:SD	1:F:581:VAL:HG11	2.50	0.52
1:F:50:THR:HG21	1:F:588:GLY:HA2	1.91	0.52
1:A:555:THR:O	1:A:563:ARG:HD3	2.10	0.52
1:A:559:GLU:OE1	1:A:559:GLU:N	2.43	0.52
1:D:199:GLN:HA	1:D:221:TRP:HZ2	1.74	0.52
1:D:387:GLY:HA2	1:D:498:TRP:CZ3	2.45	0.52
1:F:460:GLU:CB	1:F:462:LYS:HE3	2.40	0.52
1:A:383:TRP:CD1	1:A:553:LEU:HB2	2.45	0.51
1:D:488:GLU:HG3	1:D:489:ALA:N	2.24	0.51
1:E:768:TYR:HA	1:E:770:HIS:NE2	2.25	0.51
1:C:55:VAL:O	1:C:84:ARG:HD3	2.10	0.51
1:A:158:GLU:HG3	1:A:191:MET:HG2	1.93	0.51
1:E:683:LEU:HG	1:E:688:LYS:O	2.09	0.51
1:E:853:ILE:HA	1:E:858:ARG:HD3	1.92	0.51
1:F:349:PRO:HG2	1:F:590:THR:HG21	1.92	0.51
1:F:284:ARG:NH1	1:F:449:GLN:HB3	2.25	0.51
1:A:8:LEU:HD21	1:A:238:GLN:HG3	1.92	0.51
1:D:853:ILE:HG22	1:D:858:ARG:CZ	2.41	0.51
1:F:120:GLY:HA2	1:F:264:ARG:HB2	1.92	0.51
1:C:720:LEU:HD12	1:C:724:ARG:HB2	1.91	0.51
1:D:720:LEU:HD12	1:D:724:ARG:HB2	1.92	0.51
1:E:74:TYR:CE1	1:E:141:ASP:HB3	2.45	0.51
1:A:145:CYS:HB3	1:A:181:ILE:HG13	1.93	0.51
1:D:13:LYS:HG2	1:D:154:PRO:HG3	1.91	0.51
1:D:476:TRP:N	1:D:476:TRP:CD1	2.77	0.51
1:E:157:GLU:HG2	1:E:184:LEU:HD21	1.91	0.51
1:A:401:ILE:HD11	1:A:433:TRP:HZ2	1.76	0.51
1:B:633:MET:HE1	1:B:681:ARG:HD2	1.93	0.51
1:E:773:ASP:OD1	1:E:858:ARG:NE	2.40	0.51
1:B:616:ASN:HD21	1:B:667:CYS:HB3	1.76	0.51
1:C:120:GLY:O	1:C:123:ILE:HG12	2.11	0.51
1:C:266:VAL:HG22	1:C:267:VAL:H	1.76	0.51
1:D:194:THR:HG23	1:D:197:ARG:HH22	1.76	0.51
1:E:299:HIS:HB2	1:E:301:TYR:HD2	1.75	0.51
1:A:479:TRP:C	1:A:479:TRP:CD1	2.84	0.51
1:A:509:GLU:HG2	1:A:609:TYR:CE2	2.46	0.51
1:C:476:TRP:CE2	1:C:602:GLY:HA2	2.46	0.51
1:F:476:TRP:CZ3	1:F:577:LYS:HD2	2.45	0.51
1:E:518:TYR:OH	1:E:726:ILE:HA	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:LEU:HA	1:A:492:PHE:CE1	2.46	0.50
1:F:195:LEU:HD22	1:F:206:LEU:HD11	1.94	0.50
1:F:539:TRP:NE1	1:F:543:ILE:HD11	2.26	0.50
1:A:28:LYS:HZ1	1:B:45:LYS:HE2	1.75	0.50
1:C:559:GLU:OE1	1:C:559:GLU:N	2.44	0.50
1:D:102:GLY:HA3	1:D:126:LEU:HD23	1.93	0.50
1:F:330:SER:O	1:F:741:ARG:NH2	2.44	0.50
1:D:26:SER:HA	1:D:248:ARG:HD2	1.93	0.50
1:B:819:TRP:O	1:B:823:ASN:ND2	2.44	0.50
1:D:320:SER:HB2	1:D:344:MET:HB2	1.92	0.50
1:B:616:ASN:HB3	1:B:662:VAL:HG11	1.94	0.50
1:C:161:THR:O	1:C:165:LEU:HG	2.11	0.50
1:C:299:HIS:HB2	1:C:301:TYR:CD2	2.47	0.50
1:F:355:VAL:HG11	1:F:473:ARG:HA	1.94	0.50
1:A:70:TYR:O	1:A:222:VAL:HB	2.12	0.50
1:B:404:VAL:HG11	1:B:427:VAL:HG11	1.93	0.50
1:B:633:MET:CE	1:B:681:ARG:HD2	2.42	0.50
1:A:55:VAL:O	1:A:84:ARG:NH1	2.45	0.50
1:C:14:ALA:O	1:C:18:GLN:HG3	2.12	0.50
1:F:277:ILE:HG23	1:F:572:TYR:CD1	2.47	0.50
1:C:644:LYS:HA	1:C:647:ASN:HB2	1.93	0.50
1:F:186:PRO:HD2	1:F:187:TYR:CD1	2.46	0.50
1:C:78:ILE:CD1	1:C:171:TRP:HZ3	2.25	0.50
1:C:241:LEU:HD23	1:C:244:MET:SD	2.52	0.50
1:D:25:TYR:HA	1:D:28:LYS:HE2	1.94	0.50
1:D:668:VAL:HG23	1:D:710:PHE:CD1	2.47	0.50
1:E:16:LEU:HD12	1:E:19:MET:SD	2.52	0.50
1:E:35:VAL:CG2	1:E:37:ARG:CD	2.83	0.50
1:E:718:LEU:HD21	1:E:841:LEU:HD12	1.93	0.50
1:F:247:PRO:HG2	1:F:249:ARG:HG3	1.92	0.50
1:C:158:GLU:HG3	1:C:191:MET:CG	2.39	0.49
1:C:485:LEU:HA	1:C:488:GLU:HG2	1.93	0.49
1:E:278:ILE:O	1:E:282:ILE:HG12	2.10	0.49
1:A:765:GLN:HG3	1:A:778:ALA:HB1	1.95	0.49
1:B:653:GLY:O	1:B:657:LEU:HB2	2.12	0.49
1:C:80:LEU:HD12	1:C:145:CYS:SG	2.52	0.49
1:A:149:GLU:HB3	1:A:160:ARG:HD3	1.93	0.49
1:B:440:ARG:NH2	1:B:488:GLU:OE1	2.45	0.49
1:E:164:VAL:O	1:E:168:VAL:HG13	2.12	0.49
1:E:583:ARG:HG3	1:E:584:PRO:HD2	1.93	0.49
1:E:349:PRO:HG2	1:E:590:THR:HG21	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:641:ARG:HB2	1:E:644:LYS:HE3	1.94	0.49
1:B:690:ARG:NH2	1:B:697:LYS:O	2.37	0.49
1:C:78:ILE:HG21	1:C:171:TRP:CZ3	2.48	0.49
1:F:620:GLN:OE1	1:F:669:VAL:HG21	2.12	0.49
1:B:479:TRP:C	1:B:479:TRP:CD1	2.85	0.49
1:B:613:THR:HG23	1:B:662:VAL:HG12	1.94	0.49
1:D:116:VAL:HG23	1:D:118:SER:H	1.77	0.49
1:A:390:LYS:HE2	1:A:503:ASN:HB2	1.95	0.49
1:A:499:MET:HB2	1:A:509:GLU:HB2	1.95	0.49
1:C:37:ARG:NH1	1:C:56:SER:O	2.45	0.49
1:F:411:GLY:HA3	1:F:479:TRP:HA	1.95	0.49
1:B:30:SER:O	1:B:214:ASN:ND2	2.46	0.49
1:C:164:VAL:O	1:C:168:VAL:HG13	2.12	0.49
1:D:380:SER:O	1:D:384:LYS:HG3	2.12	0.49
1:C:513:LEU:HD23	1:C:516:LEU:HD12	1.94	0.49
1:F:185:CYS:O	1:F:191:MET:HG3	2.13	0.49
1:F:42:ARG:NH2	1:F:42:ARG:CG	2.73	0.49
1:F:646:THR:HA	1:F:649:LEU:HB2	1.95	0.49
1:A:357:LYS:HG3	1:A:358:GLU:HG2	1.95	0.49
1:A:569:ILE:O	1:A:573:THR:HB	2.13	0.49
1:A:686:MET:HB3	1:A:688:LYS:HZ3	1.78	0.49
1:B:20:SER:O	1:B:24:PHE:HB2	2.13	0.49
1:B:644:LYS:HA	1:B:647:ASN:HB2	1.95	0.49
1:C:83:GLY:HA3	2:C:1001:SAH:HB1	1.94	0.49
1:C:344:MET:HE1	1:C:744:PRO:HA	1.95	0.49
1:D:629:GLU:OE1	1:D:675:ARG:NH1	2.46	0.49
1:E:115:LEU:HB3	1:E:350:TYR:OH	2.13	0.49
1:A:25:TYR:HD1	1:A:28:LYS:HE2	1.78	0.48
1:C:368:GLN:OE1	1:C:637:TRP:HA	2.12	0.48
1:D:194:THR:HG23	1:D:197:ARG:NH2	2.27	0.48
1:E:157:GLU:OE1	1:E:187:TYR:OH	2.15	0.48
1:E:436:VAL:HG11	1:E:484:PHE:CE2	2.47	0.48
1:E:609:TYR:OH	1:E:663:SER:CB	2.61	0.48
1:A:104:THR:HG22	1:A:127:LYS:O	2.13	0.48
1:A:479:TRP:HD1	1:A:480:LEU:N	2.12	0.48
1:C:133:PHE:HA	1:C:167:MET:HG3	1.95	0.48
1:C:629:GLU:OE1	1:C:675:ARG:NH1	2.46	0.48
1:A:765:GLN:HE21	1:A:811:MET:HG3	1.78	0.48
1:B:102:GLY:HA3	1:B:126:LEU:HD23	1.95	0.48
1:B:344:MET:HE2	1:B:461:LYS:HG2	1.96	0.48
1:D:818:VAL:HG23	1:D:819:TRP:CD1	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:777:MET:O	1:E:781:ILE:HG13	2.13	0.48
1:F:143:LEU:HD22	1:F:172:LEU:HD23	1.95	0.48
1:F:180:CYS:HA	1:F:221:TRP:O	2.14	0.48
1:F:345:THR:HG21	1:F:462:LYS:HD2	1.95	0.48
1:A:532:TYR:CE1	1:A:677:ALA:HB2	2.49	0.48
1:B:461:LYS:HD3	1:B:742:VAL:HB	1.94	0.48
1:F:690:ARG:NH1	1:F:699:SER:OG	2.47	0.48
1:B:453:TYR:HB2	1:B:578:VAL:O	2.13	0.48
1:B:583:ARG:HG3	1:B:584:PRO:HD2	1.96	0.48
1:B:77:VAL:HG13	1:B:142:THR:HB	1.95	0.48
1:F:194:THR:HG22	1:F:198:LEU:HD22	1.96	0.48
1:F:766:LEU:HD23	1:F:805:TRP:HE3	1.78	0.48
1:C:440:ARG:NH2	1:C:488:GLU:OE1	2.47	0.48
1:D:133:PHE:CE1	1:D:163:ARG:HG2	2.49	0.48
1:D:401:ILE:HD11	1:D:433:TRP:CZ2	2.48	0.48
1:E:54:ALA:HA	1:E:259:LEU:HD11	1.95	0.48
1:A:62:LEU:HA	1:A:62:LEU:HD23	1.62	0.48
1:B:479:TRP:CD1	1:B:480:LEU:N	2.81	0.48
1:B:63:ARG:HA	1:B:90:TYR:CZ	2.48	0.48
1:C:644:LYS:HA	1:C:647:ASN:HD22	1.78	0.48
1:F:398:GLU:O	1:F:402:ASN:HB2	2.14	0.48
1:B:120:GLY:HA2	1:B:264:ARG:HB2	1.96	0.48
1:D:616:ASN:O	1:D:620:GLN:HG2	2.14	0.48
1:C:199:GLN:OE1	1:C:229:THR:HG23	2.14	0.48
1:D:8:LEU:HD23	1:D:237:SER:HB2	1.94	0.48
1:D:521:GLU:O	1:D:525:ARG:HG3	2.13	0.48
1:E:284:ARG:O	1:E:287:SER:OG	2.29	0.48
1:F:113:PRO:HD2	1:F:466:PHE:CD1	2.49	0.48
1:D:411:GLY:O	1:D:413:ILE:HG13	2.14	0.47
1:F:42:ARG:CZ	1:F:42:ARG:CB	2.92	0.47
1:F:580:LYS:HE2	1:F:592:MET:HG2	1.96	0.47
1:A:12:TRP:NE1	1:A:240:LEU:HB3	2.29	0.47
1:A:34:GLU:HG2	1:A:35:VAL:H	1.77	0.47
1:B:78:ILE:HD12	1:B:140:CYS:HB3	1.95	0.47
1:C:320:SER:HB2	1:C:344:MET:HB2	1.95	0.47
1:F:765:GLN:HG3	1:F:778:ALA:HB1	1.96	0.47
1:A:461:LYS:CE	1:A:744:PRO:HG3	2.43	0.47
1:D:330:SER:HB3	1:D:777:MET:SD	2.54	0.47
1:F:853:ILE:HA	1:F:858:ARG:HD3	1.95	0.47
1:A:13:LYS:HG2	1:A:154:PRO:HG3	1.96	0.47
1:A:653:GLY:O	1:A:657:LEU:HB2	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:PHE:CE1	1:B:163:ARG:HG2	2.49	0.47
1:B:458:LYS:HD3	1:B:460:GLU:CD	2.35	0.47
1:E:479:TRP:CZ2	1:E:481:GLY:HA3	2.48	0.47
1:E:656:ARG:HA	1:E:659:ARG:HD2	1.96	0.47
1:B:41:ARG:HH22	1:B:57:ARG:HH21	1.62	0.47
1:C:154:PRO:HA	1:C:157:GLU:HB2	1.96	0.47
1:D:293:TRP:CZ2	1:D:308:GLY:HA3	2.49	0.47
1:E:580:LYS:HG2	1:E:592:MET:SD	2.55	0.47
1:F:367:PRO:HG3	1:F:686:MET:HA	1.96	0.47
1:F:532:TYR:CE1	1:F:677:ALA:HB2	2.50	0.47
1:F:460:GLU:CD	1:F:462:LYS:CE	2.76	0.47
1:A:532:TYR:CZ	1:A:677:ALA:HB2	2.50	0.47
1:B:199:GLN:NE2	1:B:227:SER:O	2.46	0.47
1:E:368:GLN:HB2	1:E:636:LEU:O	2.13	0.47
1:E:476:TRP:CE2	1:E:602:GLY:HA2	2.50	0.47
1:E:489:ALA:HB2	1:E:569:ILE:HD12	1.95	0.47
1:F:133:PHE:CD1	1:F:167:MET:HB2	2.50	0.47
1:A:656:ARG:HA	1:A:659:ARG:HD2	1.97	0.47
1:B:628:GLU:HA	1:B:675:ARG:NH2	2.30	0.47
1:E:401:ILE:HD11	1:E:433:TRP:CZ2	2.50	0.47
1:F:853:ILE:HG22	1:F:858:ARG:CZ	2.44	0.47
1:B:783:SER:HA	1:B:883:MET:O	2.15	0.47
1:F:25:TYR:HA	1:F:28:LYS:HE2	1.96	0.47
1:F:476:TRP:N	1:F:476:TRP:CD1	2.83	0.47
1:F:873:ARG:HG2	1:F:882:TYR:CD1	2.50	0.47
1:C:620:GLN:NE2	1:C:667:CYS:SG	2.87	0.47
1:D:383:TRP:CD1	1:D:553:LEU:HB2	2.50	0.47
1:D:717:LYS:HE2	1:D:725:SER:HB2	1.97	0.47
1:E:461:LYS:NZ	1:E:760:TYR:OH	2.43	0.47
1:A:116:VAL:HG23	1:A:118:SER:H	1.79	0.46
1:A:29:LYS:HE3	1:B:45:LYS:NZ	2.30	0.46
1:B:476:TRP:N	1:B:476:TRP:CD1	2.83	0.46
1:E:158:GLU:HG3	1:E:191:MET:HG2	1.97	0.46
1:A:371:THR:HG23	1:A:682:PHE:HD2	1.80	0.46
1:C:162:LEU:HG	1:C:191:MET:SD	2.56	0.46
1:E:690:ARG:NH2	1:E:694:GLN:O	2.46	0.46
1:F:783:SER:HA	1:F:883:MET:O	2.15	0.46
1:E:77:VAL:HG22	1:E:142:THR:HB	1.97	0.46
1:A:435:LEU:HD23	1:A:438:LYS:HD2	1.97	0.46
1:B:49:ALA:HB1	1:B:117:GLN:H	1.79	0.46
1:C:342:ILE:HD12	1:C:738:GLY:HA3	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:392:PRO:HB3	1:C:492:PHE:CZ	2.50	0.46
1:C:733:GLN:OE1	1:C:851:SER:HA	2.14	0.46
2:E:1001:SAH:H2'	2:E:1001:SAH:H8	1.67	0.46
1:F:12:TRP:CZ2	1:F:240:LEU:HD13	2.50	0.46
1:A:784:SER:HB2	1:A:872:VAL:HB	1.98	0.46
2:B:1001:SAH:H8	2:B:1001:SAH:H2'	1.65	0.46
1:D:195:LEU:HD22	1:D:206:LEU:HD21	1.97	0.46
1:D:301:TYR:OH	1:D:593:ASP:OD2	2.22	0.46
1:F:161:THR:O	1:F:165:LEU:HG	2.16	0.46
1:A:183:VAL:O	1:A:218:GLU:HA	2.15	0.46
1:B:656:ARG:HA	1:B:659:ARG:HD2	1.97	0.46
1:C:194:THR:HG23	1:C:197:ARG:HH22	1.80	0.46
1:D:125:ARG:NH2	3:D:1003:PO4:O1	2.44	0.46
1:D:386:LEU:HD23	1:D:386:LEU:HA	1.75	0.46
1:D:450:SER:O	1:D:452:VAL:N	2.48	0.46
1:F:387:GLY:HA3	1:F:557:GLN:OE1	2.16	0.46
1:F:717:LYS:HE2	1:F:725:SER:HB2	1.97	0.46
1:A:209:VAL:HG23	1:A:212:SER:CB	2.46	0.46
1:A:810:ASP:O	1:A:814:VAL:HG23	2.15	0.46
1:B:352:GLN:HE22	1:B:455:MET:HG2	1.79	0.46
1:C:199:GLN:NE2	1:C:227:SER:O	2.45	0.46
1:C:416:GLU:HG3	1:C:417:GLU:HG3	1.97	0.46
1:D:652:ASN:HB3	1:D:656:ARG:CZ	2.46	0.46
1:E:411:GLY:O	1:E:413:ILE:HG13	2.16	0.46
1:F:597:ARG:NE	1:F:599:ASP:OD1	2.49	0.46
1:A:306:TYR:HA	1:A:595:ILE:HG22	1.98	0.46
1:B:733:GLN:OE1	1:B:851:SER:HA	2.16	0.46
1:C:476:TRP:CZ2	1:C:602:GLY:HA2	2.51	0.46
1:E:762:GLN:HB3	1:E:811:MET:SD	2.56	0.46
1:F:214:ASN:CG	1:F:243:ARG:HH21	2.18	0.46
1:C:34:GLU:HG2	1:C:35:VAL:H	1.81	0.46
1:D:401:ILE:HD11	1:D:433:TRP:HZ2	1.81	0.46
1:A:853:ILE:HG22	1:A:858:ARG:CZ	2.46	0.46
1:C:278:ILE:O	1:C:282:ILE:HG12	2.16	0.46
1:C:853:ILE:HG22	1:C:858:ARG:CZ	2.46	0.46
1:D:208:ARG:HH12	1:D:218:GLU:N	2.14	0.46
1:F:42:ARG:NH2	1:F:42:ARG:CB	2.79	0.46
1:F:771:ARG:HG3	1:F:774:LEU:HD12	1.96	0.46
1:A:327:ARG:HH22	1:B:160:ARG:NH2	2.14	0.45
1:B:25:TYR:HD1	1:B:28:LYS:HE2	1.81	0.45
1:B:357:LYS:HG3	1:B:358:GLU:HG2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:VAL:HG23	1:B:37:ARG:CG	2.37	0.45
1:C:853:ILE:HA	1:C:858:ARG:HD3	1.96	0.45
1:E:137:ALA:HA	1:E:171:TRP:CE2	2.51	0.45
1:E:367:PRO:HG3	1:E:686:MET:HA	1.97	0.45
1:E:646:THR:HA	1:E:649:LEU:HB2	1.98	0.45
1:E:717:LYS:HE2	1:E:725:SER:HB2	1.97	0.45
1:F:101:LYS:HD3	1:F:103:TYR:OH	2.16	0.45
1:C:71:LEU:HD22	1:C:180:CYS:HB2	1.98	0.45
1:D:414:PHE:HZ	1:D:452:VAL:HG21	1.81	0.45
1:E:133:PHE:HA	1:E:167:MET:HG3	1.98	0.45
1:E:304:TRP:CZ2	1:E:597:ARG:HD2	2.50	0.45
1:F:157:GLU:HB3	1:F:185:CYS:HB2	1.99	0.45
1:A:359:LYS:HZ1	1:A:473:ARG:CD	2.05	0.45
1:A:359:LYS:HZ3	1:A:473:ARG:HG2	1.76	0.45
1:D:530:ARG:O	1:D:671:PRO:HD2	2.16	0.45
1:E:8:LEU:HD21	1:E:238:GLN:HG3	1.98	0.45
1:E:32:ILE:HD13	1:E:213:ARG:HA	1.99	0.45
1:F:278:ILE:O	1:F:282:ILE:HG12	2.16	0.45
1:F:42:ARG:CZ	1:F:42:ARG:HB2	2.47	0.45
1:A:883:MET:HE2	1:A:885:TYR:CD2	2.52	0.45
1:B:115:LEU:HB3	1:B:350:TYR:OH	2.16	0.45
1:A:95:ARG:O	1:A:264:ARG:NH1	2.50	0.45
1:A:397:LYS:HG3	1:A:433:TRP:CH2	2.51	0.45
1:E:424:VAL:HA	1:E:427:VAL:HG22	1.98	0.45
1:E:499:MET:HB2	1:E:509:GLU:HG3	1.98	0.45
1:A:771:ARG:HB2	1:A:774:LEU:HB2	1.97	0.45
1:C:276:LYS:HD3	1:C:276:LYS:HA	1.52	0.45
1:C:580:LYS:HG2	1:C:592:MET:SD	2.56	0.45
1:E:286:ARG:HG3	1:E:293:TRP:NE1	2.32	0.45
1:F:577:LYS:CE	1:F:600:GLN:O	2.64	0.45
1:A:101:LYS:HD3	1:A:103:TYR:OH	2.17	0.45
1:A:158:GLU:HG3	1:A:191:MET:SD	2.57	0.45
1:B:349:PRO:HG2	1:B:590:THR:HG21	1.99	0.45
1:C:490:LEU:HA	1:C:492:PHE:CE1	2.51	0.45
1:D:33:THR:O	1:D:211:LEU:HA	2.17	0.45
1:E:118:SER:O	1:E:121:TRP:HD1	2.00	0.45
1:E:516:LEU:HB2	1:E:715:PHE:CZ	2.52	0.45
1:F:192:MET:HE2	1:F:230:ILE:HG12	1.99	0.45
1:F:637:TRP:CZ2	1:F:638:LEU:HD12	2.52	0.45
1:F:706:GLU:OE1	1:F:716:ASN:ND2	2.47	0.45
1:A:616:ASN:HB3	1:A:662:VAL:HG11	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:739:ARG:NH1	3:D:1005:PO4:O2	2.50	0.45
1:E:256:ASP:OD1	1:E:257:VAL:N	2.50	0.45
1:E:784:SER:HB2	1:E:872:VAL:CG1	2.47	0.45
1:F:82:CYS:SG	1:F:104:THR:HB	2.57	0.45
1:F:783:SER:OG	1:F:885:TYR:HB2	2.16	0.45
1:B:567:LEU:HD23	1:B:570:ILE:HD12	1.98	0.45
1:C:533:ALA:CB	1:C:668:VAL:HG22	2.47	0.45
1:D:214:ASN:HD21	1:D:243:ARG:HH21	1.63	0.45
1:D:62:LEU:HD23	1:D:62:LEU:HA	1.69	0.45
1:E:599:ASP:OD1	1:E:599:ASP:N	2.50	0.45
1:A:280:ASN:HB2	1:A:448:CYS:O	2.17	0.45
1:A:320:SER:HB2	1:A:344:MET:HB2	1.98	0.45
1:B:323:ASN:OD1	1:B:757:ALA:HB2	2.18	0.45
1:B:559:GLU:N	1:B:559:GLU:OE1	2.49	0.45
1:B:616:ASN:ND2	1:B:667:CYS:HB3	2.31	0.45
1:B:62:LEU:HD12	1:B:87:TRP:HA	1.98	0.45
1:C:293:TRP:HE1	1:C:295:PHE:HE1	1.65	0.45
1:D:383:TRP:CE3	1:D:554:ILE:HD13	2.52	0.45
1:E:37:ARG:NE	1:E:57:ARG:HG2	2.32	0.45
1:F:411:GLY:O	1:F:413:ILE:HG13	2.17	0.45
1:F:771:ARG:HH21	1:F:851:SER:HB2	1.82	0.45
1:B:448:CYS:SG	1:B:451:CYS:HB2	2.58	0.44
1:D:551:GLU:OE2	1:D:615:THR:OG1	2.32	0.44
1:E:416:GLU:HG3	1:E:417:GLU:HG3	1.99	0.44
1:E:77:VAL:HG13	1:E:142:THR:HB	1.99	0.44
1:F:158:GLU:HG3	1:F:191:MET:HG2	1.99	0.44
1:A:28:LYS:HZ2	1:B:45:LYS:HE2	1.80	0.44
1:B:70:TYR:CD1	1:B:225:ALA:HB2	2.52	0.44
1:B:555:THR:O	1:B:563:ARG:HD3	2.17	0.44
1:C:66:VAL:HG22	1:C:71:LEU:HB3	1.99	0.44
1:C:74:TYR:OH	1:C:177:GLY:HA3	2.16	0.44
1:D:718:LEU:HD23	1:D:718:LEU:HA	1.86	0.44
1:B:101:LYS:HD3	1:B:103:TYR:OH	2.18	0.44
1:B:15:ARG:O	1:B:19:MET:HG3	2.17	0.44
1:B:239:LEU:HA	1:B:239:LEU:HD12	1.89	0.44
1:A:480:LEU:HA	1:A:480:LEU:HD12	1.78	0.44
1:E:722:ASP:OD1	1:E:723:GLY:N	2.49	0.44
1:B:292:THR:O	1:B:294:PHE:HD1	2.00	0.44
1:B:8:LEU:HD23	1:B:237:SER:HB2	2.00	0.44
1:C:70:TYR:HB3	1:C:222:VAL:HG21	2.00	0.44
1:C:367:PRO:HD2	1:C:546:PHE:CE2	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:818:VAL:HG23	1:C:819:TRP:CD1	2.53	0.44
1:D:117:GLN:NE2	1:D:350:TYR:HB2	2.32	0.44
1:A:20:SER:O	1:A:24:PHE:HB2	2.18	0.44
1:A:417:GLU:HB2	1:A:479:TRP:CZ2	2.30	0.44
1:B:120:GLY:O	1:B:123:ILE:HG12	2.18	0.44
1:C:345:THR:HB	1:C:472:SER:HB3	2.00	0.44
1:C:352:GLN:HE22	1:C:474:ALA:HB2	1.83	0.44
1:E:397:LYS:HG3	1:E:433:TRP:CH2	2.52	0.44
1:E:771:ARG:HB2	1:E:774:LEU:HB2	2.00	0.44
1:F:12:TRP:NE1	1:F:240:LEU:HB3	2.32	0.44
1:F:383:TRP:HA	1:F:383:TRP:CE3	2.53	0.44
1:F:371:THR:HG23	1:F:682:PHE:HD2	1.83	0.44
1:C:179:PHE:H	1:C:223:SER:HB3	1.82	0.44
1:C:367:PRO:HD2	1:C:546:PHE:CD2	2.52	0.44
1:C:354:ARG:NH2	1:C:469:ALA:O	2.50	0.44
1:D:416:GLU:HG3	1:D:417:GLU:HG3	2.00	0.44
1:F:521:GLU:O	1:F:525:ARG:HG3	2.18	0.44
1:A:729:PRO:O	1:A:770:HIS:NE2	2.50	0.43
1:B:50:THR:HG21	1:B:588:GLY:HA2	2.00	0.43
1:B:80:LEU:HB2	1:B:145:CYS:HA	2.00	0.43
1:C:327:ARG:HH22	1:D:160:ARG:NH2	2.13	0.43
1:C:56:SER:HB3	1:C:84:ARG:HD2	2.00	0.43
1:C:155:GLU:HB2	1:D:324:GLY:HA3	2.00	0.43
1:E:161:THR:O	1:E:165:LEU:HG	2.18	0.43
1:A:16:LEU:HA	1:A:16:LEU:HD12	1.80	0.43
1:A:690:ARG:NH2	1:A:697:LYS:O	2.42	0.43
1:B:455:MET:HB2	1:B:476:TRP:HB3	2.01	0.43
1:B:868:THR:O	1:B:872:VAL:HG23	2.18	0.43
1:C:392:PRO:HB2	1:C:558:MET:HG2	2.00	0.43
1:D:480:LEU:HD12	1:D:480:LEU:HA	1.67	0.43
1:E:352:GLN:HE21	1:E:457:GLY:CA	2.30	0.43
1:E:284:ARG:NH1	1:E:449:GLN:HB3	2.34	0.43
1:A:35:VAL:CG1	1:A:256:ASP:HB2	2.48	0.43
1:B:35:VAL:HA	1:B:254:GLU:O	2.18	0.43
1:B:581:VAL:CG1	1:B:582:LEU:N	2.81	0.43
1:C:433:TRP:HA	1:C:436:VAL:HB	2.00	0.43
1:D:206:LEU:HD13	1:D:229:THR:HG22	2.00	0.43
1:A:133:PHE:HA	1:A:167:MET:HG3	2.00	0.43
1:A:330:SER:O	1:A:741:ARG:NH2	2.51	0.43
1:A:381:TRP:CG	1:A:649:LEU:HD13	2.54	0.43
1:A:737:ILE:O	1:A:741:ARG:HG3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:TYR:HD1	1:A:118:SER:HG	1.66	0.43
1:E:411:GLY:O	1:E:479:TRP:HB2	2.18	0.43
1:A:772:ARG:HA	1:A:840:TYR:CE1	2.53	0.43
1:C:847:LEU:HD23	1:C:851:SER:O	2.17	0.43
1:D:758:LYS:HE2	1:D:762:GLN:NE2	2.33	0.43
1:E:457:GLY:HA3	1:E:472:SER:OG	2.18	0.43
1:A:89:TYR:CZ	1:A:116:VAL:HG22	2.53	0.43
1:A:417:GLU:CD	1:A:479:TRP:CE2	2.92	0.43
1:A:509:GLU:HG2	1:A:609:TYR:HE2	1.84	0.43
1:C:411:GLY:O	1:C:413:ILE:HG13	2.18	0.43
1:C:584:PRO:HA	1:C:590:THR:HG23	2.01	0.43
1:C:155:GLU:O	1:D:328:LEU:HD11	2.19	0.43
1:E:62:LEU:HA	1:E:62:LEU:HD23	1.55	0.43
1:F:49:ALA:HB1	1:F:117:GLN:N	2.34	0.43
1:F:873:ARG:HG2	1:F:882:TYR:CE1	2.52	0.43
1:A:671:PRO:HG3	1:A:676:PHE:CB	2.49	0.43
1:B:631:LEU:HD13	1:B:682:PHE:CZ	2.54	0.43
1:D:117:GLN:HG2	1:D:350:TYR:CE1	2.54	0.43
1:D:66:VAL:HG22	1:D:71:LEU:HB3	2.01	0.43
1:D:766:LEU:HD11	1:D:818:VAL:HG21	1.99	0.43
1:E:41:ARG:NH2	1:E:57:ARG:HH11	2.16	0.43
1:A:443:HIS:CE1	1:A:485:LEU:HD13	2.54	0.43
1:A:883:MET:HE1	1:A:885:TYR:CD1	2.54	0.43
1:C:392:PRO:HA	1:C:492:PHE:CE2	2.54	0.43
1:D:284:ARG:HH11	1:D:449:GLN:HB3	1.83	0.43
1:D:397:LYS:HG3	1:D:433:TRP:CH2	2.54	0.43
1:D:489:ALA:O	1:D:562:HIS:NE2	2.35	0.43
1:D:350:TYR:HA	1:D:584:PRO:HG3	2.01	0.43
1:F:208:ARG:NH2	1:F:213:ARG:O	2.52	0.43
1:F:54:ALA:HA	1:F:259:LEU:HD11	2.01	0.43
1:F:44:LEU:HD23	1:F:44:LEU:HA	1.92	0.43
1:A:473:ARG:HH22	1:A:691:LYS:NZ	2.17	0.43
1:A:717:LYS:HE2	1:A:725:SER:HB2	2.01	0.43
1:C:30:SER:O	1:C:214:ASN:ND2	2.52	0.43
1:D:8:LEU:HD21	1:D:238:GLN:HG3	2.01	0.43
1:E:45:LYS:HZ2	1:F:213:ARG:HH22	1.67	0.43
1:F:574:TYR:O	1:F:577:LYS:NZ	2.47	0.43
1:A:37:ARG:NH1	1:A:56:SER:O	2.51	0.43
1:B:289:HIS:O	1:B:293:TRP:HB2	2.19	0.43
1:C:868:THR:O	1:C:872:VAL:HG23	2.19	0.43
1:D:413:ILE:HD13	1:D:452:VAL:HB	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:315:GLN:HB2	1:D:582:LEU:HD13	2.00	0.43
1:E:292:THR:O	1:E:294:PHE:HD1	2.02	0.43
1:F:9:GLY:HA3	1:F:187:TYR:HB2	2.01	0.43
1:A:9:GLY:HA3	1:A:187:TYR:HB2	2.01	0.42
1:B:231:LYS:HB2	1:B:231:LYS:HE3	1.85	0.42
1:B:397:LYS:HG3	1:B:433:TRP:CH2	2.55	0.42
1:B:344:MET:CE	1:B:744:PRO:HA	2.49	0.42
1:C:12:TRP:CZ2	1:C:16:LEU:HD22	2.54	0.42
1:C:371:THR:HG23	1:C:682:PHE:HD2	1.84	0.42
1:A:277:ILE:HG22	1:A:281:ARG:HH12	1.83	0.42
1:A:401:ILE:HD11	1:A:433:TRP:CZ2	2.53	0.42
1:B:12:TRP:NE1	1:B:244:MET:HE3	2.34	0.42
1:B:14:ALA:O	1:B:18:GLN:HG3	2.18	0.42
1:C:25:TYR:HD1	1:C:28:LYS:HE2	1.84	0.42
1:C:463:GLN:O	1:C:470:LYS:HB2	2.18	0.42
1:E:493:LEU:HA	1:E:498:TRP:CD1	2.54	0.42
1:F:33:THR:HA	1:F:252:LYS:O	2.19	0.42
1:A:448:CYS:SG	1:A:451:CYS:HB2	2.58	0.42
1:B:304:TRP:CZ2	1:B:597:ARG:HD2	2.54	0.42
1:C:318:ALA:HB2	1:C:346:ASP:HA	2.00	0.42
1:C:309:SER:OG	1:C:593:ASP:OD1	2.37	0.42
1:C:733:GLN:NE2	1:C:773:ASP:HB2	2.34	0.42
1:C:82:CYS:O	1:C:85:GLY:N	2.53	0.42
1:D:49:ALA:HB1	1:D:117:GLN:N	2.34	0.42
1:D:635:ASP:HA	1:D:638:LEU:O	2.19	0.42
1:D:817:ARG:HA	1:D:821:GLU:HB3	2.00	0.42
1:D:63:ARG:HG2	1:D:90:TYR:OH	2.19	0.42
1:E:490:LEU:HA	1:E:492:PHE:CE1	2.55	0.42
1:F:20:SER:O	1:F:24:PHE:HB2	2.19	0.42
1:F:416:GLU:HG3	1:F:417:GLU:HG3	2.02	0.42
1:B:284:ARG:NH1	1:B:449:GLN:O	2.52	0.42
1:C:56:SER:HA	1:C:84:ARG:HH11	1.84	0.42
1:D:12:TRP:CZ2	1:D:240:LEU:HD13	2.55	0.42
1:E:293:TRP:CZ3	1:E:594:ILE:HD13	2.55	0.42
1:A:263:THR:OG1	1:A:298:ASN:O	2.31	0.42
1:A:580:LYS:HG2	1:A:592:MET:SD	2.60	0.42
1:C:413:ILE:HD13	1:C:452:VAL:HB	2.00	0.42
1:D:158:GLU:HG3	1:D:191:MET:HG2	2.01	0.42
1:D:263:THR:HG21	1:D:300:PRO:HG3	2.02	0.42
1:D:530:ARG:O	1:D:670:LYS:HD2	2.19	0.42
1:A:476:TRP:HZ3	1:A:577:LYS:HD2	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:HIS:HB2	1:A:594:ILE:O	2.20	0.42
1:B:383:TRP:CE3	1:B:383:TRP:HA	2.55	0.42
1:B:512:GLY:O	1:B:516:LEU:HG	2.20	0.42
1:B:387:GLY:HA3	1:B:557:GLN:OE1	2.19	0.42
1:B:646:THR:HA	1:B:649:LEU:HB2	2.01	0.42
1:D:34:GLU:HG2	1:D:35:VAL:H	1.83	0.42
1:F:280:ASN:HB2	1:F:448:CYS:O	2.19	0.42
1:A:499:MET:HB2	1:A:509:GLU:HG3	2.02	0.42
2:C:1001:SAH:H2'	2:C:1001:SAH:H8	1.88	0.42
1:C:146:ASP:OD2	2:C:1001:SAH:HG1	2.20	0.42
1:C:765:GLN:HG3	1:C:778:ALA:CB	2.49	0.42
1:D:719:HIS:O	1:D:839:PRO:HG3	2.20	0.42
1:E:192:MET:SD	1:E:233:VAL:HG11	2.59	0.42
2:A:1001:SAH:H2'	2:A:1001:SAH:H8	1.85	0.42
1:B:197:ARG:HG3	1:B:200:ARG:HH22	1.85	0.42
1:B:208:ARG:NH1	1:B:218:GLU:O	2.52	0.42
1:B:50:THR:HB	1:B:588:GLY:H	1.85	0.42
1:D:16:LEU:HD12	1:D:19:MET:SD	2.60	0.42
1:D:439:GLU:OE2	1:D:449:GLN:N	2.34	0.42
1:D:489:ALA:HB3	1:D:490:LEU:HG	2.01	0.42
1:E:771:ARG:NE	1:E:846:ASP:OD1	2.44	0.42
1:F:555:THR:O	1:F:563:ARG:HD3	2.19	0.42
1:A:156:VAL:HG22	1:B:328:LEU:HG	2.01	0.42
1:A:641:ARG:O	1:A:644:LYS:HG2	2.19	0.42
1:D:284:ARG:O	1:D:288:GLU:HG3	2.20	0.42
1:D:375:MET:HB3	1:D:550:ASN:ND2	2.35	0.42
1:A:71:LEU:HA	1:A:71:LEU:HD12	1.89	0.41
1:D:199:GLN:NE2	1:D:227:SER:O	2.53	0.41
1:E:199:GLN:OE1	1:E:229:THR:HG23	2.20	0.41
1:F:712:SER:OG	3:F:1002:PO4:O4	2.39	0.41
1:F:197:ARG:HA	1:F:200:ARG:CZ	2.50	0.41
1:F:387:GLY:HA3	1:F:557:GLN:HE22	1.85	0.41
1:F:624:ASN:HD21	1:F:671:PRO:HB3	1.85	0.41
1:A:179:PHE:CD2	1:A:179:PHE:N	2.87	0.41
1:A:188:THR:O	1:A:192:MET:HG3	2.21	0.41
1:A:774:LEU:HD23	1:A:774:LEU:HA	1.79	0.41
1:E:383:TRP:CD1	1:E:553:LEU:HB2	2.54	0.41
1:A:580:LYS:HE2	1:A:592:MET:HG2	2.03	0.41
1:C:646:THR:HA	1:C:649:LEU:HB2	2.03	0.41
1:E:401:ILE:HD11	1:E:433:TRP:HZ2	1.84	0.41
1:E:455:MET:CB	1:E:476:TRP:HB3	2.49	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:262:GLY:HA3	1:F:586:GLU:HB3	2.02	0.41
1:E:468:LYS:HG2	1:E:469:ALA:H	1.85	0.41
1:E:353:GLN:NE2	1:E:583:ARG:HD3	2.36	0.41
1:F:34:GLU:CG	1:F:35:VAL:H	2.30	0.41
1:F:383:TRP:O	1:F:557:GLN:NE2	2.54	0.41
1:F:424:VAL:HA	1:F:427:VAL:HG22	2.02	0.41
1:F:718:LEU:O	1:F:726:ILE:HG12	2.20	0.41
1:A:489:ALA:HB2	1:A:569:ILE:HD12	2.02	0.41
1:B:763:MET:HB2	1:B:805:TRP:CE2	2.55	0.41
1:C:35:VAL:HG23	1:C:37:ARG:CG	2.45	0.41
1:F:733:GLN:NE2	1:F:773:ASP:HB2	2.35	0.41
1:F:97:VAL:O	1:F:264:ARG:NH1	2.54	0.41
1:A:368:GLN:HB2	1:A:636:LEU:O	2.19	0.41
1:A:752:GLU:HA	1:A:755:CYS:SG	2.61	0.41
1:B:278:ILE:O	1:B:282:ILE:HG12	2.21	0.41
1:B:841:LEU:HA	1:B:841:LEU:HD12	1.96	0.41
1:C:261:SER:OG	1:C:587:LYS:HG3	2.21	0.41
1:D:442:HIS:HB3	1:D:447:GLU:O	2.20	0.41
1:F:179:PHE:HZ	1:F:204:GLY:HA3	1.86	0.41
1:F:401:ILE:O	1:F:404:VAL:HG12	2.21	0.41
1:A:625:MET:HE3	1:A:631:LEU:HD11	2.03	0.41
1:B:344:MET:HE3	1:B:744:PRO:HA	2.02	0.41
1:B:349:PRO:HG2	1:B:590:THR:CG2	2.51	0.41
1:C:80:LEU:HD22	1:C:132:VAL:HG11	2.02	0.41
1:C:27:TYR:CD1	1:C:244:MET:HA	2.55	0.41
1:A:303:THR:HG21	1:A:362:THR:C	2.41	0.41
1:A:460:GLU:HB3	1:A:462:LYS:HG2	2.02	0.41
1:B:78:ILE:HG21	1:B:171:TRP:CZ3	2.56	0.41
1:D:559:GLU:N	1:D:559:GLU:OE1	2.53	0.41
1:E:28:LYS:HG3	1:E:29:LYS:HG3	2.02	0.41
1:E:567:LEU:HD23	1:E:570:ILE:HD12	2.03	0.41
1:F:276:LYS:HA	1:F:276:LYS:HD3	1.43	0.41
1:B:641:ARG:O	1:B:644:LYS:HG2	2.20	0.41
1:C:137:ALA:HA	1:C:171:TRP:CE2	2.56	0.41
1:E:26:SER:O	1:E:30:SER:HB2	2.20	0.41
1:E:41:ARG:NH2	1:E:57:ARG:NH1	2.68	0.41
1:F:628:GLU:HA	1:F:675:ARG:NH2	2.36	0.41
1:A:160:ARG:O	1:A:164:VAL:HG23	2.21	0.41
1:A:380:SER:O	1:A:384:LYS:HG3	2.21	0.41
1:B:102:GLY:HA3	1:B:126:LEU:CD2	2.51	0.41
1:B:367:PRO:HG3	1:B:685:ASP:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:478:MET:HB3	1:C:482:ALA:HB3	2.03	0.41
1:D:458:LYS:HD2	1:D:475:ILE:HD11	2.03	0.41
1:D:771:ARG:NH2	1:D:846:ASP:OD1	2.52	0.41
1:E:476:TRP:N	1:E:476:TRP:HD1	2.17	0.41
1:F:12:TRP:HB2	1:F:241:LEU:CG	2.49	0.41
1:B:765:GLN:HG3	1:B:778:ALA:HB1	2.03	0.41
1:D:625:MET:HE3	1:D:631:LEU:HD11	2.03	0.41
1:E:101:LYS:HE2	1:E:125:ARG:HH11	1.86	0.41
1:E:277:ILE:HG23	1:E:572:TYR:CD1	2.55	0.41
1:F:551:GLU:OE1	1:F:611:LEU:HD22	2.21	0.41
1:F:717:LYS:CE	1:F:725:SER:HB2	2.51	0.41
1:F:329:LEU:HD13	1:F:781:ILE:HG12	2.03	0.41
1:A:401:ILE:O	1:A:404:VAL:HG12	2.21	0.40
1:A:41:ARG:NH1	1:A:57:ARG:HH21	2.19	0.40
1:B:714:HIS:CE1	1:B:731:ARG:HA	2.56	0.40
1:C:153:SER:HB2	1:C:155:GLU:OE1	2.21	0.40
1:C:424:VAL:HA	1:C:427:VAL:HG22	2.02	0.40
1:C:611:LEU:HA	1:C:611:LEU:HD23	1.85	0.40
1:D:15:ARG:O	1:D:19:MET:HG3	2.21	0.40
1:D:303:THR:HG21	1:D:363:ARG:HB2	2.03	0.40
1:D:416:GLU:HB2	1:D:435:LEU:HD11	2.02	0.40
1:D:498:TRP:HA	1:D:503:ASN:HD22	1.86	0.40
1:E:450:SER:O	1:E:452:VAL:N	2.54	0.40
1:F:16:LEU:HD12	1:F:19:MET:SD	2.61	0.40
1:A:675:ARG:HB2	1:A:675:ARG:HE	1.58	0.40
1:A:89:TYR:CE1	1:A:116:VAL:HG22	2.56	0.40
1:D:367:PRO:HD2	1:D:546:PHE:CD2	2.56	0.40
1:D:537:ALA:HA	1:D:691:LYS:HD2	2.02	0.40
1:D:537:ALA:HB2	1:D:691:LYS:HA	2.03	0.40
1:A:349:PRO:O	1:A:353:GLN:HG2	2.21	0.40
1:B:77:VAL:HG22	1:B:142:THR:HB	2.03	0.40
1:B:186:PRO:HD2	1:B:217:HIS:HB3	2.03	0.40
1:B:493:LEU:HA	1:B:498:TRP:CD1	2.56	0.40
1:D:63:ARG:HA	1:D:90:TYR:CZ	2.56	0.40
1:D:653:GLY:O	1:D:657:LEU:HB2	2.21	0.40
1:E:18:GLN:HE21	1:F:747:GLY:HA3	1.87	0.40
1:E:733:GLN:O	1:E:737:ILE:HG13	2.21	0.40
1:F:772:ARG:HD2	1:F:853:ILE:HD13	2.04	0.40
1:A:164:VAL:O	1:A:168:VAL:HG13	2.21	0.40
1:A:771:ARG:NE	1:A:846:ASP:OD1	2.44	0.40
1:B:536:THR:HG21	1:B:688:LYS:HB3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:437:ASP:O	1:E:441:GLU:HG3	2.21	0.40
1:E:508:VAL:HA	1:E:511:LEU:HD13	2.02	0.40
1:E:555:THR:O	1:E:563:ARG:HD3	2.21	0.40
1:A:112:GLU:OE1	1:A:466:PHE:HA	2.22	0.40
1:C:28:LYS:NZ	1:D:46:ASP:OD1	2.39	0.40
1:D:478:MET:HB3	1:D:482:ALA:HB3	2.03	0.40
1:D:583:ARG:HG3	1:D:584:PRO:HD2	2.04	0.40
1:F:345:THR:CG2	1:F:462:LYS:HD2	2.51	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%)	836 (95%)	45 (5%)	0	100	100
1	B	880/914 (96%)	837 (95%)	42 (5%)	1 (0%)	51	83
1	C	881/914 (96%)	832 (94%)	47 (5%)	2 (0%)	47	79
1	D	881/914 (96%)	829 (94%)	49 (6%)	3 (0%)	41	74
1	E	881/914 (96%)	834 (95%)	45 (5%)	2 (0%)	47	79
1	F	881/914 (96%)	835 (95%)	45 (5%)	1 (0%)	51	83
All	All	5285/5484 (96%)	5003 (95%)	273 (5%)	9 (0%)	47	79

All (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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	186	PRO
1	E	664	GLY
1	C	664	GLY
1	D	186	PRO
1	F	186	PRO

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	87
1	B	755/779 (97%)	748 (99%)	7 (1%)	78	87
1	C	756/779 (97%)	748 (99%)	8 (1%)	73	84
1	D	756/779 (97%)	747 (99%)	9 (1%)	71	83
1	E	756/779 (97%)	744 (98%)	12 (2%)	62	79
1	F	756/779 (97%)	746 (99%)	10 (1%)	69	81
All	All	4535/4674 (97%)	4482 (99%)	53 (1%)	71	83

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	281	ARG
1	A	366	ASP
1	A	476	TRP
1	A	479	TRP
1	A	656	ARG
1	A	673	ASP
1	A	722	ASP
1	B	281	ARG
1	B	366	ASP
1	B	462	LYS
1	B	476	TRP
1	B	656	ARG
1	B	673	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	722	ASP
1	C	38	GLU
1	C	281	ARG
1	C	366	ASP
1	C	476	TRP
1	C	479	TRP
1	C	514	GLN
1	C	656	ARG
1	C	673	ASP
1	D	24	PHE
1	D	38	GLU
1	D	281	ARG
1	D	366	ASP
1	D	405	ARG
1	D	476	TRP
1	D	479	TRP
1	D	514	GLN
1	D	656	ARG
1	E	24	PHE
1	E	281	ARG
1	E	359	LYS
1	E	366	ASP
1	E	462	LYS
1	E	476	TRP
1	E	479	TRP
1	E	514	GLN
1	E	656	ARG
1	E	673	ASP
1	E	856	ARG
1	E	884	ASP
1	F	39	GLU
1	F	42	ARG
1	F	281	ARG
1	F	366	ASP
1	F	476	TRP
1	F	479	TRP
1	F	514	GLN
1	F	656	ARG
1	F	673	ASP
1	F	722	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	238	GLN
1	A	274	ASN
1	A	323	ASN
1	A	352	GLN
1	A	353	GLN
1	A	428	ASN
1	A	463	GLN
1	A	576	ASN
1	A	598	GLN
1	A	652	ASN
1	A	765	GLN
1	A	864	ASN
1	B	110	HIS
1	B	428	ASN
1	B	616	ASN
1	B	762	GLN
1	B	765	GLN
1	B	864	ASN
1	C	238	GLN
1	C	274	ASN
1	C	428	ASN
1	C	576	ASN
1	C	598	GLN
1	C	620	GLN
1	C	647	ASN
1	D	238	GLN
1	D	323	ASN
1	D	463	GLN
1	D	503	ASN
1	D	576	ASN
1	D	598	GLN
1	D	733	GLN
1	D	762	GLN
1	D	770	HIS
1	D	870	ASN
1	E	18	GLN
1	E	110	HIS
1	E	323	ASN
1	E	428	ASN
1	E	864	ASN
1	E	870	ASN
1	F	238	GLN
1	F	274	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	428	ASN
1	F	442	HIS
1	F	463	GLN
1	F	494	ASN
1	F	576	ASN
1	F	624	ASN

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 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	D	1002	-	4,4,4	0.87	0	6,6,6	0.41	0
3	PO4	D	1005	-	4,4,4	0.81	0	6,6,6	0.51	0
2	SAH	E	1001	-	21,28,28	1.28	2 (9%)	20,40,40	1.84	3 (15%)
3	PO4	A	1003	-	4,4,4	0.82	0	6,6,6	0.57	0
2	SAH	C	1001	-	21,28,28	1.16	2 (9%)	20,40,40	1.69	3 (15%)
3	PO4	B	1002	-	4,4,4	0.91	0	6,6,6	0.46	0
3	PO4	A	1002	-	4,4,4	0.88	0	6,6,6	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	PO4	C	1002	-	4,4,4	0.89	0	6,6,6	0.47	0
3	PO4	F	1002	-	4,4,4	0.90	0	6,6,6	0.43	0
3	PO4	E	1002	-	4,4,4	0.87	0	6,6,6	0.51	0
2	SAH	B	1001	-	21,28,28	1.26	2 (9%)	20,40,40	1.74	3 (15%)
3	PO4	B	1003	-	4,4,4	0.92	0	6,6,6	0.42	0
2	SAH	F	1001	-	21,28,28	1.21	2 (9%)	20,40,40	1.62	4 (20%)
3	PO4	D	1003	-	4,4,4	0.94	0	6,6,6	0.48	0
2	SAH	D	1001	-	21,28,28	1.26	2 (9%)	20,40,40	1.72	3 (15%)
3	PO4	F	1003	-	4,4,4	0.90	0	6,6,6	0.34	0
3	PO4	D	1004	-	4,4,4	0.88	0	6,6,6	0.49	0
3	PO4	E	1003	-	4,4,4	0.92	0	6,6,6	0.44	0
3	PO4	F	1005	-	4,4,4	0.86	0	6,6,6	0.47	0
3	PO4	F	1004	-	4,4,4	0.86	0	6,6,6	0.47	0
2	SAH	A	1001	-	21,28,28	1.12	2 (9%)	20,40,40	1.82	3 (15%)

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	E	1001	-	-	2/7/31/31	0/3/3/3
2	SAH	C	1001	-	-	2/7/31/31	0/3/3/3
2	SAH	B	1001	-	-	3/7/31/31	0/3/3/3
2	SAH	F	1001	-	-	0/7/31/31	0/3/3/3
2	SAH	D	1001	-	-	3/7/31/31	0/3/3/3
2	SAH	A	1001	-	-	3/7/31/31	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1001	SAH	C2-N3	4.30	1.39	1.32
2	B	1001	SAH	C2-N3	4.27	1.39	1.32
2	D	1001	SAH	C2-N3	4.23	1.38	1.32
2	F	1001	SAH	C2-N3	4.22	1.38	1.32
2	C	1001	SAH	C2-N3	4.12	1.38	1.32
2	A	1001	SAH	C2-N3	3.86	1.38	1.32
2	B	1001	SAH	C2-N1	2.82	1.39	1.33
2	E	1001	SAH	C2-N1	2.56	1.38	1.33
2	D	1001	SAH	C2-N1	2.52	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1001	SAH	C2-N1	2.44	1.38	1.33
2	C	1001	SAH	C2-N1	2.42	1.38	1.33
2	A	1001	SAH	C2-N1	2.01	1.37	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1001	SAH	N3-C2-N1	-5.33	120.35	128.68
2	A	1001	SAH	N3-C2-N1	-5.33	120.35	128.68
2	D	1001	SAH	N3-C2-N1	-5.22	120.52	128.68
2	F	1001	SAH	N3-C2-N1	-5.08	120.74	128.68
2	B	1001	SAH	N3-C2-N1	-4.93	120.98	128.68
2	C	1001	SAH	N3-C2-N1	-4.80	121.18	128.68
2	E	1001	SAH	C5'-SD-CG	-4.32	89.31	102.27
2	A	1001	SAH	C5'-SD-CG	-3.93	90.49	102.27
2	C	1001	SAH	C3'-C2'-C1'	3.69	106.53	100.98
2	B	1001	SAH	C3'-C2'-C1'	3.60	106.40	100.98
2	D	1001	SAH	C5'-SD-CG	-3.49	91.80	102.27
2	A	1001	SAH	C3'-C2'-C1'	3.45	106.17	100.98
2	C	1001	SAH	C5'-SD-CG	-3.41	92.03	102.27
2	B	1001	SAH	C5'-SD-CG	-3.29	92.40	102.27
2	D	1001	SAH	C3'-C2'-C1'	3.27	105.91	100.98
2	E	1001	SAH	C3'-C2'-C1'	3.05	105.57	100.98
2	F	1001	SAH	C3'-C2'-C1'	2.71	105.05	100.98
2	F	1001	SAH	C5'-SD-CG	-2.70	94.18	102.27
2	F	1001	SAH	C2'-C3'-C4'	2.11	106.74	102.64

There are no chirality outliers.

All (13) torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

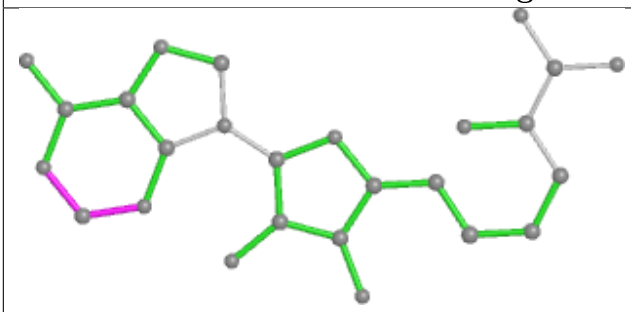
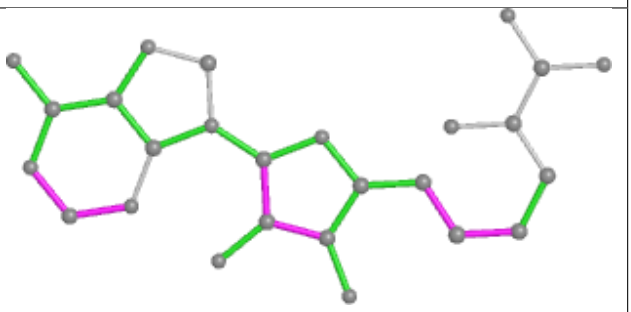
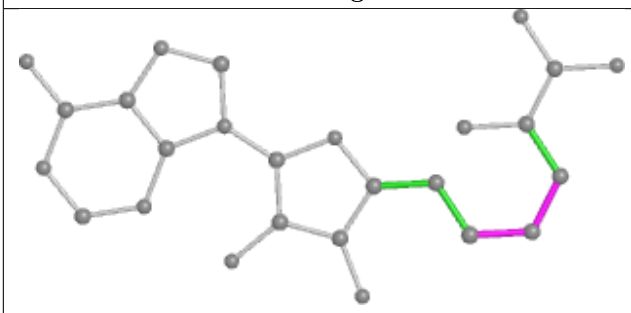
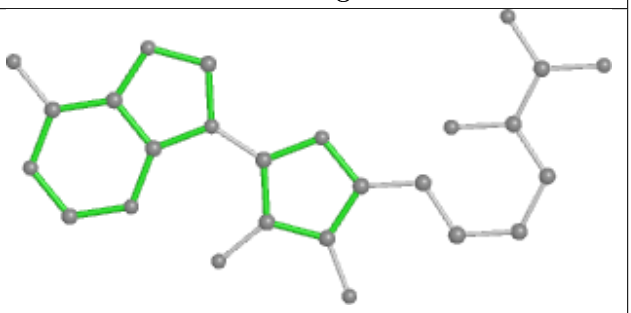
Mol	Chain	Res	Type	Atoms
2	A	1001	SAH	N-CA-CB-CG
2	C	1001	SAH	N-CA-CB-CG

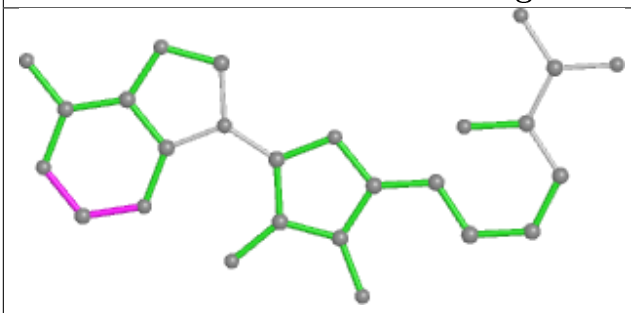
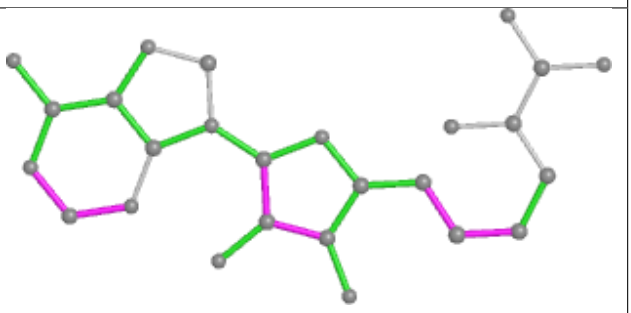
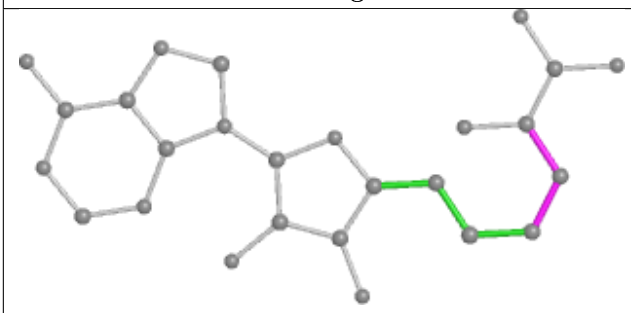
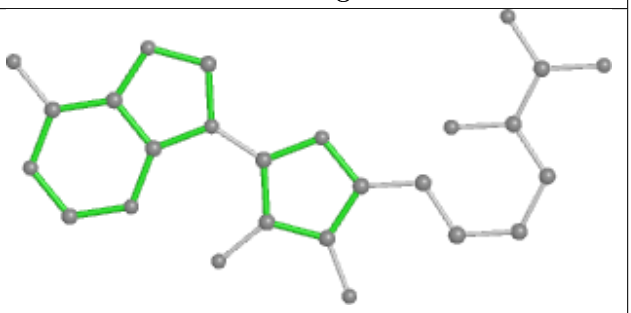
There are no ring outliers.

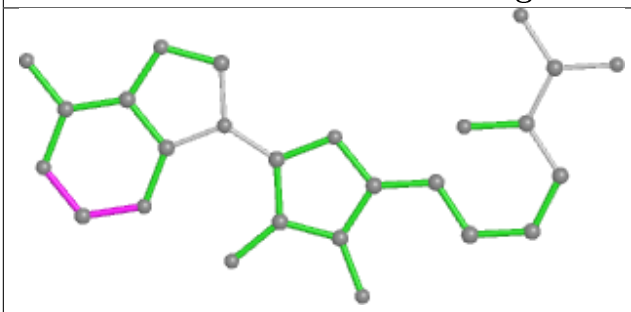
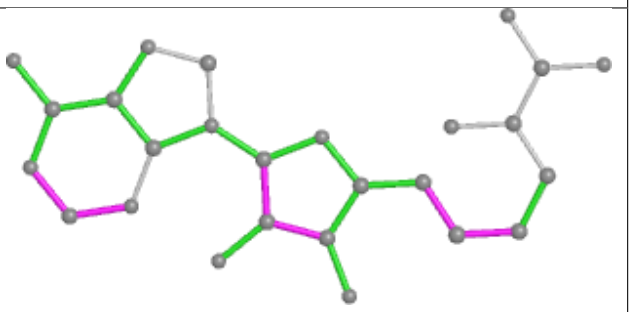
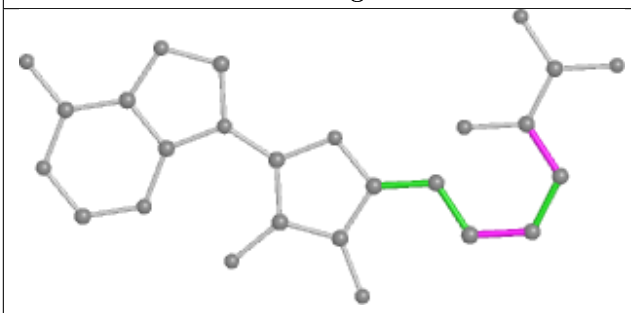
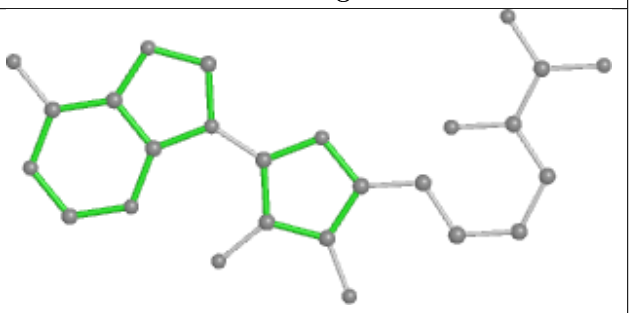
9 monomers are involved in 12 short contacts:

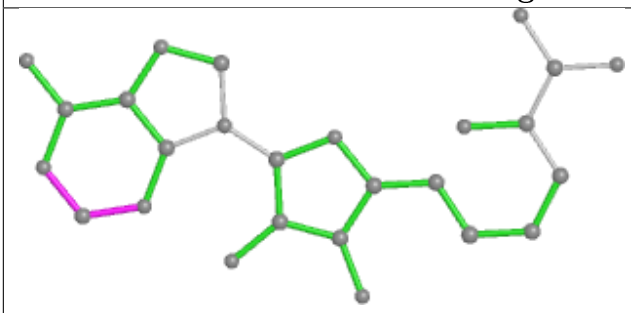
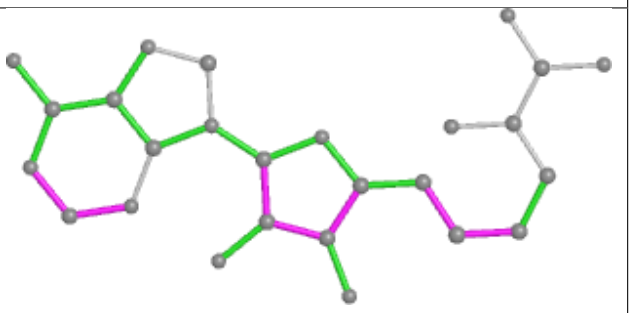
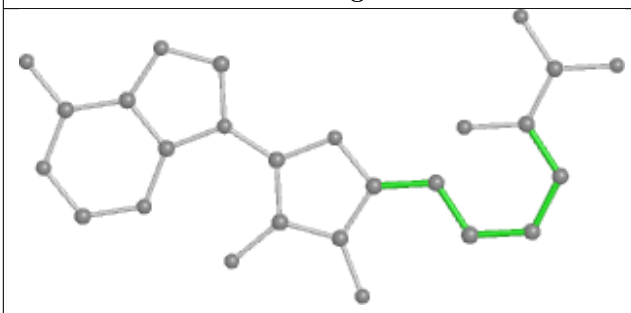
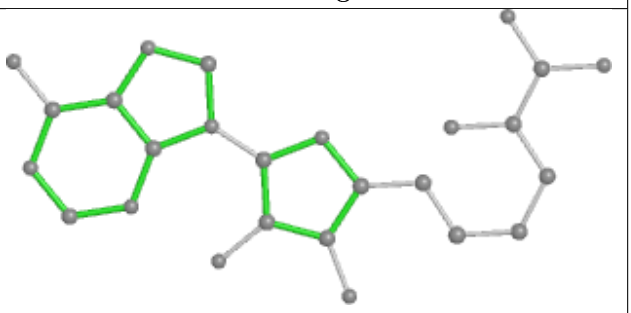
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1005	PO4	1	0
2	E	1001	SAH	1	0
2	C	1001	SAH	3	0
3	F	1002	PO4	1	0
2	B	1001	SAH	1	0
3	D	1003	PO4	2	0
2	D	1001	SAH	1	0
3	F	1003	PO4	1	0
2	A	1001	SAH	1	0

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 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.

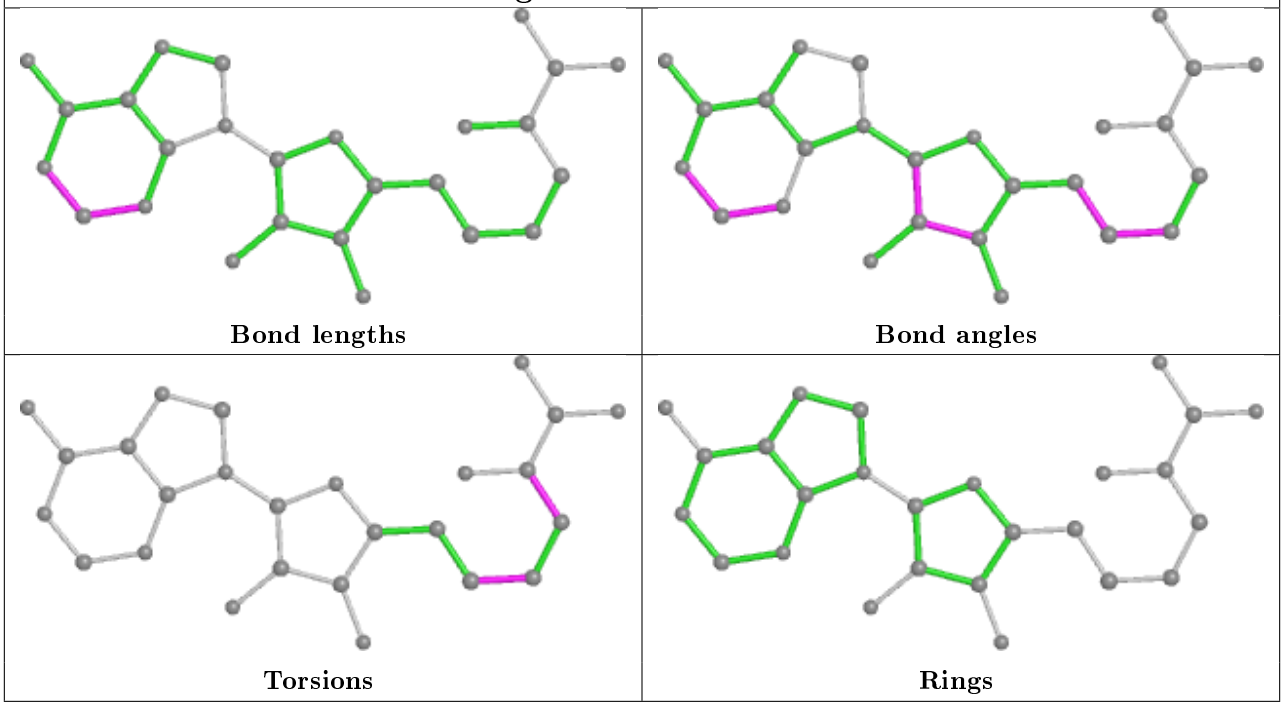
Ligand SAH E 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SAH C 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

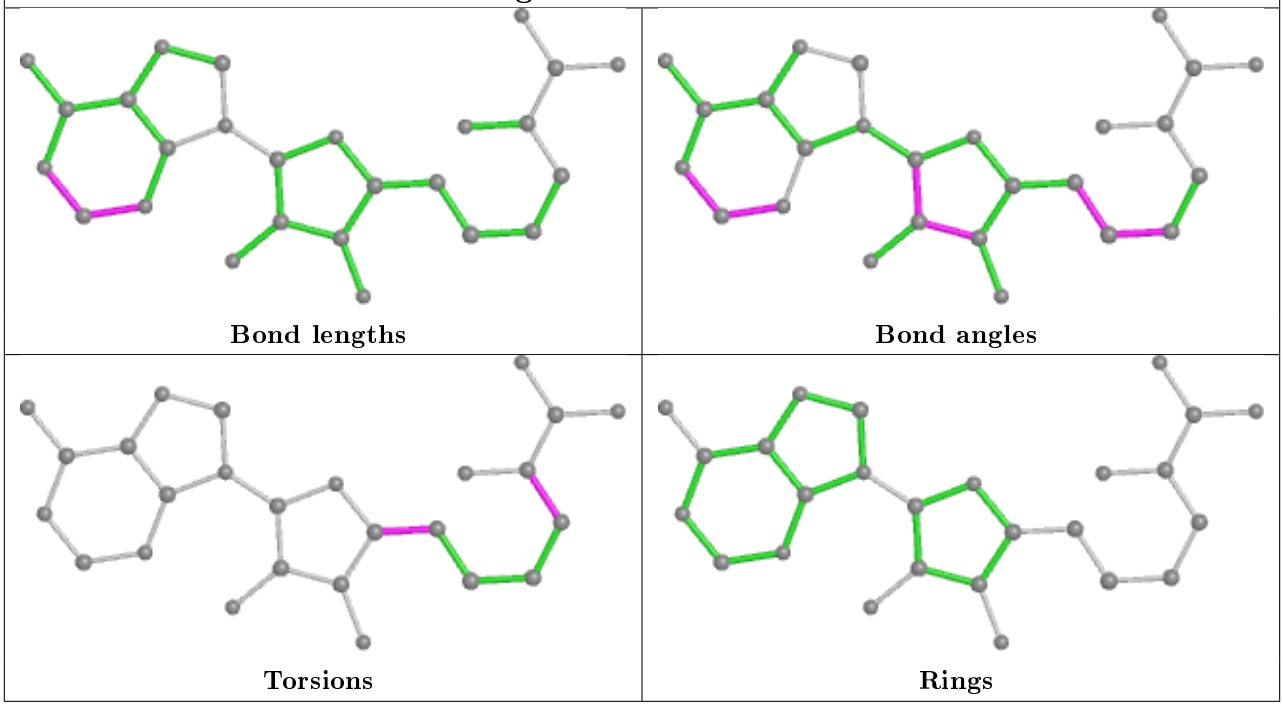
Ligand SAH B 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SAH F 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SAH D 1001



Ligand SAH A 1001



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

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%)	0.47	54 (6%)	21	17	20, 104, 182, 261	0
1	B	882/914 (96%)	0.56	62 (7%)	16	13	26, 111, 191, 253	0
1	C	883/914 (96%)	0.54	62 (7%)	16	13	18, 108, 166, 222	0
1	D	883/914 (96%)	0.35	18 (2%)	65	56	17, 77, 131, 187	0
1	E	883/914 (96%)	0.36	21 (2%)	59	49	19, 86, 156, 221	0
1	F	883/914 (96%)	0.40	37 (4%)	36	29	27, 91, 149, 195	0
All	All	5297/5484 (96%)	0.45	254 (4%)	30	25	17, 96, 171, 261	0

All (254) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	578	VAL	7.4
1	A	723	GLY	6.9
1	B	446	GLY	6.8
1	B	452	VAL	6.4
1	A	720	LEU	5.9
1	B	566	ALA	5.8
1	A	722	ASP	5.7
1	A	819	TRP	5.4
1	A	435	LEU	5.3
1	C	578	VAL	4.9
1	F	578	VAL	4.9
1	B	447	GLU	4.8
1	A	579	VAL	4.7
1	B	428	ASN	4.6
1	C	579	VAL	4.5
1	A	535	ASP	4.4
1	A	416	GLU	4.4
1	B	704	ASN	4.2
1	C	768	TYR	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	386	LEU	4.1
1	F	656	ARG	4.1
1	A	660	MET	4.1
1	D	416	GLU	4.0
1	B	445	ARG	4.0
1	D	717	LYS	3.9
1	F	593	ASP	3.9
1	B	451	CYS	3.9
1	A	839	PRO	3.9
1	C	658	LYS	3.8
1	A	417	GLU	3.8
1	B	436	VAL	3.8
1	C	661	ALA	3.7
1	C	668	VAL	3.7
1	D	415	GLU	3.7
1	E	704	ASN	3.6
1	C	506	GLY	3.6
1	A	413	ILE	3.6
1	B	793	GLY	3.6
1	C	660	MET	3.6
1	C	804	GLU	3.5
1	F	804	GLU	3.5
1	B	400	PHE	3.5
1	A	400	PHE	3.5
1	A	831	PRO	3.5
1	A	879	GLU	3.5
1	A	661	ALA	3.4
1	C	745	GLY	3.4
1	C	505	GLY	3.4
1	F	800	HIS	3.4
1	A	717	LYS	3.4
1	E	416	GLU	3.4
1	A	657	LEU	3.3
1	C	746	ALA	3.3
1	B	206	LEU	3.3
1	C	278	ILE	3.3
1	B	574	TYR	3.3
1	E	796	THR	3.3
1	C	580	LYS	3.3
1	C	703	ASP	3.3
1	C	416	GLU	3.3
1	B	575	GLN	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	490	LEU	3.2
1	C	726	ILE	3.2
1	E	654	TRP	3.1
1	D	746	ALA	3.1
1	C	744	PRO	3.1
1	B	577	LYS	3.1
1	C	518	TYR	3.1
1	A	821	GLU	3.1
1	E	794	ARG	3.1
1	C	654	TRP	3.1
1	A	721	LYS	3.1
1	F	795	THR	3.1
1	C	577	LYS	3.1
1	B	414	PHE	3.1
1	F	357	LYS	3.1
1	B	523	MET	3.0
1	B	16	LEU	3.0
1	A	428	ASN	3.0
1	A	577	LYS	3.0
1	C	354	ARG	2.9
1	D	413	ILE	2.9
1	C	576	ASN	2.9
1	D	206	LEU	2.9
1	E	400	PHE	2.9
1	C	727	VAL	2.9
1	B	448	CYS	2.9
1	F	594	ILE	2.9
1	B	416	GLU	2.8
1	D	414	PHE	2.8
1	D	516	LEU	2.8
1	F	580	LYS	2.8
1	F	669	VAL	2.8
1	B	631	LEU	2.8
1	E	797	TRP	2.8
1	A	278	ILE	2.8
1	C	631	LEU	2.8
1	B	514	GLN	2.8
1	E	705	TRP	2.7
1	A	793	GLY	2.7
1	C	525	ARG	2.7
1	C	717	LYS	2.7
1	F	579	VAL	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	453	TYR	2.7
1	F	654	TRP	2.7
1	A	414	PHE	2.7
1	B	147	ILE	2.7
1	B	417	GLU	2.7
1	A	726	ILE	2.6
1	A	536	THR	2.6
1	D	435	LEU	2.6
1	F	386	LEU	2.6
1	F	536	THR	2.6
1	F	432	PHE	2.6
1	B	551	GLU	2.6
1	A	484	PHE	2.6
1	F	446	GLY	2.6
1	D	793	GLY	2.6
1	A	630	VAL	2.6
1	E	586	GLU	2.6
1	B	17	ASN	2.6
1	C	447	GLU	2.6
1	B	317	SER	2.6
1	F	565	LEU	2.6
1	F	668	VAL	2.6
1	A	834	LYS	2.6
1	C	716	ASN	2.6
1	E	709	PRO	2.6
1	F	416	GLU	2.6
1	B	159	ALA	2.6
1	B	320	SER	2.6
1	C	282	ILE	2.5
1	F	796	THR	2.5
1	A	300	PRO	2.5
1	B	382	LEU	2.5
1	A	432	PHE	2.5
1	B	595	ILE	2.5
1	A	815	TRP	2.5
1	B	482	ALA	2.5
1	E	34	GLU	2.5
1	A	658	LYS	2.5
1	B	403	LYS	2.5
1	F	827	GLU	2.5
1	D	747	GLY	2.5
1	C	837	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	707	GLU	2.4
1	B	353	GLN	2.4
1	C	645	VAL	2.4
1	C	317	SER	2.4
1	E	576	ASN	2.4
1	F	34	GLU	2.4
1	C	767	LEU	2.4
1	D	578	VAL	2.4
1	F	414	PHE	2.4
1	A	832	VAL	2.4
1	E	531	MET	2.4
1	C	534	ASP	2.4
1	B	569	ILE	2.4
1	A	506	GLY	2.4
1	A	452	VAL	2.4
1	C	414	PHE	2.4
1	D	217	HIS	2.4
1	C	158	GLU	2.3
1	C	277	ILE	2.3
1	C	533	ALA	2.3
1	B	84	ARG	2.3
1	F	688	LYS	2.3
1	F	408	ALA	2.3
1	C	669	VAL	2.3
1	B	18	GLN	2.3
1	A	284	ARG	2.3
1	C	646	THR	2.3
1	F	253	TYR	2.3
1	B	156	VAL	2.3
1	C	586	GLU	2.3
1	C	793	GLY	2.3
1	C	760	TYR	2.3
1	F	881	LYS	2.3
1	A	573	THR	2.3
1	B	801	GLY	2.3
1	A	744	PRO	2.3
1	B	803	GLY	2.3
1	B	220	TYR	2.3
1	B	354	ARG	2.2
1	C	329	LEU	2.2
1	C	455	MET	2.2
1	F	186	PRO	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	705	TRP	2.2
1	C	130	VAL	2.2
1	C	704	ASN	2.2
1	E	837	ASP	2.2
1	E	707	GLU	2.2
1	A	654	TRP	2.2
1	B	804	GLU	2.2
1	F	57	ARG	2.2
1	A	282	ILE	2.2
1	A	386	LEU	2.2
1	C	523	MET	2.2
1	F	566	ALA	2.2
1	F	506	GLY	2.2
1	B	819	TRP	2.2
1	B	153	SER	2.2
1	B	707	GLU	2.2
1	B	768	TYR	2.1
1	C	327	ARG	2.1
1	B	186	PRO	2.1
1	A	515	ARG	2.1
1	B	13	LYS	2.1
1	D	124	VAL	2.1
1	A	522	GLU	2.1
1	F	263	THR	2.1
1	A	259	LEU	2.1
1	A	390	LYS	2.1
1	E	523	MET	2.1
1	C	838	ILE	2.1
1	D	186	PRO	2.1
1	B	441	GLU	2.1
1	B	184	LEU	2.1
1	B	533	ALA	2.1
1	C	432	PHE	2.1
1	D	575	GLN	2.1
1	B	576	ASN	2.1
1	C	314	THR	2.1
1	A	621	LEU	2.1
1	B	630	VAL	2.1
1	B	181	ILE	2.1
1	D	577	LYS	2.1
1	E	16	LEU	2.1
1	E	716	ASN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	413	ILE	2.1
1	C	758	LYS	2.1
1	F	413	ILE	2.1
1	C	461	LYS	2.1
1	B	790	VAL	2.1
1	C	504	SER	2.1
1	C	682	PHE	2.1
1	E	59	SER	2.1
1	B	658	LYS	2.0
1	E	577	LYS	2.0
1	F	658	LYS	2.0
1	C	819	TRP	2.0
1	F	705	TRP	2.0
1	A	382	LEU	2.0
1	A	94	ILE	2.0
1	B	40	ALA	2.0
1	F	285	ILE	2.0
1	E	25	TYR	2.0
1	B	471	GLY	2.0
1	C	747	GLY	2.0
1	C	452	VAL	2.0
1	A	505	GLY	2.0
1	A	640	ARG	2.0
1	B	476	TRP	2.0
1	F	221	TRP	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

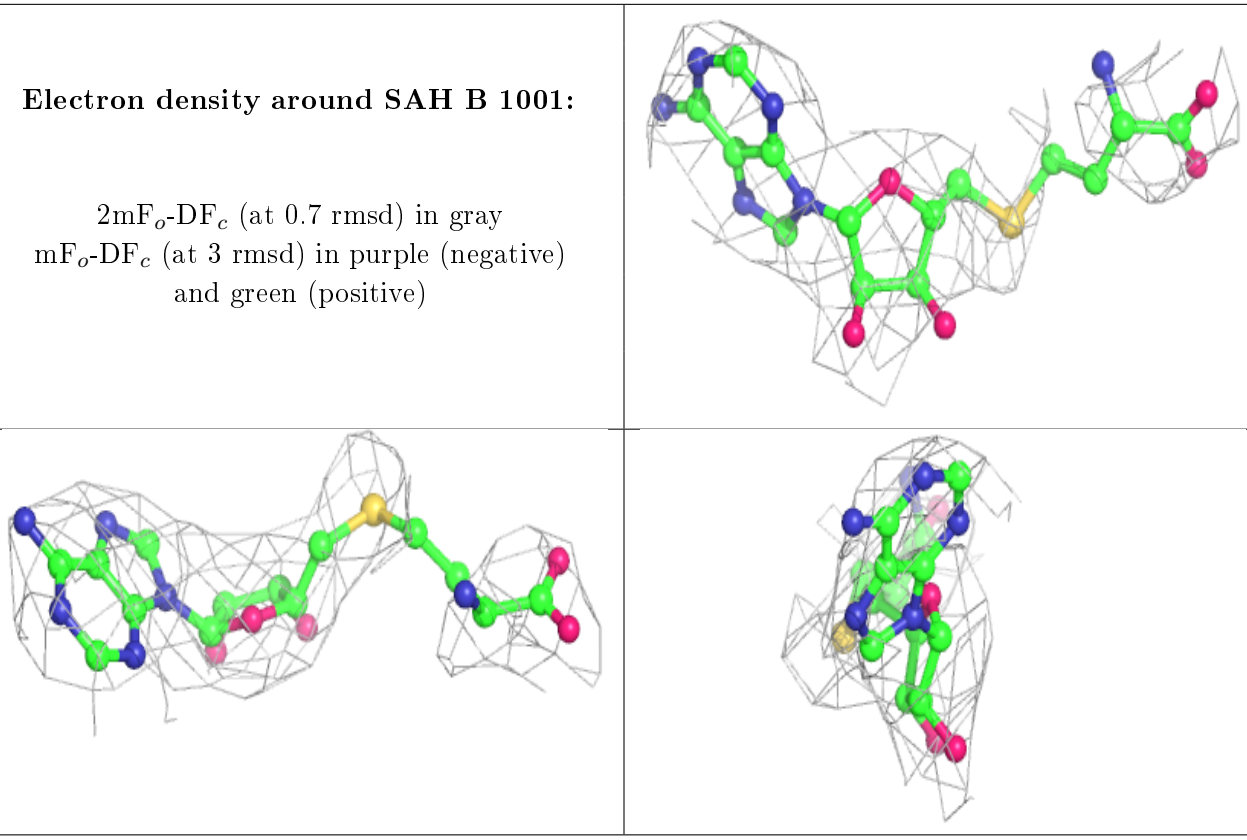
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PO4	F	1005	5/5	0.39	0.26	163,195,212,227	0
3	PO4	E	1003	5/5	0.39	0.24	168,181,230,239	0
3	PO4	D	1002	5/5	0.67	0.24	123,143,182,184	0
3	PO4	D	1004	5/5	0.73	0.17	156,179,206,209	0
3	PO4	C	1002	5/5	0.73	0.23	110,129,154,157	0
3	PO4	A	1002	5/5	0.74	0.25	127,148,153,161	0
3	PO4	B	1003	5/5	0.74	0.17	157,184,212,213	0
3	PO4	D	1005	5/5	0.78	0.24	119,125,139,152	0
3	PO4	F	1003	5/5	0.81	0.18	103,138,171,194	0
3	PO4	D	1003	5/5	0.82	0.15	151,169,206,225	0
3	PO4	F	1004	5/5	0.89	0.19	79,90,144,173	0
2	SAH	B	1001	26/26	0.89	0.52	68,105,131,138	0
2	SAH	C	1001	26/26	0.90	0.39	43,74,103,125	0
3	PO4	B	1002	5/5	0.90	0.16	94,109,127,135	0
2	SAH	F	1001	26/26	0.92	0.38	43,81,100,140	0
2	SAH	D	1001	26/26	0.92	0.41	31,85,110,128	0
2	SAH	A	1001	26/26	0.93	0.34	44,65,92,141	0
3	PO4	E	1002	5/5	0.94	0.18	78,104,111,113	0
3	PO4	F	1002	5/5	0.95	0.18	70,78,116,131	0
3	PO4	A	1003	5/5	0.95	0.15	88,95,130,137	0
2	SAH	E	1001	26/26	0.95	0.43	38,67,106,137	0
4	ZN	A	1005	1/1	0.97	0.15	154,154,154,154	0
4	ZN	E	1004	1/1	0.97	0.19	156,156,156,156	0
4	ZN	C	1003	1/1	0.97	0.22	68,68,68,68	0
4	ZN	A	1004	1/1	0.98	0.20	73,73,73,73	0
4	ZN	F	1007	1/1	0.99	0.16	118,118,118,118	0
4	ZN	C	1004	1/1	0.99	0.16	142,142,142,142	0
4	ZN	B	1004	1/1	0.99	0.21	32,32,32,32	0
4	ZN	E	1005	1/1	0.99	0.22	10,10,10,10	0
4	ZN	F	1006	1/1	0.99	0.17	57,57,57,57	0
4	ZN	D	1006	1/1	0.99	0.20	44,44,44,44	0
4	ZN	D	1007	1/1	1.00	0.24	51,51,51,51	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.

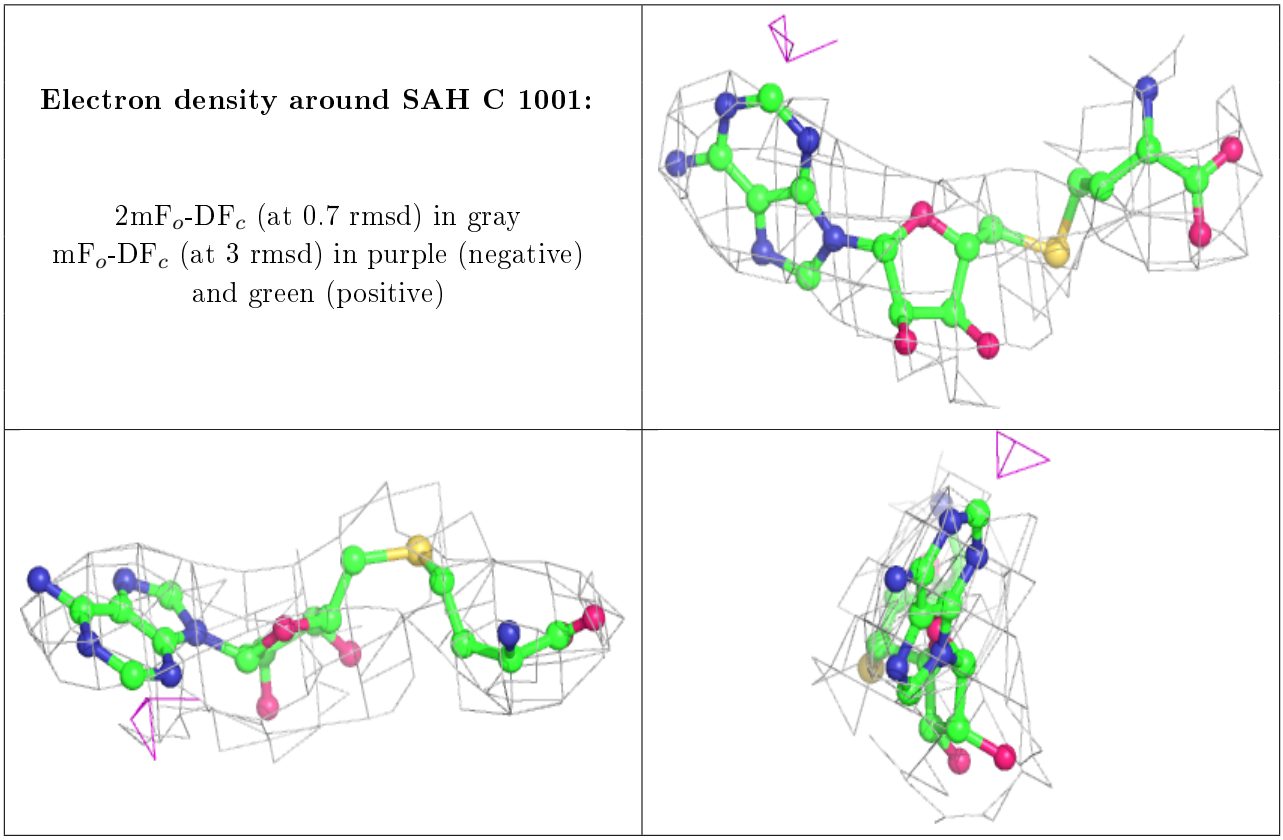
Electron density around SAH B 1001:

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



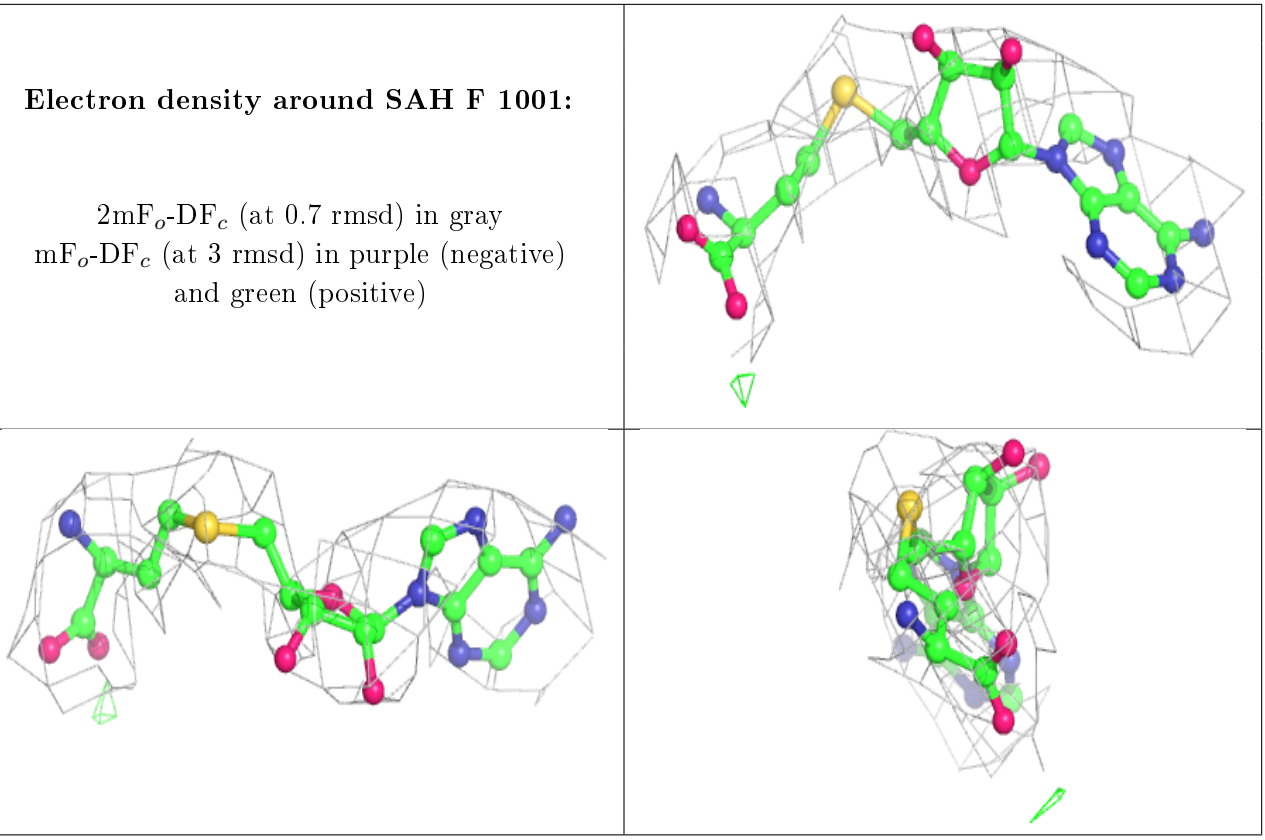
Electron density around SAH C 1001:

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



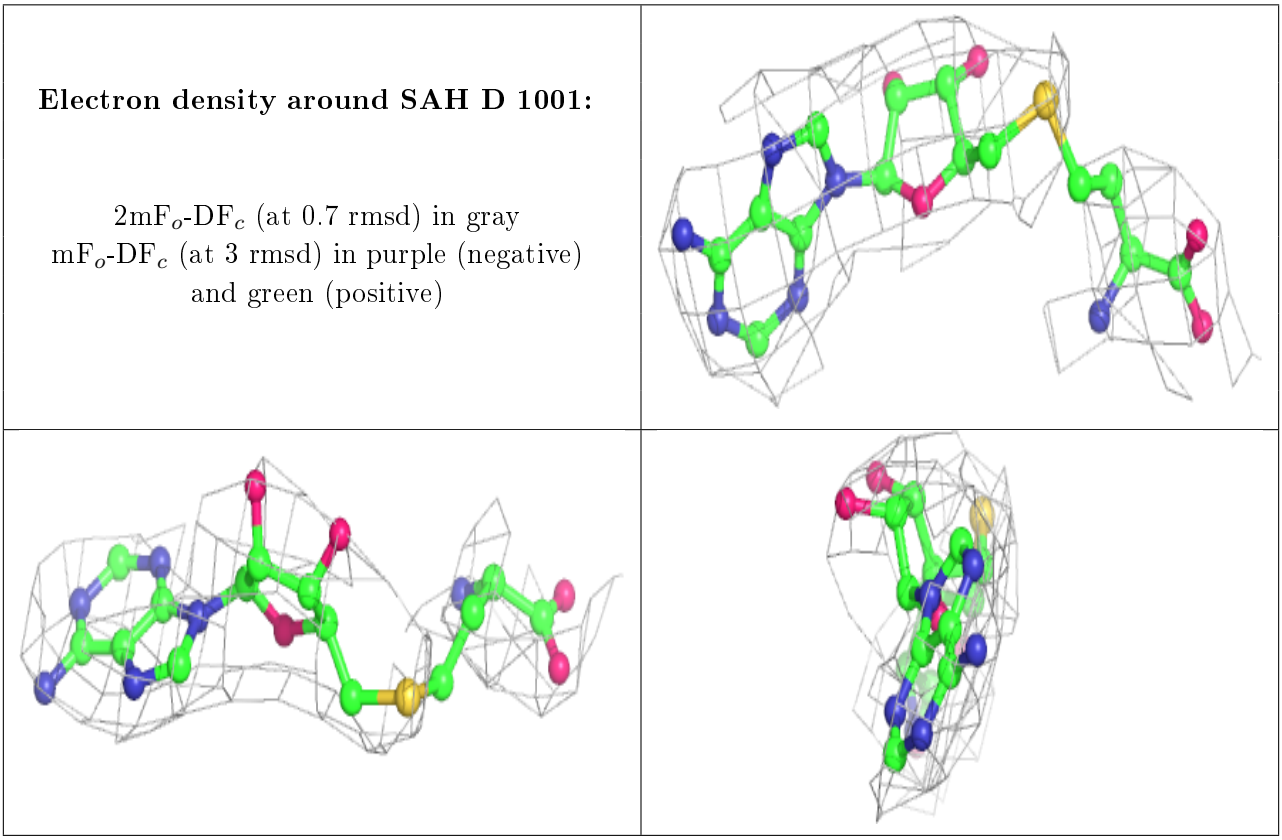
Electron density around SAH F 1001:

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



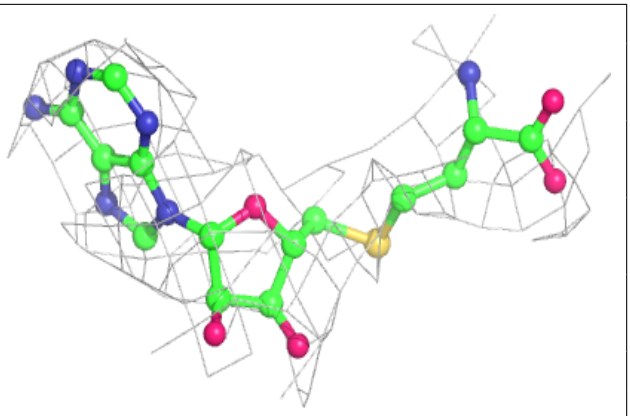
Electron density around SAH D 1001:

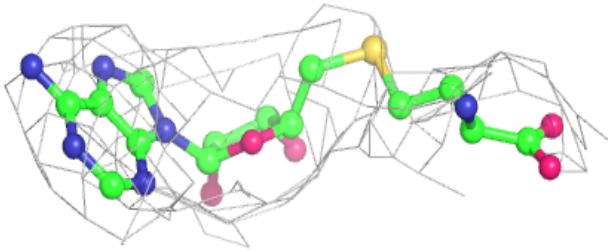
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

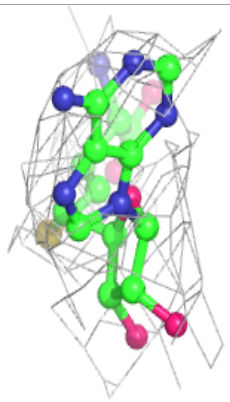


Electron density around SAH A 1001:

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

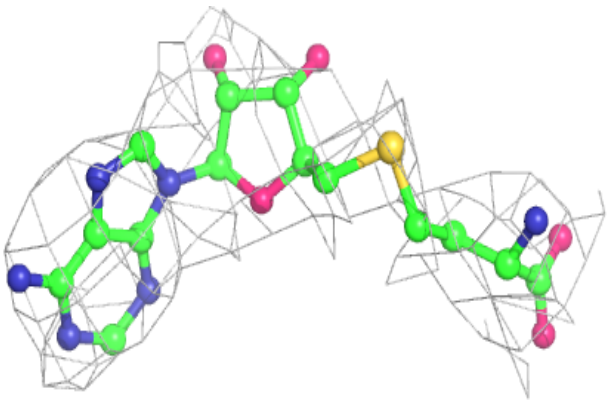


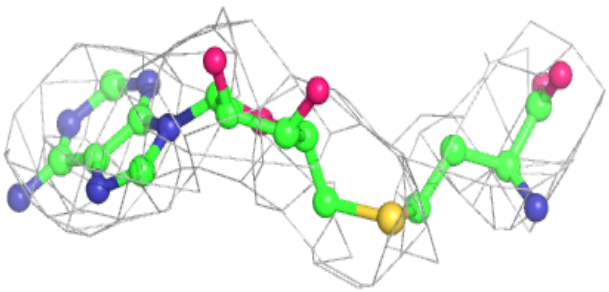


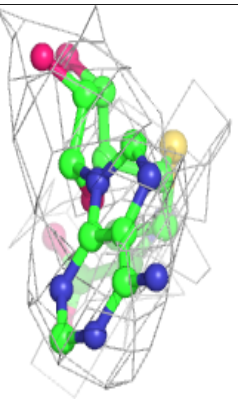


Electron density around SAH E 1001:

$2mF_o$-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.