



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 02:38 pm BST

PDB ID : 6DUQ
Title : Structure of a Rho-NusG KOW domain complex
Authors : Berger, J.M.; Lawson, M.R.
Deposited on : 2018-06-21
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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

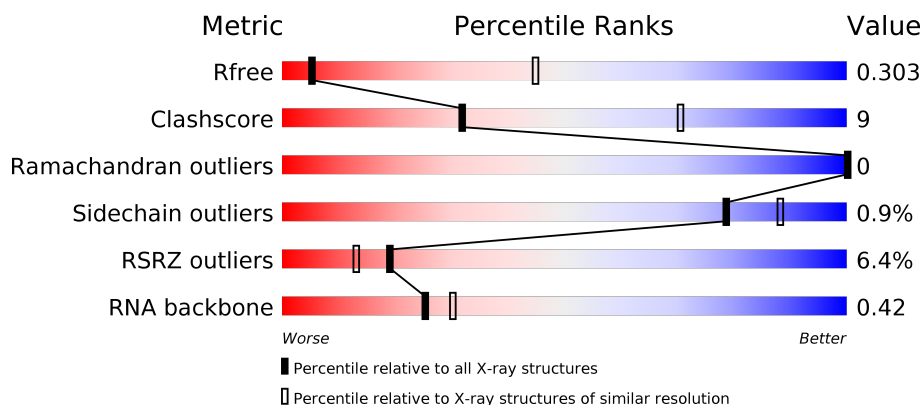
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)
RNA backbone	3102	1027 (4.40-3.00)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	422	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>20%</div> <div>..</div> </div> </div>
1	B	422	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>20%</div> <div>.</div> </div> </div>
1	C	422	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>21%</div> <div>..</div> </div> </div>
1	D	422	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div>.</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	422	
1	F	422	
1	G	422	
1	H	422	
1	I	422	
1	J	422	
1	K	422	
1	L	422	
2	M	60	
2	N	60	
2	O	60	
2	P	60	
2	Q	60	
2	R	60	
2	S	60	
2	T	60	
2	U	60	
2	V	60	
2	W	60	
2	X	60	
3	Y	12	
3	Z	12	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 43612 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 Transcription termination factor Rho.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	409	Total	C	N	O	S	0	0	0
			3207	2019	566	606	16			
1	A	414	Total	C	N	O	S	0	0	0
			3232	2034	571	611	16			
1	G	414	Total	C	N	O	S	0	0	0
			3232	2034	571	611	16			
1	B	409	Total	C	N	O	S	0	0	0
			3207	2019	566	606	16			
1	H	409	Total	C	N	O	S	0	0	0
			3207	2019	566	606	16			
1	C	414	Total	C	N	O	S	0	0	0
			3232	2034	571	611	16			
1	I	414	Total	C	N	O	S	0	0	0
			3232	2034	571	611	16			
1	D	409	Total	C	N	O	S	0	0	0
			3207	2019	566	606	16			
1	K	414	Total	C	N	O	S	0	0	0
			3232	2034	571	611	16			
1	F	409	Total	C	N	O	S	0	0	0
			3207	2019	566	606	16			
1	J	409	Total	C	N	O	S	0	0	0
			3207	2019	566	606	16			
1	E	414	Total	C	N	O	S	0	0	0
			3232	2034	571	611	16			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	-2	MET	-	initiating methionine	UNP F4TMM7
L	-1	GLY	-	expression tag	UNP F4TMM7
L	0	HIS	-	expression tag	UNP F4TMM7
A	-2	MET	-	initiating methionine	UNP F4TMM7
A	-1	GLY	-	expression tag	UNP F4TMM7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP F4TMM7
G	-2	MET	-	initiating methionine	UNP F4TMM7
G	-1	GLY	-	expression tag	UNP F4TMM7
G	0	HIS	-	expression tag	UNP F4TMM7
B	-2	MET	-	initiating methionine	UNP F4TMM7
B	-1	GLY	-	expression tag	UNP F4TMM7
B	0	HIS	-	expression tag	UNP F4TMM7
H	-2	MET	-	initiating methionine	UNP F4TMM7
H	-1	GLY	-	expression tag	UNP F4TMM7
H	0	HIS	-	expression tag	UNP F4TMM7
C	-2	MET	-	initiating methionine	UNP F4TMM7
C	-1	GLY	-	expression tag	UNP F4TMM7
C	0	HIS	-	expression tag	UNP F4TMM7
I	-2	MET	-	initiating methionine	UNP F4TMM7
I	-1	GLY	-	expression tag	UNP F4TMM7
I	0	HIS	-	expression tag	UNP F4TMM7
D	-2	MET	-	initiating methionine	UNP F4TMM7
D	-1	GLY	-	expression tag	UNP F4TMM7
D	0	HIS	-	expression tag	UNP F4TMM7
K	-2	MET	-	initiating methionine	UNP F4TMM7
K	-1	GLY	-	expression tag	UNP F4TMM7
K	0	HIS	-	expression tag	UNP F4TMM7
F	-2	MET	-	initiating methionine	UNP F4TMM7
F	-1	GLY	-	expression tag	UNP F4TMM7
F	0	HIS	-	expression tag	UNP F4TMM7
J	-2	MET	-	initiating methionine	UNP F4TMM7
J	-1	GLY	-	expression tag	UNP F4TMM7
J	0	HIS	-	expression tag	UNP F4TMM7
E	-2	MET	-	initiating methionine	UNP F4TMM7
E	-1	GLY	-	expression tag	UNP F4TMM7
E	0	HIS	-	expression tag	UNP F4TMM7

- Molecule 2 is a protein called Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	43	Total	C	N	O	S	0	0	0
			323	206	51	65	1			
2	N	43	Total	C	N	O	S	0	0	0
			323	206	51	65	1			
2	O	43	Total	C	N	O	S	0	0	0
			323	206	51	65	1			
2	P	43	Total	C	N	O	S	0	0	0
			323	206	51	65	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Q	43	Total	C	N	O	S	0	0	0
			323	206	51	65	1			
2	R	43	Total	C	N	O	S	0	0	0
			323	206	51	65	1			
2	S	43	Total	C	N	O	S	0	0	0
			323	206	51	65	1			
2	T	43	Total	C	N	O	S	0	0	0
			323	206	51	65	1			
2	U	43	Total	C	N	O	S	0	0	0
			323	206	51	65	1			
2	V	43	Total	C	N	O	S	0	0	0
			323	206	51	65	1			
2	W	43	Total	C	N	O	S	0	0	0
			319	204	51	63	1			
2	X	43	Total	C	N	O	S	0	0	0
			319	204	51	63	1			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	122	SER	-	expression tag	UNP F4T6L5
M	123	ASN	-	expression tag	UNP F4T6L5
M	124	ALA	-	expression tag	UNP F4T6L5
N	122	SER	-	expression tag	UNP F4T6L5
N	123	ASN	-	expression tag	UNP F4T6L5
N	124	ALA	-	expression tag	UNP F4T6L5
O	122	SER	-	expression tag	UNP F4T6L5
O	123	ASN	-	expression tag	UNP F4T6L5
O	124	ALA	-	expression tag	UNP F4T6L5
P	122	SER	-	expression tag	UNP F4T6L5
P	123	ASN	-	expression tag	UNP F4T6L5
P	124	ALA	-	expression tag	UNP F4T6L5
Q	122	SER	-	expression tag	UNP F4T6L5
Q	123	ASN	-	expression tag	UNP F4T6L5
Q	124	ALA	-	expression tag	UNP F4T6L5
R	122	SER	-	expression tag	UNP F4T6L5
R	123	ASN	-	expression tag	UNP F4T6L5
R	124	ALA	-	expression tag	UNP F4T6L5
S	122	SER	-	expression tag	UNP F4T6L5
S	123	ASN	-	expression tag	UNP F4T6L5
S	124	ALA	-	expression tag	UNP F4T6L5
T	122	SER	-	expression tag	UNP F4T6L5
T	123	ASN	-	expression tag	UNP F4T6L5

Continued on next page...

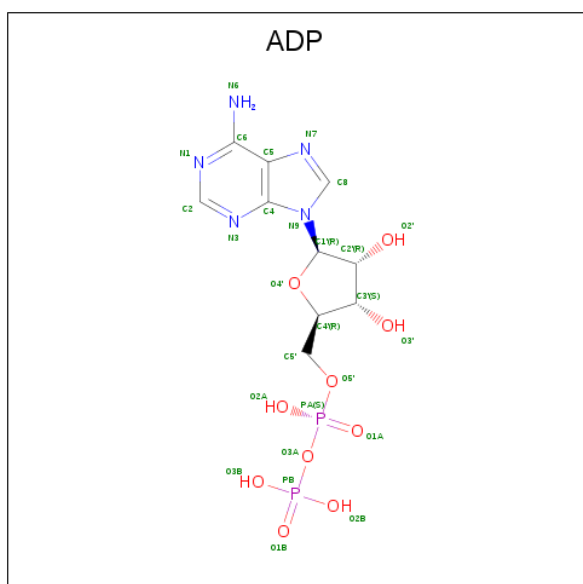
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
T	124	ALA	-	expression tag	UNP F4T6L5
U	122	SER	-	expression tag	UNP F4T6L5
U	123	ASN	-	expression tag	UNP F4T6L5
U	124	ALA	-	expression tag	UNP F4T6L5
V	122	SER	-	expression tag	UNP F4T6L5
V	123	ASN	-	expression tag	UNP F4T6L5
V	124	ALA	-	expression tag	UNP F4T6L5
W	122	SER	-	expression tag	UNP F4T6L5
W	123	ASN	-	expression tag	UNP F4T6L5
W	124	ALA	-	expression tag	UNP F4T6L5
X	122	SER	-	expression tag	UNP F4T6L5
X	123	ASN	-	expression tag	UNP F4T6L5
X	124	ALA	-	expression tag	UNP F4T6L5

- Molecule 3 is a RNA chain called rU12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Y	6	Total	C	N	O	P	0	6	0
			363	162	36	147	18			
3	Z	6	Total	C	N	O	P	0	6	0
			363	162	36	147	18			

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

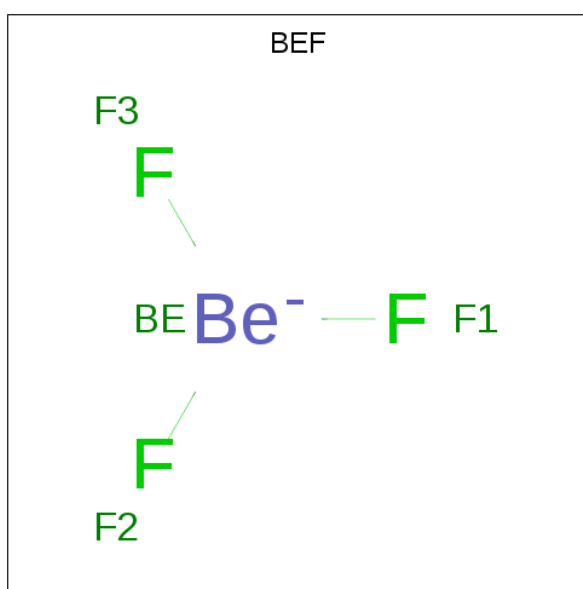
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Mg	0	0
			1	1		
5	J	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	K	1	Total	Mg	0	0
			1	1		
5	E	1	Total	Mg	0	0
			1	1		
5	H	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		
5	I	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total 1	Mg 1	0	0
5	A	1	Total 1	Mg 1	0	0
5	L	1	Total 1	Mg 1	0	0
5	F	1	Total 1	Mg 1	0	0

- Molecule 6 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total 4	Be 1	F 3	0	0
6	A	1	Total 4	Be 1	F 3	0	0
6	G	1	Total 4	Be 1	F 3	0	0
6	B	1	Total 4	Be 1	F 3	0	0
6	H	1	Total 4	Be 1	F 3	0	0
6	C	1	Total 4	Be 1	F 3	0	0
6	I	1	Total 4	Be 1	F 3	0	0

Continued on next page...

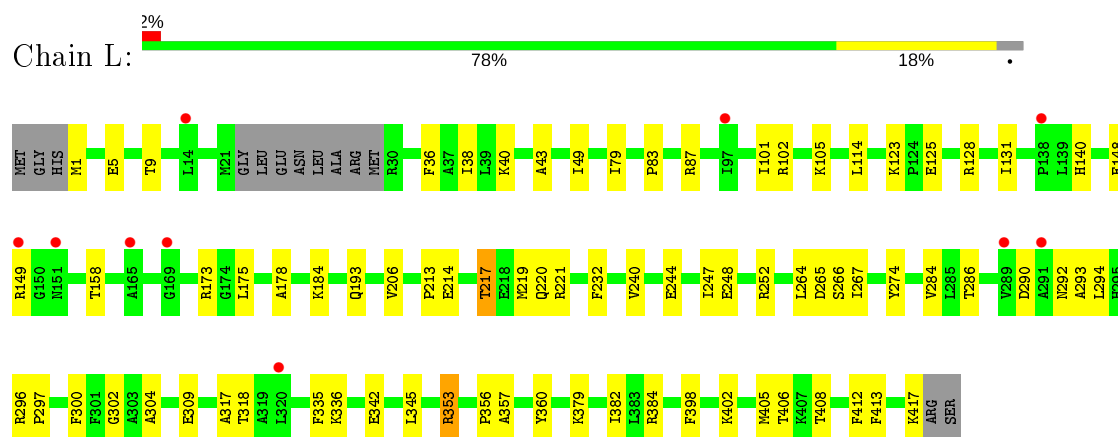
Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total 4	Be 1	F 3	0	0
6	K	1	Total 4	Be 1	F 3	0	0
6	F	1	Total 4	Be 1	F 3	0	0
6	J	1	Total 4	Be 1	F 3	0	0
6	E	1	Total 4	Be 1	F 3	0	0

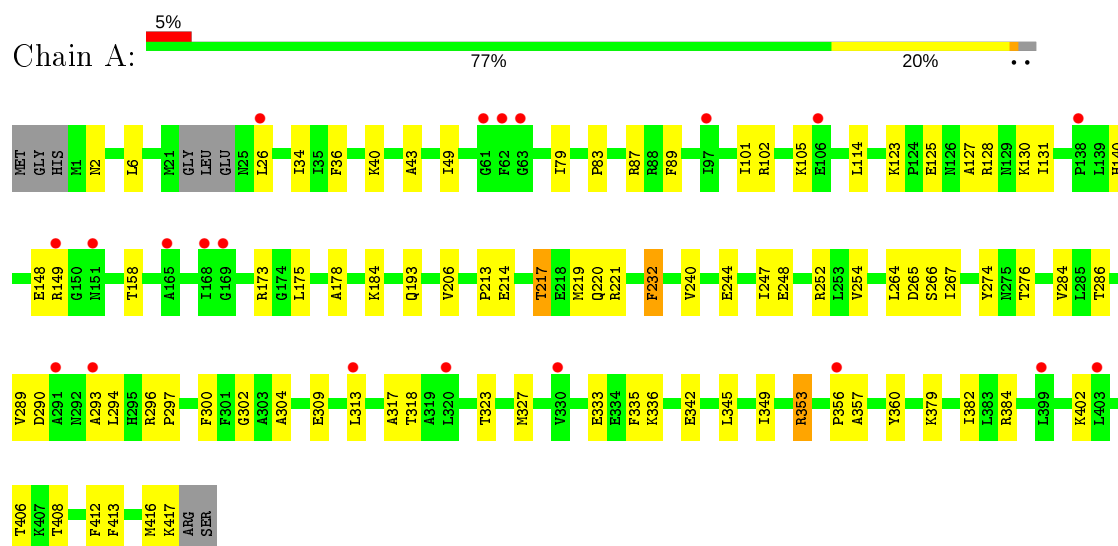
3 Residue-property plots [i](#)

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.

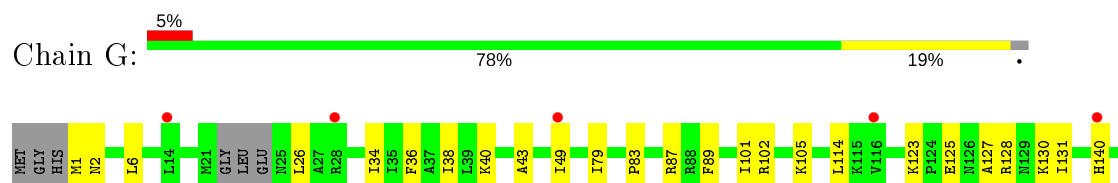
• Molecule 1: Transcription termination factor Rho

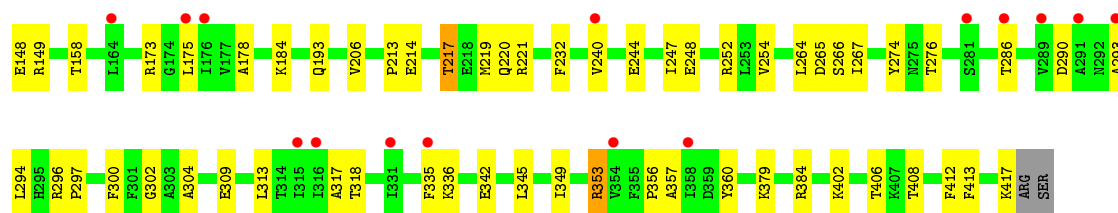


• Molecule 1: Transcription termination factor Rho

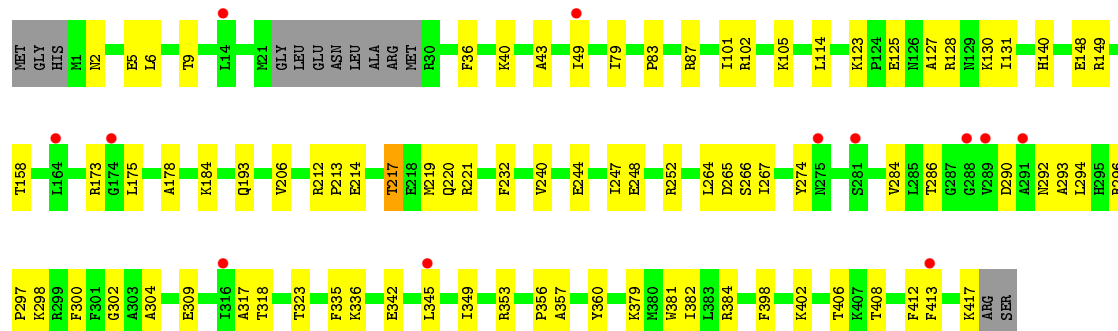
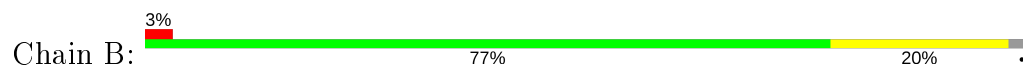


• Molecule 1: Transcription termination factor Rho

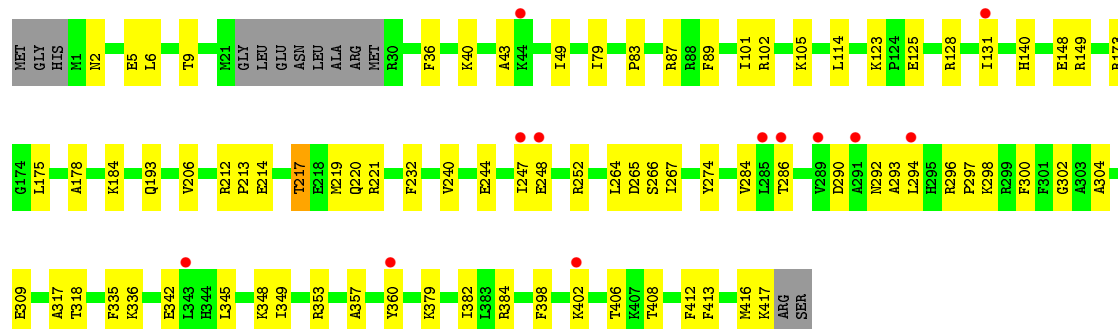
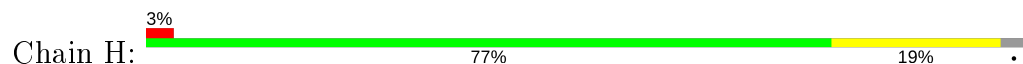




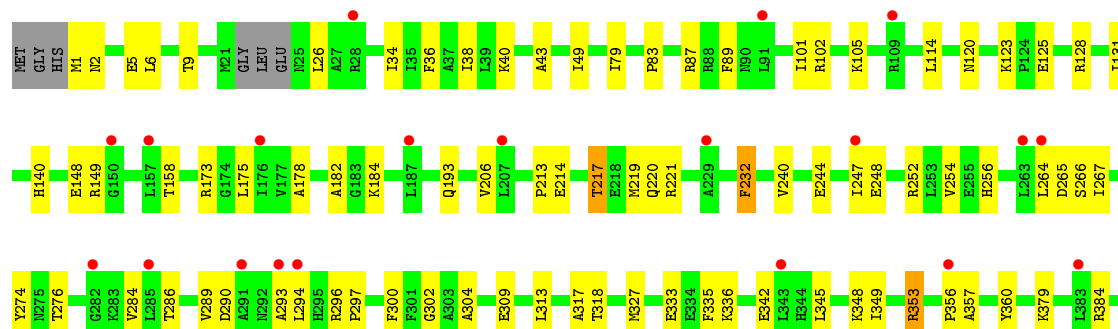
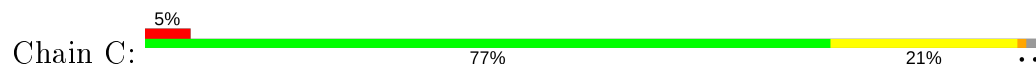
• Molecule 1: Transcription termination factor Rho

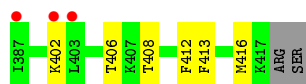


• Molecule 1: Transcription termination factor Rho

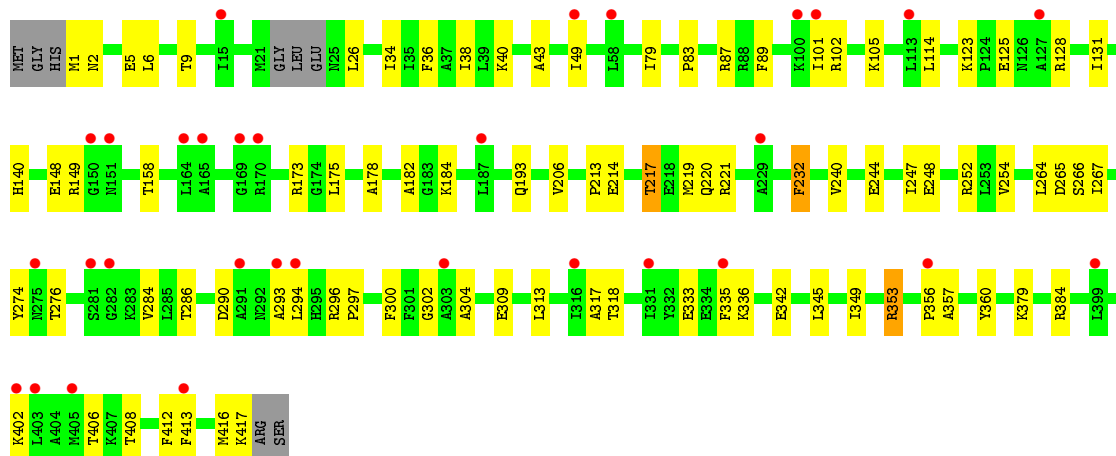
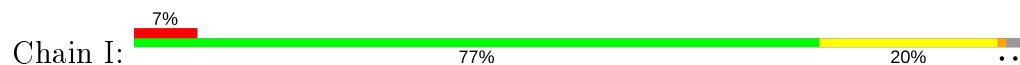


• Molecule 1: Transcription termination factor Rho

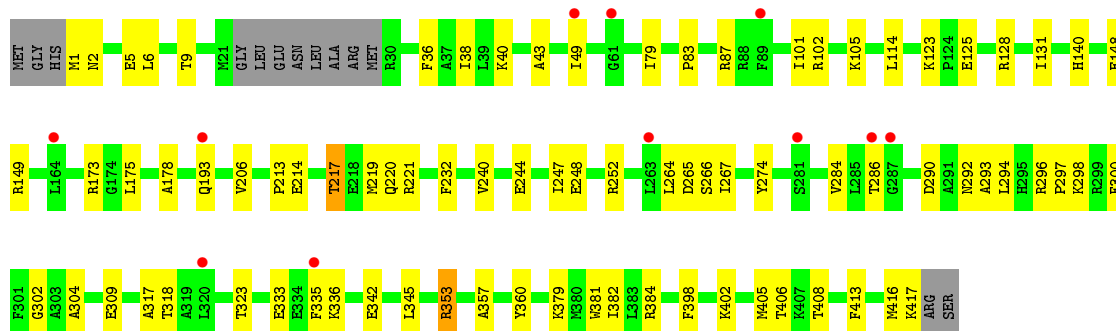
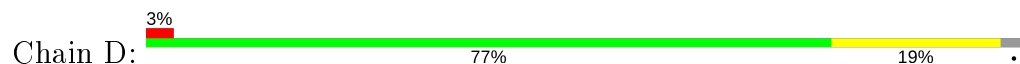




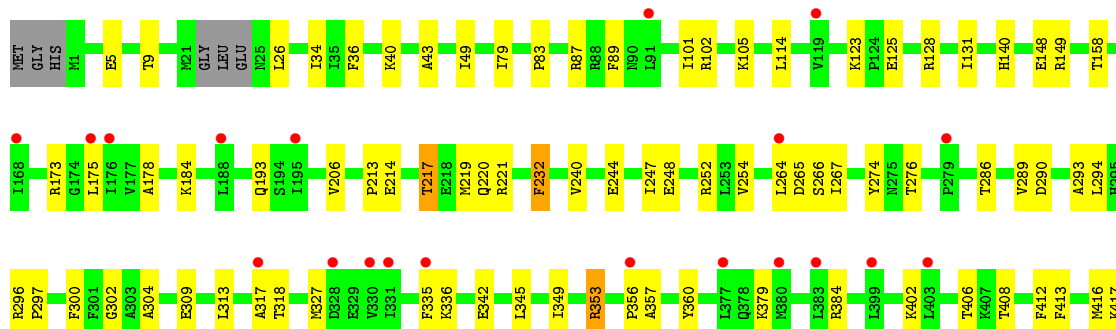
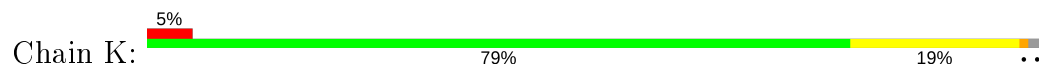
• Molecule 1: Transcription termination factor Rho



• Molecule 1: Transcription termination factor Rho




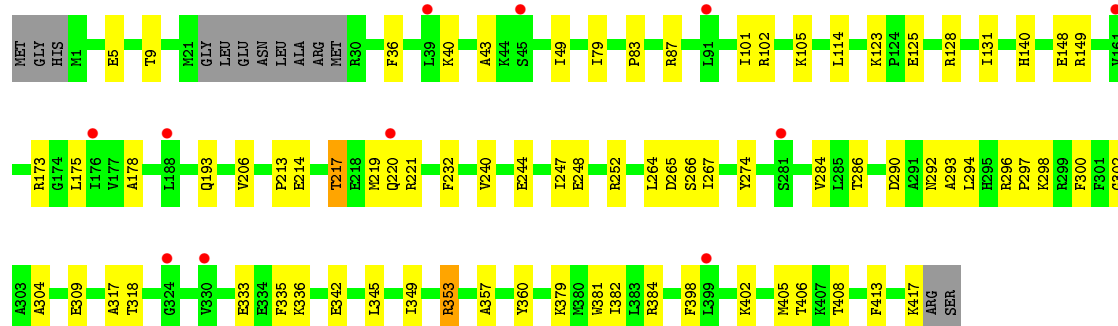
• Molecule 1: Transcription termination factor Rho




ARG
SER

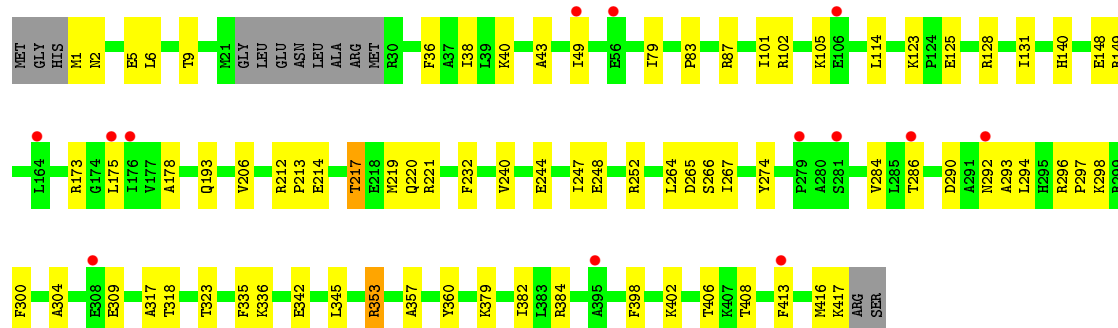
• Molecule 1: Transcription termination factor Rho

Chain F: 




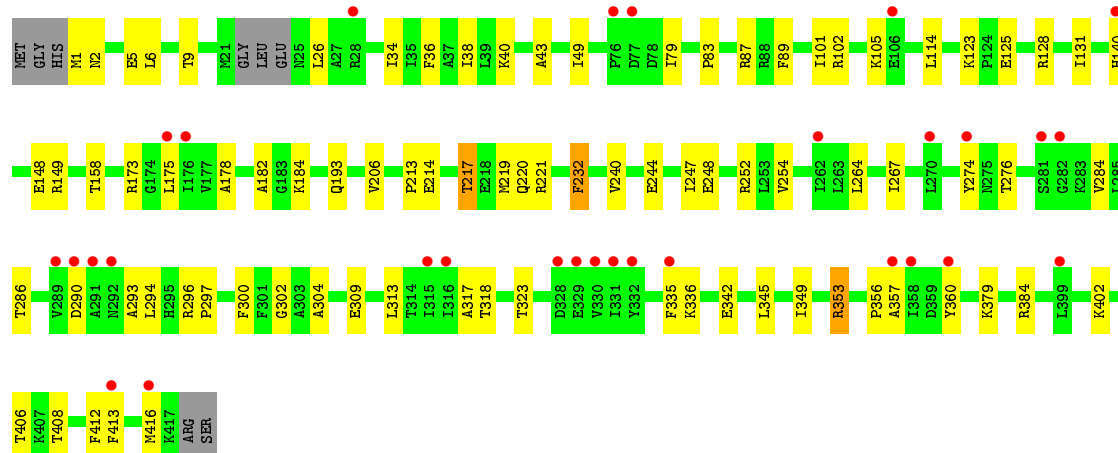
• Molecule 1: Transcription termination factor Rho

Chain J: 

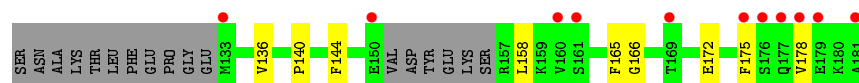


• Molecule 1: Transcription termination factor Rho

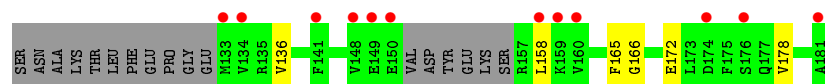
Chain E: 



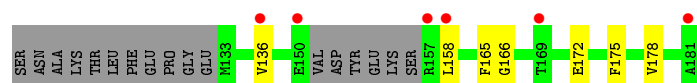
• Molecule 2: Transcription termination/antitermination protein NusG



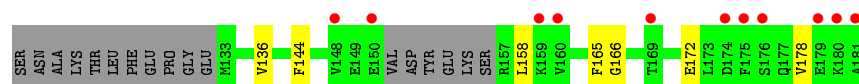
- Molecule 2: Transcription termination/antitermination protein NusG



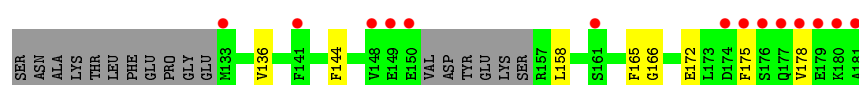
- Molecule 2: Transcription termination/antitermination protein NusG



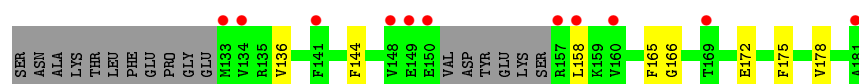
- Molecule 2: Transcription termination/antitermination protein NusG



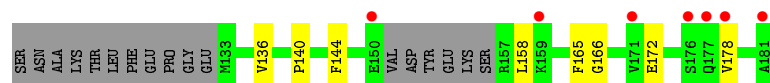
- Molecule 2: Transcription termination/antitermination protein NusG



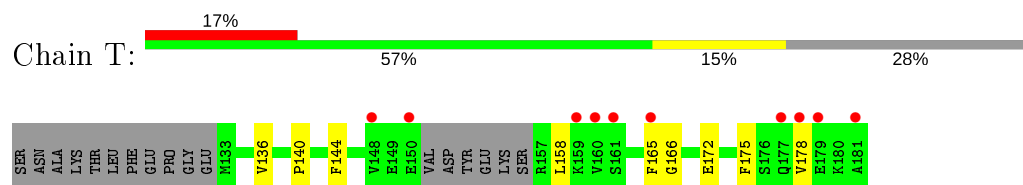
- Molecule 2: Transcription termination/antitermination protein NusG



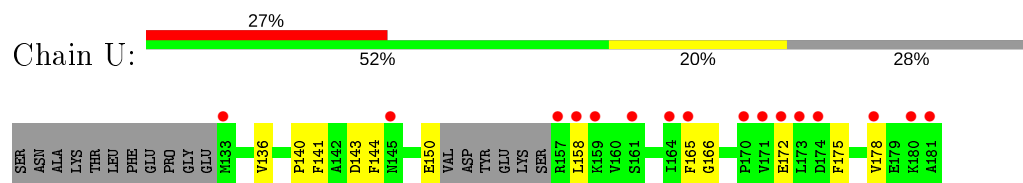
- Molecule 2: Transcription termination/antitermination protein NusG



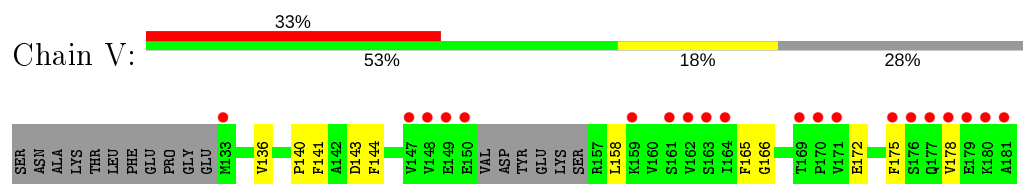
- Molecule 2: Transcription termination/antitermination protein NusG



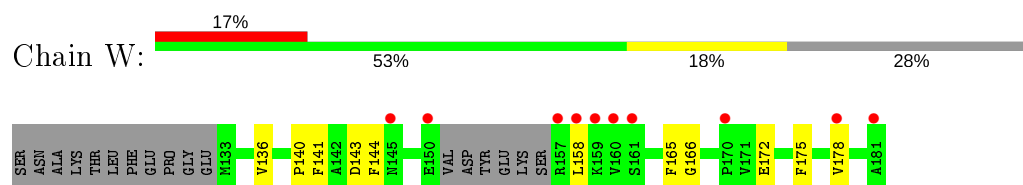
- Molecule 2: Transcription termination/antitermination protein NusG



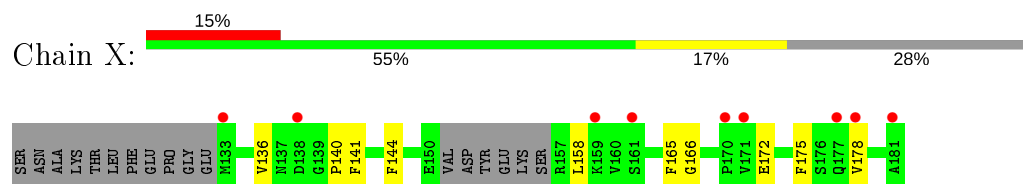
- Molecule 2: Transcription termination/antitermination protein NusG



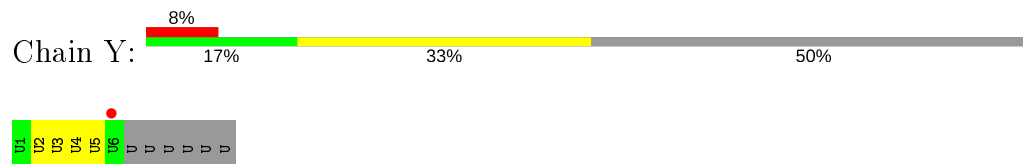
- Molecule 2: Transcription termination/antitermination protein NusG



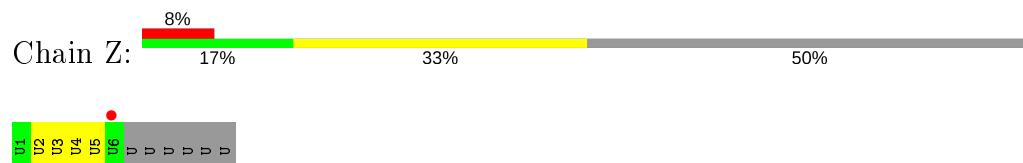
- Molecule 2: Transcription termination/antitermination protein NusG



- Molecule 3: rU12



- Molecule 3: rU12



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	126.35Å 126.32Å 166.82Å 89.94° 89.90° 60.01°	Depositor
Resolution (Å)	39.03 – 3.70 39.03 – 3.40	Depositor EDS
% Data completeness (in resolution range)	97.7 (39.03-3.70) 96.7 (39.03-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 3.40Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.287 , 0.300 0.289 , 0.303	Depositor DCC
R_{free} test set	1958 reflections (1.63%)	wwPDB-VP
Wilson B-factor (Å ²)	103.0	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 99.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.317 for h-k,h,l 0.317 for k,-h+k,l 0.307 for -k,h-k,l 0.307 for -h+k,-h,l 0.126 for -h+k,k,-l 0.127 for h,h-k,-l 0.316 for -h,-k,l 0.125 for k,h,-l 0.126 for -k,-h,-l 0.126 for h-k,-k,-l 0.125 for -h,-h+k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	43612	wwPDB-VP
Average B, all atoms (Å ²)	201.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.00 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6248e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BEF, ADP

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	0.31	0/3280	0.48	0/4422
1	B	0.34	0/3255	0.50	0/4387
1	C	0.32	0/3280	0.48	0/4422
1	D	0.33	0/3255	0.50	0/4387
1	E	0.32	0/3280	0.48	0/4422
1	F	0.34	0/3255	0.50	0/4387
1	G	0.32	0/3280	0.48	0/4422
1	H	0.33	0/3255	0.49	0/4387
1	I	0.32	0/3280	0.48	0/4422
1	J	0.33	0/3255	0.50	0/4387
1	K	0.31	0/3280	0.48	0/4422
1	L	0.34	0/3255	0.50	0/4387
2	M	0.41	0/327	0.60	0/440
2	N	0.40	0/327	0.60	0/440
2	O	0.40	0/327	0.60	0/440
2	P	0.40	0/327	0.60	0/440
2	Q	0.39	0/327	0.60	0/440
2	R	0.40	0/327	0.60	0/440
2	S	0.55	0/327	0.69	0/440
2	T	0.55	0/327	0.69	0/440
2	U	0.58	0/327	0.71	0/440
2	V	0.47	0/327	0.64	0/440
2	W	0.44	0/323	0.61	0/435
2	X	0.54	0/323	0.69	0/435
3	Y	0.48	0/396	1.02	0/600
3	Z	0.48	0/396	1.05	0/600
All	All	0.34	0/43918	0.52	0/59324

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3232	0	3273	62	0
1	B	3207	0	3260	69	0
1	C	3232	0	3273	62	0
1	D	3207	0	3260	68	0
1	E	3232	0	3273	61	0
1	F	3207	0	3260	67	0
1	G	3232	0	3273	54	0
1	H	3207	0	3260	67	0
1	I	3232	0	3273	60	0
1	J	3207	0	3260	69	0
1	K	3232	0	3273	58	0
1	L	3207	0	3260	63	0
2	M	323	0	307	6	0
2	N	323	0	307	3	0
2	O	323	0	307	4	0
2	P	323	0	307	4	0
2	Q	323	0	307	5	0
2	R	323	0	307	5	0
2	S	323	0	307	15	0
2	T	323	0	307	16	0
2	U	323	0	307	19	0
2	V	323	0	307	14	0
2	W	319	0	303	20	0
2	X	319	0	303	15	0
3	Y	363	0	183	22	0
3	Z	363	0	183	16	0
4	A	27	0	12	0	0
4	B	27	0	12	0	0
4	C	27	0	12	0	0
4	D	27	0	12	0	0
4	E	27	0	12	0	0
4	F	27	0	12	0	0
4	G	27	0	12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	27	0	12	0	0
4	I	27	0	12	0	0
4	J	27	0	12	0	0
4	K	27	0	12	0	0
4	L	27	0	12	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
6	A	4	0	0	0	0
6	B	4	0	0	0	0
6	C	4	0	0	0	0
6	D	4	0	0	0	0
6	E	4	0	0	0	0
6	F	4	0	0	0	0
6	G	4	0	0	0	0
6	H	4	0	0	0	0
6	I	4	0	0	0	0
6	J	4	0	0	0	0
6	K	4	0	0	0	0
6	L	4	0	0	0	0
All	All	43612	0	43384	776	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 9.

All (776) 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:F:402:LYS:HG3	2:U:165:PHE:HE1	1.17	1.08
1:K:286:THR:HA	3:Z:5[A]:U:H4'	1.48	0.95
1:F:402:LYS:HG3	2:U:165:PHE:CE1	2.05	0.92
1:J:402:LYS:HG3	2:W:165:PHE:HE1	1.38	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:286:THR:HA	3:Z:5[B]:U:H4'	1.56	0.88
1:B:402:LYS:HG3	2:S:165:PHE:HE1	1.39	0.87
1:E:286:THR:HA	3:Y:5[A]:U:H4'	1.60	0.83
1:B:417:LYS:HA	2:S:144:PHE:HE1	1.46	0.80
1:A:286:THR:HA	3:Y:5[B]:U:H4'	1.62	0.80
1:J:398:PHE:CE1	2:W:165:PHE:CZ	2.70	0.80
1:D:402:LYS:HG3	2:T:165:PHE:CE1	2.15	0.80
1:C:286:THR:HA	3:Y:5[C]:U:H4'	1.63	0.79
1:B:417:LYS:HA	2:S:144:PHE:CE1	2.19	0.78
1:B:402:LYS:HG3	2:S:165:PHE:CE1	2.20	0.76
1:D:125:GLU:HA	1:D:128:ARG:HD3	1.69	0.75
1:D:402:LYS:HG3	2:T:165:PHE:HE1	1.51	0.74
1:B:125:GLU:HA	1:B:128:ARG:HD3	1.70	0.74
1:L:417:LYS:HA	2:X:144:PHE:HE1	1.51	0.74
1:D:417:LYS:HA	2:T:144:PHE:CE1	2.22	0.74
1:C:125:GLU:HA	1:C:128:ARG:HD3	1.70	0.74
1:G:125:GLU:HA	1:G:128:ARG:HD3	1.70	0.74
1:L:125:GLU:HA	1:L:128:ARG:HD3	1.70	0.74
1:I:125:GLU:HA	1:I:128:ARG:HD3	1.70	0.73
1:A:125:GLU:HA	1:A:128:ARG:HD3	1.70	0.73
1:F:125:GLU:HA	1:F:128:ARG:HD3	1.70	0.73
1:J:125:GLU:HA	1:J:128:ARG:HD3	1.70	0.73
1:L:417:LYS:HA	2:X:144:PHE:CE1	2.23	0.73
1:H:125:GLU:HA	1:H:128:ARG:HD3	1.71	0.73
1:D:417:LYS:HA	2:T:144:PHE:HE1	1.52	0.73
1:K:125:GLU:HA	1:K:128:ARG:HD3	1.70	0.72
1:J:286:THR:HA	3:Z:4[C]:U:H5''	1.72	0.72
1:E:125:GLU:HA	1:E:128:ARG:HD3	1.71	0.72
1:H:417:LYS:HA	2:V:144:PHE:HE1	1.54	0.72
1:D:286:THR:HA	3:Y:4[C]:U:H5''	1.72	0.72
1:I:286:THR:HA	3:Z:5[C]:U:H4'	1.71	0.71
1:J:417:LYS:HA	2:W:144:PHE:CE1	2.27	0.69
2:U:165:PHE:CD2	2:U:166:GLY:N	2.60	0.68
1:H:417:LYS:HA	2:V:144:PHE:CE1	2.28	0.68
1:L:402:LYS:HG3	2:X:165:PHE:HE1	1.57	0.68
1:H:286:THR:HA	3:Z:4[B]:U:H5''	1.77	0.67
1:A:382:ILE:HD11	2:M:140:PRO:HB2	1.75	0.67
1:J:382:ILE:HD11	2:W:140:PRO:O	1.94	0.67
1:B:284:VAL:HB	3:Y:2[A]:U:H5'	1.77	0.65
1:A:417:LYS:HA	2:M:144:PHE:HE1	1.60	0.64
1:H:87:ARG:NH2	2:U:150:GLU:OE2	2.30	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:TYR:HE2	1:A:384:ARG:HG2	1.62	0.64
1:G:360:TYR:HE2	1:G:384:ARG:HG2	1.61	0.63
1:H:398:PHE:HE1	2:V:165:PHE:CZ	2.16	0.63
1:K:360:TYR:HE2	1:K:384:ARG:HG2	1.63	0.63
1:H:382:ILE:HD11	2:V:140:PRO:O	1.99	0.63
2:T:165:PHE:CD2	2:T:166:GLY:N	2.66	0.62
1:K:214:GLU:HG3	1:J:140:HIS:CE1	2.35	0.62
1:I:360:TYR:HE2	1:I:384:ARG:HG2	1.63	0.62
1:J:398:PHE:HE1	2:W:165:PHE:CZ	2.17	0.62
1:H:284:VAL:HB	3:Z:2[A]:U:H5'	1.80	0.62
1:L:43:ALA:HB2	1:L:49:ILE:HD11	1.82	0.62
1:L:382:ILE:HD11	2:X:140:PRO:O	1.99	0.62
1:D:43:ALA:HB2	1:D:49:ILE:HD11	1.81	0.62
1:A:43:ALA:HB2	1:A:49:ILE:HD11	1.82	0.61
1:G:43:ALA:HB2	1:G:49:ILE:HD11	1.82	0.61
1:E:360:TYR:HE2	1:E:384:ARG:HG2	1.64	0.61
1:F:286:THR:HA	3:Y:4[A]:U:H5''	1.83	0.61
1:J:417:LYS:HD2	2:W:143:ASP:O	2.01	0.61
1:J:43:ALA:HB2	1:J:49:ILE:HD11	1.82	0.61
1:I:43:ALA:HB2	1:I:49:ILE:HD11	1.82	0.61
1:K:43:ALA:HB2	1:K:49:ILE:HD11	1.82	0.60
1:F:382:ILE:HD11	2:U:140:PRO:O	2.00	0.60
1:B:43:ALA:HB2	1:B:49:ILE:HD11	1.83	0.60
1:E:43:ALA:HB2	1:E:49:ILE:HD11	1.83	0.60
1:F:417:LYS:HA	2:U:144:PHE:CE1	2.37	0.60
1:L:286:THR:HA	3:Z:4[A]:U:H5''	1.83	0.60
1:F:43:ALA:HB2	1:F:49:ILE:HD11	1.82	0.60
1:C:43:ALA:HB2	1:C:49:ILE:HD11	1.82	0.60
1:D:140:HIS:CE1	1:E:214:GLU:HG3	2.37	0.60
1:H:43:ALA:HB2	1:H:49:ILE:HD11	1.82	0.60
1:C:360:TYR:HE2	1:C:384:ARG:HG2	1.65	0.59
1:B:382:ILE:HD11	2:S:140:PRO:O	2.02	0.59
2:U:140:PRO:HG2	2:U:141:PHE:CD2	2.37	0.59
1:F:402:LYS:HZ3	2:U:165:PHE:HZ	1.50	0.59
1:D:284:VAL:O	3:Y:3[C]:U:O2'	2.20	0.59
1:J:402:LYS:HG3	2:W:165:PHE:CE1	2.29	0.58
1:L:284:VAL:HB	3:Z:2[C]:U:H5'	1.83	0.58
1:F:382:ILE:HG12	2:U:140:PRO:HB2	1.86	0.58
1:J:267:ILE:HB	1:J:317:ALA:HB1	1.86	0.58
2:S:165:PHE:CD2	2:S:166:GLY:N	2.72	0.58
2:U:165:PHE:HD2	2:U:166:GLY:H	1.50	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:GLU:HG3	1:F:140:HIS:CE1	2.38	0.58
1:B:398:PHE:CE1	2:S:165:PHE:CZ	2.91	0.58
1:B:123:LYS:HD2	1:B:125:GLU:HB2	1.85	0.57
1:B:284:VAL:O	3:Y:3[B]:U:O2'	2.22	0.57
1:L:123:LYS:HD2	1:L:125:GLU:HB2	1.85	0.57
1:F:398:PHE:CE1	2:U:165:PHE:CZ	2.92	0.57
1:E:267:ILE:HB	1:E:317:ALA:HB1	1.86	0.57
1:D:267:ILE:HB	1:D:317:ALA:HB1	1.86	0.57
1:F:123:LYS:HD2	1:F:125:GLU:HB2	1.86	0.57
1:H:123:LYS:HD2	1:H:125:GLU:HB2	1.86	0.57
2:T:165:PHE:HD2	2:T:166:GLY:H	1.52	0.57
1:J:402:LYS:CG	2:W:165:PHE:HE1	2.13	0.57
1:A:123:LYS:HD2	1:A:125:GLU:HB2	1.87	0.57
1:D:402:LYS:HG3	2:T:165:PHE:CZ	2.40	0.57
1:K:267:ILE:HB	1:K:317:ALA:HB1	1.86	0.57
1:F:267:ILE:HB	1:F:317:ALA:HB1	1.86	0.57
1:G:267:ILE:HB	1:G:317:ALA:HB1	1.86	0.57
1:B:267:ILE:HB	1:B:317:ALA:HB1	1.86	0.57
1:D:382:ILE:HD11	2:T:140:PRO:O	2.05	0.56
1:J:123:LYS:HD2	1:J:125:GLU:HB2	1.86	0.56
1:A:267:ILE:HB	1:A:317:ALA:HB1	1.86	0.56
1:B:83:PRO:O	1:B:87:ARG:HG3	2.05	0.56
1:I:267:ILE:HB	1:I:317:ALA:HB1	1.87	0.56
2:W:165:PHE:CD2	2:W:166:GLY:N	2.74	0.56
2:X:165:PHE:CD2	2:X:166:GLY:N	2.73	0.56
1:D:123:LYS:HD2	1:D:125:GLU:HB2	1.86	0.56
1:E:123:LYS:HD2	1:E:125:GLU:HB2	1.87	0.56
1:H:140:HIS:CE1	1:I:214:GLU:HG3	2.41	0.56
1:A:217:THR:O	1:A:221:ARG:HD3	2.06	0.56
1:G:123:LYS:HD2	1:G:125:GLU:HB2	1.87	0.56
1:D:398:PHE:CE1	2:T:165:PHE:CZ	2.94	0.56
1:H:267:ILE:HB	1:H:317:ALA:HB1	1.86	0.56
1:I:140:HIS:CE1	1:J:214:GLU:HG3	2.41	0.56
1:K:123:LYS:HD2	1:K:125:GLU:HB2	1.88	0.56
1:C:267:ILE:HB	1:C:317:ALA:HB1	1.87	0.55
1:F:402:LYS:HE3	1:F:405:MET:CE	2.37	0.55
1:C:123:LYS:HD2	1:C:125:GLU:HB2	1.87	0.55
1:L:267:ILE:HB	1:L:317:ALA:HB1	1.87	0.55
2:V:165:PHE:CD2	2:V:166:GLY:N	2.74	0.55
1:G:178:ALA:HB2	1:G:345:LEU:HB2	1.89	0.55
1:A:178:ALA:HB2	1:A:345:LEU:HB2	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:178:ALA:HB2	1:K:345:LEU:HB2	1.89	0.55
1:F:417:LYS:HD2	2:U:143:ASP:O	2.07	0.55
1:D:217:THR:O	1:D:221:ARG:HD3	2.06	0.55
1:G:217:THR:O	1:G:221:ARG:HD3	2.07	0.54
1:K:232:PHE:HB2	1:J:298:LYS:HE2	1.88	0.54
1:A:360:TYR:CE2	1:A:384:ARG:HG2	2.41	0.54
1:E:178:ALA:HB2	1:E:345:LEU:HB2	1.90	0.54
1:F:284:VAL:O	3:Y:3[A]:U:O2'	2.22	0.54
1:B:382:ILE:HG12	2:S:140:PRO:HB2	1.90	0.54
1:C:178:ALA:HB2	1:C:345:LEU:HB2	1.90	0.54
1:H:178:ALA:HB2	1:H:345:LEU:HB2	1.90	0.54
1:I:123:LYS:HD2	1:I:125:GLU:HB2	1.88	0.54
1:F:178:ALA:HB2	1:F:345:LEU:HB2	1.90	0.54
1:J:217:THR:O	1:J:221:ARG:HD3	2.08	0.54
1:L:178:ALA:HB2	1:L:345:LEU:HB2	1.90	0.54
1:E:217:THR:O	1:E:221:ARG:HD3	2.08	0.54
1:I:360:TYR:CE2	1:I:384:ARG:HG2	2.43	0.54
1:H:398:PHE:CE1	2:V:165:PHE:CZ	2.95	0.54
1:B:286:THR:HA	3:Y:4[B]:U:H5''	1.88	0.54
1:D:178:ALA:HB2	1:D:345:LEU:HB2	1.90	0.54
1:G:360:TYR:CE2	1:G:384:ARG:HG2	2.41	0.54
1:K:217:THR:O	1:K:221:ARG:HD3	2.08	0.54
1:F:217:THR:O	1:F:221:ARG:HD3	2.08	0.54
1:L:214:GLU:HG3	1:K:140:HIS:CE1	2.43	0.54
1:B:178:ALA:HB2	1:B:345:LEU:HB2	1.90	0.54
1:F:214:GLU:HG3	1:E:140:HIS:CE1	2.43	0.54
1:D:102:ARG:HB3	1:D:114:LEU:HD21	1.90	0.53
1:L:83:PRO:O	1:L:87:ARG:HG3	2.07	0.53
1:E:284:VAL:N	3:Y:2[C]:U:O2'	2.39	0.53
1:I:178:ALA:HB2	1:I:345:LEU:HB2	1.90	0.53
1:D:298:LYS:HE2	1:E:232:PHE:HB2	1.89	0.53
1:H:102:ARG:HB3	1:H:114:LEU:HD21	1.90	0.53
1:B:36:PHE:CZ	1:B:40:LYS:HD2	2.43	0.53
1:L:402:LYS:HG3	2:X:165:PHE:CE1	2.42	0.53
1:A:102:ARG:HB3	1:A:114:LEU:HD21	1.91	0.53
1:H:36:PHE:CZ	1:H:40:LYS:HD2	2.44	0.53
1:J:178:ALA:HB2	1:J:345:LEU:HB2	1.91	0.53
1:C:217:THR:O	1:C:221:ARG:HD3	2.08	0.53
1:I:102:ARG:HB3	1:I:114:LEU:HD21	1.91	0.53
1:K:276:THR:HG23	1:J:292:ASN:OD1	2.09	0.53
1:B:284:VAL:HB	3:Y:2[A]:U:C5'	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:79:ILE:HD13	1:G:101:ILE:HG21	1.91	0.53
1:D:36:PHE:CZ	1:D:40:LYS:HD2	2.44	0.53
1:J:36:PHE:CZ	1:J:40:LYS:HD2	2.44	0.53
1:D:206:VAL:HG11	1:D:219:MET:HG2	1.91	0.53
1:E:360:TYR:CE2	1:E:384:ARG:HG2	2.43	0.53
1:J:83:PRO:O	1:J:87:ARG:HG3	2.09	0.53
1:L:102:ARG:HB3	1:L:114:LEU:HD21	1.91	0.53
1:B:140:HIS:CE1	1:C:214:GLU:HG3	2.43	0.53
1:C:102:ARG:HB3	1:C:114:LEU:HD21	1.90	0.53
1:C:206:VAL:HG11	1:C:219:MET:HG2	1.91	0.53
1:E:102:ARG:HB3	1:E:114:LEU:HD21	1.91	0.53
1:E:36:PHE:CZ	1:E:40:LYS:HD2	2.44	0.53
1:J:102:ARG:HB3	1:J:114:LEU:HD21	1.91	0.53
1:I:36:PHE:CZ	1:I:40:LYS:HD2	2.44	0.52
1:F:284:VAL:HB	3:Y:2[C]:U:H5'	1.91	0.52
1:B:102:ARG:HB3	1:B:114:LEU:HD21	1.91	0.52
1:B:360:TYR:HE2	1:B:384:ARG:HG2	1.73	0.52
1:C:79:ILE:HD13	1:C:101:ILE:HG21	1.92	0.52
1:G:206:VAL:HG11	1:G:219:MET:HG2	1.90	0.52
1:D:292:ASN:OD1	1:E:276:THR:HG23	2.09	0.52
1:K:360:TYR:CE2	1:K:384:ARG:HG2	2.42	0.52
1:L:140:HIS:CE1	1:G:214:GLU:HG3	2.45	0.52
1:L:360:TYR:HE2	1:L:384:ARG:HG2	1.74	0.52
1:C:140:HIS:CE1	1:D:214:GLU:HG3	2.45	0.52
1:F:102:ARG:HB3	1:F:114:LEU:HD21	1.91	0.52
1:F:36:PHE:CZ	1:F:40:LYS:HD2	2.45	0.52
1:F:417:LYS:HA	2:U:144:PHE:CD1	2.44	0.52
1:G:102:ARG:HB3	1:G:114:LEU:HD21	1.91	0.52
1:I:379:LYS:HD3	1:I:413:PHE:HB3	1.91	0.52
1:C:360:TYR:CE2	1:C:384:ARG:HG2	2.44	0.52
1:F:206:VAL:HG11	1:F:219:MET:HG2	1.90	0.52
1:H:83:PRO:O	1:H:87:ARG:HG3	2.09	0.52
1:I:206:VAL:HG11	1:I:219:MET:HG2	1.92	0.52
1:K:36:PHE:CZ	1:K:40:LYS:HD2	2.45	0.52
1:C:379:LYS:HD3	1:C:413:PHE:HB3	1.91	0.52
1:D:175:LEU:HD11	1:D:335:PHE:HB3	1.92	0.52
1:I:79:ILE:HD13	1:I:101:ILE:HG21	1.91	0.52
1:H:384:ARG:HD2	1:I:353:ARG:NH1	2.25	0.52
1:G:417:LYS:HA	2:P:144:PHE:HE1	1.74	0.52
1:K:379:LYS:HD3	1:K:413:PHE:HB3	1.91	0.52
1:A:206:VAL:HG11	1:A:219:MET:HG2	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:VAL:HG11	1:B:219:MET:HG2	1.91	0.51
1:H:206:VAL:HG11	1:H:219:MET:HG2	1.92	0.51
1:H:360:TYR:HE2	1:H:384:ARG:HG2	1.74	0.51
1:H:379:LYS:HD3	1:H:413:PHE:HB3	1.92	0.51
1:F:379:LYS:HD3	1:F:413:PHE:HB3	1.92	0.51
1:I:217:THR:O	1:I:221:ARG:HD3	2.09	0.51
1:J:398:PHE:HE1	2:W:165:PHE:CE2	2.28	0.51
1:C:36:PHE:CZ	1:C:40:LYS:HD2	2.45	0.51
1:L:379:LYS:HD3	1:L:413:PHE:HB3	1.92	0.51
1:A:36:PHE:CZ	1:A:40:LYS:HD2	2.45	0.51
1:L:206:VAL:HG11	1:L:219:MET:HG2	1.91	0.51
1:L:284:VAL:O	3:Z:3[A]:U:O2'	2.23	0.51
1:L:382:ILE:HG12	2:X:140:PRO:HB2	1.92	0.51
1:B:379:LYS:HD3	1:B:413:PHE:HB3	1.91	0.51
1:E:79:ILE:HD13	1:E:101:ILE:HG21	1.91	0.51
1:E:83:PRO:O	1:E:87:ARG:HG3	2.10	0.51
1:A:379:LYS:HD3	1:A:413:PHE:HB3	1.92	0.51
1:E:379:LYS:HD3	1:E:413:PHE:HB3	1.91	0.51
1:J:206:VAL:HG11	1:J:219:MET:HG2	1.93	0.51
1:L:36:PHE:CZ	1:L:40:LYS:HD2	2.44	0.51
1:E:206:VAL:HG11	1:E:219:MET:HG2	1.92	0.51
1:H:284:VAL:HB	3:Z:2[A]:U:C5'	2.39	0.51
1:I:274:TYR:CD2	1:I:297:PRO:HG3	2.46	0.51
1:K:206:VAL:HG11	1:K:219:MET:HG2	1.92	0.51
1:D:379:LYS:HD3	1:D:413:PHE:HB3	1.92	0.51
1:D:384:ARG:HD2	1:E:353:ARG:NH1	2.25	0.51
1:K:79:ILE:HD13	1:K:101:ILE:HG21	1.92	0.51
1:L:217:THR:O	1:L:221:ARG:HD3	2.11	0.51
1:K:102:ARG:HB3	1:K:114:LEU:HD21	1.92	0.51
1:B:79:ILE:HD13	1:B:101:ILE:HG21	1.93	0.50
1:C:83:PRO:O	1:C:87:ARG:HG3	2.11	0.50
1:E:274:TYR:CD2	1:E:297:PRO:HG3	2.46	0.50
1:A:276:THR:HG23	1:F:292:ASN:OD1	2.10	0.50
1:G:36:PHE:CZ	1:G:40:LYS:HD2	2.45	0.50
1:G:379:LYS:HD3	1:G:413:PHE:HB3	1.91	0.50
1:L:284:VAL:HB	3:Z:2[C]:U:C5'	2.40	0.50
1:E:175:LEU:HD11	1:E:335:PHE:HB3	1.93	0.50
1:G:274:TYR:CD2	1:G:297:PRO:HG3	2.45	0.50
1:G:83:PRO:O	1:G:87:ARG:HG3	2.10	0.50
1:H:175:LEU:HD11	1:H:335:PHE:HB3	1.92	0.50
1:J:175:LEU:HD11	1:J:335:PHE:HB3	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:PRO:O	1:A:87:ARG:HG3	2.11	0.50
1:F:360:TYR:HE2	1:F:384:ARG:HG2	1.77	0.50
1:A:274:TYR:CD2	1:A:297:PRO:HG3	2.45	0.50
1:G:175:LEU:HD11	1:G:335:PHE:HB3	1.93	0.50
1:I:149:ARG:HH21	1:I:193:GLN:HB3	1.77	0.50
1:I:175:LEU:HD11	1:I:335:PHE:HB3	1.93	0.50
1:K:274:TYR:CD2	1:K:297:PRO:HG3	2.45	0.50
1:B:274:TYR:CD2	1:B:297:PRO:HG3	2.46	0.50
1:G:140:HIS:CE1	1:H:214:GLU:HG3	2.46	0.50
1:H:274:TYR:CD2	1:H:297:PRO:HG3	2.47	0.50
1:K:83:PRO:O	1:K:87:ARG:HG3	2.11	0.50
1:A:79:ILE:HD13	1:A:101:ILE:HG21	1.92	0.50
1:D:274:TYR:CD2	1:D:297:PRO:HG3	2.47	0.50
1:F:284:VAL:HB	3:Y:2[C]:U:C5'	2.42	0.50
1:A:286:THR:HA	3:Y:5[B]:U:C4'	2.40	0.49
2:Q:158:LEU:O	2:Q:172:GLU:HA	2.12	0.49
1:C:175:LEU:HD11	1:C:335:PHE:HB3	1.93	0.49
1:B:217:THR:O	1:B:221:ARG:HD3	2.12	0.49
1:C:149:ARG:HH21	1:C:193:GLN:HB3	1.77	0.49
1:E:149:ARG:HH21	1:E:193:GLN:HB3	1.78	0.49
1:G:336:LYS:HE3	1:G:342:GLU:OE1	2.13	0.49
1:J:417:LYS:HA	2:W:144:PHE:HE1	1.75	0.49
1:J:79:ILE:HD13	1:J:101:ILE:HG21	1.92	0.49
1:A:286:THR:HA	3:Y:5[B]:U:C5'	2.42	0.49
1:A:140:HIS:CE1	1:B:214:GLU:HG3	2.48	0.49
1:A:175:LEU:HD11	1:A:335:PHE:HB3	1.93	0.49
1:H:402:LYS:HE2	2:V:165:PHE:CE1	2.47	0.49
1:L:292:ASN:OD1	1:G:276:THR:HG23	2.13	0.49
1:I:83:PRO:O	1:I:87:ARG:HG3	2.12	0.49
1:J:274:TYR:CD2	1:J:297:PRO:HG3	2.47	0.49
1:J:379:LYS:HD3	1:J:413:PHE:HB3	1.93	0.49
1:F:175:LEU:HD11	1:F:335:PHE:HB3	1.93	0.49
1:J:336:LYS:HE3	1:J:342:GLU:OE1	2.12	0.49
1:J:382:ILE:HG12	2:W:140:PRO:HB2	1.94	0.49
1:K:149:ARG:HH21	1:K:193:GLN:HB3	1.78	0.49
2:P:158:LEU:O	2:P:172:GLU:HA	2.12	0.49
1:A:284:VAL:N	3:Y:2[A]:U:O2'	2.38	0.49
1:D:148:GLU:OE1	1:D:408:THR:HA	2.13	0.49
1:F:290:ASP:HB3	1:F:293:ALA:HB2	1.95	0.49
1:J:290:ASP:HB3	1:J:293:ALA:HB2	1.95	0.49
1:K:175:LEU:HD11	1:K:335:PHE:HB3	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:158:LEU:O	2:O:172:GLU:HA	2.13	0.49
1:F:83:PRO:O	1:F:87:ARG:HG3	2.12	0.49
1:H:298:LYS:HE2	1:I:232:PHE:HB2	1.95	0.49
1:H:79:ILE:HD13	1:H:101:ILE:HG21	1.95	0.49
1:B:381:TRP:CZ3	2:S:140:PRO:HG3	2.48	0.49
1:A:232:PHE:HB2	1:F:298:LYS:HE2	1.95	0.49
1:D:79:ILE:HD13	1:D:101:ILE:HG21	1.94	0.49
1:D:336:LYS:HE3	1:D:342:GLU:OE1	2.13	0.49
1:D:83:PRO:O	1:D:87:ARG:HG3	2.12	0.49
1:H:217:THR:O	1:H:221:ARG:HD3	2.11	0.49
1:C:274:TYR:CD2	1:C:297:PRO:HG3	2.48	0.48
1:D:149:ARG:HH21	1:D:193:GLN:HB3	1.79	0.48
1:D:360:TYR:HE2	1:D:384:ARG:HG2	1.77	0.48
2:R:158:LEU:O	2:R:172:GLU:HA	2.13	0.48
2:M:158:LEU:O	2:M:172:GLU:HA	2.13	0.48
1:B:292:ASN:OD1	1:C:276:THR:HG23	2.12	0.48
1:D:240:VAL:O	1:D:244:GLU:HG2	2.13	0.48
1:A:353:ARG:NH1	1:F:384:ARG:HD2	2.29	0.48
1:G:290:ASP:HB3	1:G:293:ALA:HB2	1.94	0.48
1:K:353:ARG:NH1	1:J:384:ARG:HD2	2.27	0.48
2:N:158:LEU:O	2:N:172:GLU:HA	2.13	0.48
1:C:284:VAL:N	3:Y:2[B]:U:O2'	2.41	0.48
1:I:265:ASP:HA	1:I:266:SER:HA	1.61	0.48
1:L:175:LEU:HD11	1:L:335:PHE:HB3	1.94	0.48
1:L:148:GLU:OE1	1:L:408:THR:HA	2.13	0.48
1:B:175:LEU:HD11	1:B:335:PHE:HB3	1.95	0.48
1:B:384:ARG:HD2	1:C:353:ARG:NH1	2.28	0.48
1:F:79:ILE:HD13	1:F:101:ILE:HG21	1.94	0.48
1:G:248:GLU:O	1:G:252:ARG:HG2	2.14	0.48
1:L:149:ARG:HH21	1:L:193:GLN:HB3	1.79	0.48
1:G:149:ARG:HH21	1:G:193:GLN:HB3	1.78	0.48
1:A:149:ARG:HH21	1:A:193:GLN:HB3	1.79	0.48
1:B:213:PRO:HD3	1:B:232:PHE:CZ	2.49	0.48
1:D:265:ASP:HA	1:D:266:SER:HA	1.62	0.48
1:H:292:ASN:OD1	1:I:276:THR:HG23	2.13	0.48
1:J:265:ASP:HA	1:J:266:SER:HA	1.61	0.48
1:F:417:LYS:HG2	2:U:144:PHE:CE1	2.49	0.48
1:F:148:GLU:OE1	1:F:408:THR:HA	2.13	0.48
1:D:284:VAL:HB	3:Y:2[B]:U:C5'	2.44	0.48
1:C:148:GLU:OE1	1:C:408:THR:HA	2.14	0.48
1:F:149:ARG:HH21	1:F:193:GLN:HB3	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:148:GLU:OE1	1:H:408:THR:HA	2.14	0.48
1:L:274:TYR:CD2	1:L:297:PRO:HG3	2.48	0.48
2:S:158:LEU:O	2:S:172:GLU:HA	2.14	0.48
1:A:148:GLU:OE1	1:A:408:THR:HA	2.14	0.47
1:C:265:ASP:HA	1:C:266:SER:HA	1.62	0.47
1:D:36:PHE:CE1	1:D:40:LYS:HD2	2.49	0.47
1:L:398:PHE:CE1	2:X:165:PHE:CZ	3.02	0.47
1:J:149:ARG:HH21	1:J:193:GLN:HB3	1.79	0.47
1:F:336:LYS:HE3	1:F:342:GLU:OE1	2.14	0.47
1:G:265:ASP:HA	1:G:266:SER:HA	1.62	0.47
1:D:381:TRP:CZ3	2:T:140:PRO:HG3	2.49	0.47
1:G:240:VAL:O	1:G:244:GLU:HG2	2.14	0.47
1:H:149:ARG:HH21	1:H:193:GLN:HB3	1.79	0.47
1:J:148:GLU:OE1	1:J:408:THR:HA	2.13	0.47
1:L:336:LYS:HE3	1:L:342:GLU:OE1	2.14	0.47
1:I:148:GLU:OE1	1:I:408:THR:HA	2.15	0.47
1:J:213:PRO:HD3	1:J:232:PHE:CZ	2.49	0.47
1:C:290:ASP:HB3	1:C:293:ALA:HB2	1.96	0.47
1:H:213:PRO:HD3	1:H:232:PHE:CZ	2.50	0.47
1:H:284:VAL:O	3:Z:3[B]:U:O2'	2.24	0.47
1:I:36:PHE:CE1	1:I:40:LYS:HD2	2.50	0.47
1:A:290:ASP:HB3	1:A:293:ALA:HB2	1.96	0.47
1:G:36:PHE:CE1	1:G:40:LYS:HD2	2.50	0.47
1:J:360:TYR:HE2	1:J:384:ARG:HG2	1.79	0.47
1:B:148:GLU:OE1	1:B:408:THR:HA	2.14	0.47
1:B:36:PHE:CE1	1:B:40:LYS:HD2	2.50	0.47
1:I:290:ASP:HB3	1:I:293:ALA:HB2	1.96	0.47
1:L:79:ILE:HD13	1:L:101:ILE:HG21	1.95	0.47
1:I:417:LYS:HA	2:Q:144:PHE:HE1	1.80	0.47
2:T:158:LEU:O	2:T:172:GLU:HA	2.15	0.47
1:G:148:GLU:OE1	1:G:408:THR:HA	2.14	0.47
1:I:248:GLU:O	1:I:252:ARG:HG2	2.14	0.47
1:K:286:THR:HA	3:Z:5[A]:U:C4'	2.34	0.47
1:L:1:MET:HE3	1:L:38:ILE:HG22	1.97	0.47
1:G:213:PRO:HD3	1:G:232:PHE:CZ	2.50	0.47
1:L:384:ARG:HD2	1:G:353:ARG:NH1	2.29	0.47
1:K:148:GLU:OE1	1:K:408:THR:HA	2.15	0.47
1:K:213:PRO:HD3	1:K:232:PHE:CZ	2.50	0.47
1:A:36:PHE:CE1	1:A:40:LYS:HD2	2.50	0.47
1:E:248:GLU:O	1:E:252:ARG:HG2	2.14	0.47
1:E:290:ASP:HB3	1:E:293:ALA:HB2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:36:PHE:CE1	1:H:40:LYS:HD2	2.50	0.47
1:I:247:ILE:HB	1:I:300:PHE:CE1	2.50	0.47
2:X:158:LEU:O	2:X:172:GLU:HA	2.15	0.47
1:J:417:LYS:HA	2:W:144:PHE:CD1	2.49	0.46
1:K:290:ASP:HB3	1:K:293:ALA:HB2	1.97	0.46
1:L:398:PHE:HE1	2:X:165:PHE:CZ	2.34	0.46
1:A:248:GLU:O	1:A:252:ARG:HG2	2.14	0.46
1:B:360:TYR:CE2	1:B:384:ARG:HG2	2.50	0.46
1:F:240:VAL:O	1:F:244:GLU:HG2	2.15	0.46
1:G:267:ILE:HG22	1:G:318:THR:O	2.16	0.46
2:U:158:LEU:O	2:U:172:GLU:HA	2.15	0.46
1:C:248:GLU:O	1:C:252:ARG:HG2	2.15	0.46
1:D:284:VAL:HB	3:Y:2[B]:U:H5'	1.97	0.46
1:F:274:TYR:CD2	1:F:297:PRO:HG3	2.49	0.46
1:J:240:VAL:O	1:J:244:GLU:HG2	2.15	0.46
1:K:240:VAL:O	1:K:244:GLU:HG2	2.15	0.46
1:C:36:PHE:CE1	1:C:40:LYS:HD2	2.50	0.46
1:L:290:ASP:HB3	1:L:293:ALA:HB2	1.97	0.46
1:L:36:PHE:CE1	1:L:40:LYS:HD2	2.51	0.46
2:V:158:LEU:O	2:V:172:GLU:HA	2.14	0.46
1:A:240:VAL:O	1:A:244:GLU:HG2	2.15	0.46
1:E:213:PRO:HD3	1:E:232:PHE:CZ	2.50	0.46
1:E:247:ILE:HB	1:E:300:PHE:CE1	2.51	0.46
1:E:148:GLU:OE1	1:E:408:THR:HA	2.15	0.46
1:G:294:LEU:C	1:G:297:PRO:HD2	2.36	0.46
1:I:336:LYS:HE3	1:I:342:GLU:OE1	2.15	0.46
2:W:158:LEU:O	2:W:172:GLU:HA	2.15	0.46
1:B:336:LYS:HE3	1:B:342:GLU:OE1	2.16	0.46
1:C:294:LEU:C	1:C:297:PRO:HD2	2.35	0.46
1:D:290:ASP:HB3	1:D:293:ALA:HB2	1.97	0.46
1:F:213:PRO:HD3	1:F:232:PHE:CZ	2.51	0.46
1:K:248:GLU:O	1:K:252:ARG:HG2	2.15	0.46
1:B:149:ARG:HH21	1:B:193:GLN:HB3	1.79	0.46
1:E:36:PHE:CE1	1:E:40:LYS:HD2	2.50	0.46
1:K:336:LYS:HE3	1:K:342:GLU:OE1	2.16	0.46
1:A:213:PRO:HD3	1:A:232:PHE:CZ	2.51	0.46
1:E:336:LYS:HE3	1:E:342:GLU:OE1	2.16	0.46
1:F:294:LEU:C	1:F:297:PRO:HD2	2.36	0.46
1:G:89:PHE:HA	1:G:128:ARG:HG3	1.97	0.46
1:J:36:PHE:CE1	1:J:40:LYS:HD2	2.50	0.46
2:N:165:PHE:CD2	2:N:166:GLY:N	2.84	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:379:LYS:HB3	1:E:416:MET:HE1	1.98	0.46
1:J:248:GLU:O	1:J:252:ARG:HG2	2.15	0.46
1:C:267:ILE:HG22	1:C:318:THR:O	2.15	0.46
1:D:247:ILE:HB	1:D:300:PHE:CE1	2.51	0.46
1:J:402:LYS:HD3	1:J:402:LYS:HA	1.58	0.46
1:K:217:THR:HA	1:K:220:GLN:HG2	1.98	0.46
1:K:36:PHE:CE1	1:K:40:LYS:HD2	2.50	0.46
2:X:140:PRO:HG2	2:X:141:PHE:CD2	2.51	0.46
1:A:336:LYS:HE3	1:A:342:GLU:OE1	2.16	0.45
1:F:264:LEU:O	1:F:317:ALA:HA	2.16	0.45
1:F:36:PHE:CE1	1:F:40:LYS:HD2	2.51	0.45
1:A:264:LEU:O	1:A:317:ALA:HA	2.17	0.45
1:C:336:LYS:HE3	1:C:342:GLU:OE1	2.16	0.45
1:D:175:LEU:HA	1:D:317:ALA:O	2.16	0.45
1:A:175:LEU:HA	1:A:317:ALA:O	2.16	0.45
1:F:381:TRP:CE3	2:U:140:PRO:HB3	2.51	0.45
1:K:173:ARG:NH1	1:K:304:ALA:O	2.49	0.45
1:K:289:VAL:HG22	1:K:327:MET:HE2	1.99	0.45
1:A:247:ILE:HB	1:A:300:PHE:CE1	2.52	0.45
1:B:247:ILE:HB	1:B:300:PHE:CE1	2.51	0.45
1:C:213:PRO:HD3	1:C:232:PHE:CZ	2.51	0.45
1:L:402:LYS:HB3	1:L:412:PHE:HE1	1.81	0.45
2:N:136:VAL:HG22	2:N:178:VAL:HG12	1.99	0.45
1:B:382:ILE:CG1	2:S:140:PRO:HB2	2.46	0.45
1:G:127:ALA:O	1:G:130:LYS:HD2	2.16	0.45
1:G:178:ALA:CB	1:G:345:LEU:HB2	2.47	0.45
1:G:264:LEU:O	1:G:317:ALA:HA	2.16	0.45
1:H:417:LYS:HG2	2:V:144:PHE:CE1	2.52	0.45
1:B:240:VAL:O	1:B:244:GLU:HG2	2.16	0.45
1:D:248:GLU:O	1:D:252:ARG:HG2	2.16	0.45
1:D:267:ILE:HG22	1:D:318:THR:O	2.17	0.45
1:F:402:LYS:HE3	1:F:405:MET:HE1	1.99	0.45
1:I:267:ILE:HG22	1:I:318:THR:O	2.17	0.45
1:K:294:LEU:C	1:K:297:PRO:HD2	2.37	0.45
1:L:247:ILE:HB	1:L:300:PHE:CE1	2.52	0.45
2:M:165:PHE:CD2	2:M:166:GLY:N	2.84	0.45
1:B:217:THR:HA	1:B:220:GLN:HG2	1.99	0.45
1:C:102:ARG:NH1	1:C:105:LYS:HG3	2.32	0.45
1:E:175:LEU:HA	1:E:317:ALA:O	2.17	0.45
1:K:264:LEU:O	1:K:317:ALA:HA	2.16	0.45
2:O:165:PHE:CD2	2:O:166:GLY:N	2.84	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:ARG:NH1	1:B:304:ALA:O	2.50	0.45
1:E:217:THR:HA	1:E:220:GLN:HG2	1.99	0.45
1:H:217:THR:HA	1:H:220:GLN:HG2	1.99	0.45
1:H:248:GLU:O	1:H:252:ARG:HG2	2.16	0.45
1:I:217:THR:HA	1:I:220:GLN:HG2	1.99	0.45
1:I:240:VAL:O	1:I:244:GLU:HG2	2.16	0.45
1:A:178:ALA:CB	1:A:345:LEU:HB2	2.47	0.45
1:B:290:ASP:HB3	1:B:293:ALA:HB2	1.98	0.45
1:B:175:LEU:HA	1:B:317:ALA:O	2.16	0.45
1:C:240:VAL:O	1:C:244:GLU:HG2	2.16	0.45
1:C:264:LEU:O	1:C:317:ALA:HA	2.16	0.45
1:E:240:VAL:O	1:E:244:GLU:HG2	2.16	0.45
1:E:264:LEU:O	1:E:317:ALA:HA	2.17	0.45
1:F:173:ARG:NH1	1:F:304:ALA:O	2.49	0.45
1:H:240:VAL:O	1:H:244:GLU:HG2	2.16	0.45
1:I:384:ARG:HD2	1:J:353:ARG:NH1	2.32	0.45
1:J:173:ARG:NH1	1:J:304:ALA:O	2.49	0.45
1:L:213:PRO:HD3	1:L:232:PHE:CZ	2.52	0.45
1:L:240:VAL:O	1:L:244:GLU:HG2	2.16	0.45
1:L:264:LEU:O	1:L:317:ALA:HA	2.17	0.45
1:L:360:TYR:CE2	1:L:384:ARG:HG2	2.51	0.45
1:B:248:GLU:O	1:B:252:ARG:HG2	2.18	0.45
1:H:360:TYR:CE2	1:H:384:ARG:HG2	2.51	0.45
1:I:102:ARG:NH1	1:I:105:LYS:HG3	2.32	0.45
1:I:175:LEU:HA	1:I:317:ALA:O	2.17	0.45
1:J:175:LEU:HA	1:J:317:ALA:O	2.18	0.45
2:O:136:VAL:HG22	2:O:178:VAL:HG12	1.99	0.45
2:Q:136:VAL:HG22	2:Q:178:VAL:HG12	1.99	0.45
2:R:165:PHE:CD2	2:R:166:GLY:N	2.84	0.45
1:B:178:ALA:CB	1:B:345:LEU:HB2	2.47	0.44
1:C:89:PHE:HA	1:C:128:ARG:HG3	1.99	0.44
1:D:173:ARG:NH1	1:D:304:ALA:O	2.50	0.44
1:D:213:PRO:HD3	1:D:232:PHE:CZ	2.52	0.44
1:F:247:ILE:HB	1:F:300:PHE:CE1	2.52	0.44
1:G:173:ARG:NH1	1:G:304:ALA:O	2.51	0.44
1:H:290:ASP:HB3	1:H:293:ALA:HB2	1.98	0.44
1:J:267:ILE:HG22	1:J:318:THR:O	2.17	0.44
1:K:178:ALA:CB	1:K:345:LEU:HB2	2.47	0.44
1:L:294:LEU:C	1:L:297:PRO:HD2	2.38	0.44
2:P:136:VAL:HG22	2:P:178:VAL:HG12	1.99	0.44
2:Q:165:PHE:CD2	2:Q:166:GLY:N	2.84	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:136:VAL:HG22	2:M:178:VAL:HG12	1.99	0.44
1:A:294:LEU:C	1:A:297:PRO:HD2	2.38	0.44
1:C:247:ILE:HB	1:C:300:PHE:CE1	2.52	0.44
1:D:402:LYS:HA	1:D:402:LYS:HD3	1.50	0.44
1:G:1:MET:HE3	1:G:38:ILE:HG22	1.99	0.44
1:H:267:ILE:HG22	1:H:318:THR:O	2.17	0.44
1:I:213:PRO:HD3	1:I:232:PHE:CZ	2.52	0.44
1:I:264:LEU:O	1:I:317:ALA:HA	2.17	0.44
2:R:136:VAL:HG22	2:R:178:VAL:HG12	2.00	0.44
1:B:267:ILE:HG22	1:B:318:THR:O	2.18	0.44
1:D:294:LEU:C	1:D:297:PRO:HD2	2.37	0.44
1:D:382:ILE:HG12	2:T:140:PRO:HB2	1.99	0.44
1:E:89:PHE:HA	1:E:128:ARG:HG3	1.98	0.44
1:G:247:ILE:HB	1:G:300:PHE:CE1	2.52	0.44
1:J:284:VAL:O	3:Z:3[C]:U:O2'	2.32	0.44
2:P:165:PHE:CD2	2:P:166:GLY:N	2.84	0.44
1:F:265:ASP:HA	1:F:266:SER:HA	1.61	0.44
1:J:294:LEU:C	1:J:297:PRO:HD2	2.37	0.44
1:L:175:LEU:HA	1:L:317:ALA:O	2.17	0.44
2:X:136:VAL:HG22	2:X:178:VAL:HG12	2.00	0.44
1:A:127:ALA:O	1:A:130:LYS:HD2	2.18	0.44
1:A:217:THR:HA	1:A:220:GLN:HG2	1.99	0.44
1:B:298:LYS:HE2	1:C:232:PHE:HB2	2.00	0.44
1:G:102:ARG:NH1	1:G:105:LYS:HG3	2.32	0.44
1:I:294:LEU:C	1:I:297:PRO:HD2	2.37	0.44
1:K:265:ASP:HA	1:K:266:SER:HA	1.61	0.44
1:L:178:ALA:CB	1:L:345:LEU:HB2	2.48	0.44
1:L:267:ILE:HG22	1:L:318:THR:O	2.17	0.44
1:L:402:LYS:HA	1:L:402:LYS:HD3	1.28	0.44
1:C:178:ALA:CB	1:C:345:LEU:HB2	2.48	0.44
1:F:175:LEU:HA	1:F:317:ALA:O	2.18	0.44
1:F:217:THR:HA	1:F:220:GLN:HG2	2.00	0.44
1:H:178:ALA:CB	1:H:345:LEU:HB2	2.47	0.44
1:J:296:ARG:HB2	1:J:297:PRO:HD3	2.00	0.44
1:K:417:LYS:HA	2:R:144:PHE:HE1	1.82	0.44
1:L:173:ARG:NH1	1:L:304:ALA:O	2.49	0.44
2:S:136:VAL:HG22	2:S:178:VAL:HG12	1.99	0.44
2:V:136:VAL:HG22	2:V:178:VAL:HG12	2.00	0.44
1:G:175:LEU:HA	1:G:317:ALA:O	2.17	0.44
1:J:264:LEU:O	1:J:317:ALA:HA	2.17	0.44
1:K:102:ARG:NH1	1:K:105:LYS:HG3	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:131:ILE:HD12	1:K:309:GLU:HG2	2.00	0.44
1:K:175:LEU:HA	1:K:317:ALA:O	2.17	0.44
1:A:89:PHE:HA	1:A:128:ARG:HG3	1.99	0.44
1:C:217:THR:HA	1:C:220:GLN:HG2	2.00	0.44
1:D:178:ALA:CB	1:D:345:LEU:HB2	2.48	0.44
1:E:178:ALA:CB	1:E:345:LEU:HB2	2.47	0.44
1:F:248:GLU:O	1:F:252:ARG:HG2	2.17	0.44
1:G:217:THR:HA	1:G:220:GLN:HG2	1.99	0.44
1:H:294:LEU:C	1:H:297:PRO:HD2	2.37	0.44
1:H:175:LEU:HA	1:H:317:ALA:O	2.17	0.44
1:K:89:PHE:HA	1:K:128:ARG:HG3	1.99	0.44
1:J:284:VAL:HB	3:Z:2[B]:U:C5'	2.48	0.44
1:A:102:ARG:NH1	1:A:105:LYS:HG3	2.32	0.43
1:D:264:LEU:O	1:D:317:ALA:HA	2.18	0.43
1:F:296:ARG:HB2	1:F:297:PRO:HD3	2.00	0.43
1:J:247:ILE:HB	1:J:300:PHE:CE1	2.53	0.43
1:K:247:ILE:HB	1:K:300:PHE:CE1	2.53	0.43
1:L:248:GLU:O	1:L:252:ARG:HG2	2.17	0.43
2:T:136:VAL:HG22	2:T:178:VAL:HG12	2.00	0.43
2:W:165:PHE:CG	2:W:166:GLY:N	2.85	0.43
1:B:381:TRP:HZ3	2:S:140:PRO:HG3	1.83	0.43
1:C:173:ARG:HD2	1:C:302:GLY:HA2	2.01	0.43
1:H:102:ARG:NH1	1:H:105:LYS:HG3	2.34	0.43
1:H:89:PHE:HA	1:H:128:ARG:HG3	2.00	0.43
1:H:402:LYS:HA	1:H:402:LYS:HD3	1.66	0.43
1:H:402:LYS:HB3	1:H:412:PHE:HE1	1.83	0.43
1:I:178:ALA:CB	1:I:345:LEU:HB2	2.48	0.43
1:K:267:ILE:HG22	1:K:318:THR:O	2.18	0.43
1:C:173:ARG:NH1	1:C:304:ALA:O	2.51	0.43
1:E:294:LEU:C	1:E:297:PRO:HD2	2.38	0.43
1:E:296:ARG:HB2	1:E:297:PRO:HD3	2.00	0.43
1:F:267:ILE:HG22	1:F:318:THR:O	2.18	0.43
1:F:360:TYR:CE2	1:F:384:ARG:HG2	2.53	0.43
1:H:247:ILE:HB	1:H:300:PHE:CE1	2.52	0.43
1:H:173:ARG:HD2	1:H:302:GLY:HA2	2.01	0.43
1:A:173:ARG:NH1	1:A:304:ALA:O	2.50	0.43
1:B:296:ARG:HB2	1:B:297:PRO:HD3	1.99	0.43
1:D:398:PHE:CZ	2:T:165:PHE:CZ	3.06	0.43
1:D:379:LYS:HB3	1:D:416:MET:HE1	2.01	0.43
1:E:102:ARG:NH1	1:E:105:LYS:HG3	2.33	0.43
1:F:178:ALA:CB	1:F:345:LEU:HB2	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:173:ARG:NH1	1:H:304:ALA:O	2.51	0.43
1:I:296:ARG:HB2	1:I:297:PRO:HD3	1.99	0.43
1:L:217:THR:HA	1:L:220:GLN:HG2	2.00	0.43
1:B:102:ARG:NH1	1:B:105:LYS:HG3	2.34	0.43
1:I:345:LEU:HA	1:I:357:ALA:O	2.19	0.43
1:L:345:LEU:HA	1:L:357:ALA:O	2.19	0.43
1:H:336:LYS:HE3	1:H:342:GLU:OE1	2.18	0.43
2:V:165:PHE:HD2	2:V:166:GLY:H	1.65	0.43
2:W:136:VAL:HG22	2:W:178:VAL:HG12	2.00	0.43
1:C:175:LEU:HA	1:C:317:ALA:O	2.17	0.43
1:D:345:LEU:HA	1:D:357:ALA:O	2.19	0.43
1:C:384:ARG:HD2	1:D:353:ARG:NH1	2.33	0.43
1:E:402:LYS:HB3	1:E:412:PHE:HE1	1.84	0.43
1:H:264:LEU:O	1:H:317:ALA:HA	2.18	0.43
1:K:232:PHE:CB	1:J:298:LYS:HE2	2.49	0.43
1:K:402:LYS:HB3	1:K:412:PHE:HE1	1.84	0.43
2:U:136:VAL:HG22	2:U:178:VAL:HG12	2.00	0.43
1:B:345:LEU:HA	1:B:357:ALA:O	2.19	0.43
1:D:296:ARG:HB2	1:D:297:PRO:HD3	2.00	0.43
1:E:267:ILE:HG22	1:E:318:THR:O	2.18	0.43
1:J:402:LYS:HZ3	2:W:165:PHE:HZ	1.63	0.43
1:D:217:THR:HA	1:D:220:GLN:HG2	2.01	0.43
1:D:360:TYR:CE2	1:D:384:ARG:HG2	2.53	0.43
1:E:173:ARG:NH1	1:E:304:ALA:O	2.51	0.43
1:E:254:VAL:HG21	1:E:313:LEU:HB2	2.01	0.43
1:E:345:LEU:HA	1:E:357:ALA:O	2.19	0.43
1:F:345:LEU:HA	1:F:357:ALA:O	2.19	0.43
1:I:254:VAL:HG21	1:I:313:LEU:HB2	2.01	0.43
1:L:296:ARG:HB2	1:L:297:PRO:HD3	2.00	0.43
1:A:131:ILE:HD12	1:A:309:GLU:HG2	2.01	0.43
1:B:131:ILE:HD12	1:B:309:GLU:HG2	2.01	0.43
1:B:294:LEU:C	1:B:297:PRO:HD2	2.39	0.43
1:F:402:LYS:HD3	1:F:402:LYS:HA	1.50	0.43
1:G:131:ILE:HD12	1:G:309:GLU:HG2	2.01	0.43
1:I:173:ARG:HD2	1:I:302:GLY:HA2	2.01	0.43
1:I:173:ARG:NH1	1:I:304:ALA:O	2.52	0.43
1:L:417:LYS:HG2	2:X:144:PHE:CE1	2.54	0.43
1:B:264:LEU:O	1:B:317:ALA:HA	2.19	0.42
1:D:381:TRP:HE1	1:E:353:ARG:HB3	1.84	0.42
1:E:1:MET:HE3	1:E:38:ILE:HG22	1.99	0.42
1:F:353:ARG:NH1	1:E:384:ARG:HD2	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1:MET:HE3	1:I:38:ILE:HG22	2.00	0.42
1:J:345:LEU:HA	1:J:357:ALA:O	2.19	0.42
1:L:131:ILE:HD12	1:L:309:GLU:HG2	2.02	0.42
1:L:402:LYS:HE3	1:L:405:MET:CE	2.50	0.42
1:I:379:LYS:HB3	1:I:416:MET:HE1	2.01	0.42
1:F:102:ARG:NH1	1:F:105:LYS:HG3	2.34	0.42
1:G:345:LEU:HA	1:G:357:ALA:O	2.20	0.42
1:J:178:ALA:CB	1:J:345:LEU:HB2	2.49	0.42
1:J:217:THR:HA	1:J:220:GLN:HG2	2.01	0.42
2:S:165:PHE:HD2	2:S:166:GLY:H	1.62	0.42
1:A:345:LEU:HA	1:A:357:ALA:O	2.19	0.42
1:C:333:GLU:HG2	1:D:323:THR:O	2.20	0.42
1:F:131:ILE:HD12	1:F:309:GLU:HG2	2.01	0.42
1:I:402:LYS:HB3	1:I:412:PHE:HE1	1.85	0.42
1:H:417:LYS:HD2	2:V:143:ASP:O	2.19	0.42
1:K:345:LEU:HA	1:K:357:ALA:O	2.20	0.42
1:L:265:ASP:HA	1:L:266:SER:HA	1.62	0.42
2:U:136:VAL:HG11	2:U:141:PHE:HB2	2.00	0.42
1:A:333:GLU:HG2	1:B:323:THR:HA	2.02	0.42
1:D:102:ARG:NH1	1:D:105:LYS:HG3	2.35	0.42
1:H:296:ARG:HB2	1:H:297:PRO:HD3	2.00	0.42
1:K:254:VAL:HG21	1:K:313:LEU:HB2	2.02	0.42
1:L:353:ARG:NH1	1:K:384:ARG:HD2	2.35	0.42
2:X:136:VAL:HG11	2:X:141:PHE:HB2	2.01	0.42
1:C:131:ILE:HD12	1:C:309:GLU:HG2	2.02	0.42
1:E:131:ILE:HD12	1:E:309:GLU:HG2	2.01	0.42
1:K:296:ARG:HB2	1:K:297:PRO:HD3	2.01	0.42
1:I:284:VAL:N	3:Z:2[B]:U:O2'	2.46	0.42
1:A:296:ARG:HB2	1:A:297:PRO:HD3	2.00	0.42
1:C:254:VAL:HG21	1:C:313:LEU:HB2	2.01	0.42
1:C:349:ILE:HB	1:C:357:ALA:HB1	2.02	0.42
1:F:173:ARG:HD2	1:F:302:GLY:HA2	2.01	0.42
1:H:382:ILE:HG21	1:H:382:ILE:HD13	1.82	0.42
1:I:333:GLU:HG2	1:J:323:THR:O	2.20	0.42
1:I:89:PHE:HA	1:I:128:ARG:HG3	2.02	0.42
1:J:131:ILE:HD12	1:J:309:GLU:HG2	2.01	0.42
1:L:102:ARG:NH1	1:L:105:LYS:HG3	2.34	0.42
1:L:5:GLU:O	1:L:9:THR:HG23	2.19	0.42
2:W:136:VAL:HG11	2:W:141:PHE:HB2	2.01	0.42
1:A:254:VAL:HG21	1:A:313:LEU:HB2	2.02	0.42
1:D:5:GLU:O	1:D:9:THR:HG23	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:178:ALA:HB3	1:H:184:LYS:CG	2.50	0.42
1:H:2:ASN:O	1:H:6:LEU:HD13	2.20	0.42
1:H:345:LEU:HA	1:H:357:ALA:O	2.19	0.42
2:V:175:PHE:CD1	2:V:175:PHE:N	2.88	0.42
1:C:345:LEU:HA	1:C:357:ALA:O	2.19	0.42
1:D:402:LYS:HE3	1:D:405:MET:HE1	2.01	0.42
1:D:2:ASN:O	1:D:6:LEU:HD13	2.20	0.42
1:E:173:ARG:HD2	1:E:302:GLY:HA2	2.02	0.42
1:G:296:ARG:HB2	1:G:297:PRO:HD3	2.01	0.42
1:G:173:ARG:HD2	1:G:302:GLY:HA2	2.02	0.42
1:J:360:TYR:CE2	1:J:384:ARG:HG2	2.54	0.42
1:K:379:LYS:HB3	1:K:416:MET:HE1	2.02	0.42
2:R:175:PHE:CD1	2:R:175:PHE:N	2.88	0.42
1:A:265:ASP:HA	1:A:266:SER:HA	1.61	0.41
1:A:267:ILE:HG22	1:A:318:THR:O	2.19	0.41
1:B:265:ASP:HA	1:B:266:SER:HA	1.62	0.41
1:B:158:THR:HA	1:B:356:PRO:HG3	2.02	0.41
1:B:5:GLU:O	1:B:9:THR:HG23	2.20	0.41
1:C:296:ARG:HB2	1:C:297:PRO:HD3	2.00	0.41
1:E:284:VAL:HB	3:Y:3[C]:U:C4'	2.50	0.41
1:H:131:ILE:HD12	1:H:309:GLU:HG2	2.02	0.41
2:M:175:PHE:CD1	2:M:175:PHE:N	2.88	0.41
1:A:402:LYS:HB3	1:A:412:PHE:HE1	1.84	0.41
1:F:131:ILE:H	1:F:131:ILE:HG12	1.70	0.41
1:J:102:ARG:NH1	1:J:105:LYS:HG3	2.34	0.41
1:B:382:ILE:HD13	1:B:382:ILE:HG21	1.80	0.41
1:C:402:LYS:HB3	1:C:412:PHE:HE1	1.85	0.41
1:G:254:VAL:HG21	1:G:313:LEU:HB2	2.01	0.41
1:H:348:LYS:HB2	1:H:348:LYS:HE3	1.87	0.41
1:J:379:LYS:HB3	1:J:416:MET:HE1	2.02	0.41
1:K:173:ARG:HD2	1:K:302:GLY:HA2	2.02	0.41
1:B:212:ARG:HA	1:B:232:PHE:CE2	2.55	0.41
1:B:173:ARG:HD2	1:B:302:GLY:HA2	2.02	0.41
1:E:178:ALA:HB3	1:E:184:LYS:CG	2.50	0.41
1:G:158:THR:HA	1:G:356:PRO:HG3	2.02	0.41
1:I:178:ALA:HB3	1:I:184:LYS:CG	2.50	0.41
1:J:2:ASN:O	1:J:6:LEU:HD13	2.20	0.41
1:E:5:GLU:O	1:E:9:THR:HG23	2.21	0.41
1:I:26:LEU:O	1:I:34:ILE:HD11	2.20	0.41
1:J:1:MET:HE3	1:J:38:ILE:HG22	2.00	0.41
2:V:136:VAL:HG11	2:V:141:PHE:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:175:PHE:CD1	2:X:175:PHE:N	2.88	0.41
1:G:26:LEU:O	1:G:34:ILE:HD11	2.20	0.41
1:G:349:ILE:HB	1:G:357:ALA:HB1	2.02	0.41
1:K:349:ILE:HB	1:K:357:ALA:HB1	2.02	0.41
1:A:173:ARG:HD2	1:A:302:GLY:HA2	2.02	0.41
1:B:127:ALA:O	1:B:130:LYS:HD2	2.21	0.41
1:D:131:ILE:HD12	1:D:309:GLU:HG2	2.01	0.41
1:E:349:ILE:HB	1:E:357:ALA:HB1	2.02	0.41
1:F:402:LYS:HE3	1:F:405:MET:HE3	2.02	0.41
1:I:349:ILE:HB	1:I:357:ALA:HB1	2.02	0.41
1:K:158:THR:HA	1:K:356:PRO:HG3	2.03	0.41
1:A:158:THR:HA	1:A:356:PRO:HG3	2.03	0.41
1:B:402:LYS:HB3	1:B:412:PHE:HE1	1.86	0.41
1:D:333:GLU:HG2	1:E:323:THR:O	2.20	0.41
1:D:1:MET:HE3	1:D:38:ILE:HG22	2.02	0.41
1:K:178:ALA:HB3	1:K:184:LYS:CG	2.50	0.41
1:L:173:ARG:HD2	1:L:302:GLY:HA2	2.02	0.41
1:L:158:THR:HA	1:L:356:PRO:HG3	2.03	0.41
1:B:398:PHE:HE1	2:S:165:PHE:CZ	2.37	0.41
2:T:175:PHE:CD1	2:T:175:PHE:N	2.88	0.41
1:A:289:VAL:HG22	1:A:327:MET:HE2	2.03	0.41
1:B:349:ILE:HB	1:B:357:ALA:HB1	2.02	0.41
1:C:120:ASN:HB2	1:C:256:HIS:CE1	2.56	0.41
1:C:26:LEU:O	1:C:34:ILE:HD11	2.21	0.41
1:E:26:LEU:O	1:E:34:ILE:HD11	2.20	0.41
1:H:5:GLU:O	1:H:9:THR:HG23	2.21	0.41
1:K:5:GLU:O	1:K:9:THR:HG23	2.21	0.41
2:O:175:PHE:N	2:O:175:PHE:CD1	2.88	0.41
1:A:379:LYS:HB3	1:A:416:MET:HE1	2.01	0.41
1:C:178:ALA:HB3	1:C:184:LYS:CG	2.51	0.41
1:C:348:LYS:HB2	1:C:348:LYS:HE3	1.87	0.41
1:J:212:ARG:HA	1:J:232:PHE:CE2	2.56	0.41
1:J:5:GLU:O	1:J:9:THR:HG23	2.21	0.41
1:F:349:ILE:HB	1:F:357:ALA:HB1	2.02	0.41
1:I:131:ILE:HD12	1:I:309:GLU:HG2	2.02	0.41
1:I:178:ALA:HB1	1:I:182:ALA:HB3	2.03	0.41
1:I:5:GLU:O	1:I:9:THR:HG23	2.21	0.41
1:A:349:ILE:HB	1:A:357:ALA:HB1	2.02	0.40
1:A:26:LEU:O	1:A:34:ILE:HD11	2.21	0.40
1:B:2:ASN:O	1:B:6:LEU:HD13	2.20	0.40
1:C:1:MET:HE3	1:C:38:ILE:HG22	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:212:ARG:HA	1:H:232:PHE:CE2	2.56	0.40
1:J:417:LYS:NZ	2:W:143:ASP:OD1	2.42	0.40
1:E:286:THR:HG23	3:Y:5[A]:U:H5"	2.02	0.40
1:C:178:ALA:HB1	1:C:182:ALA:HB3	2.03	0.40
1:F:5:GLU:O	1:F:9:THR:HG23	2.22	0.40
1:I:158:THR:HA	1:I:356:PRO:HG3	2.03	0.40
1:L:178:ALA:HB3	1:L:184:LYS:CG	2.51	0.40
2:Q:175:PHE:N	2:Q:175:PHE:CD1	2.88	0.40
1:A:323:THR:O	1:F:333:GLU:HG2	2.21	0.40
1:G:2:ASN:O	1:G:6:LEU:HD13	2.20	0.40
1:H:265:ASP:HA	1:H:266:SER:HA	1.62	0.40
1:H:379:LYS:HB3	1:H:416:MET:HE1	2.03	0.40
1:I:2:ASN:O	1:I:6:LEU:HD13	2.22	0.40
1:K:26:LEU:O	1:K:34:ILE:HD11	2.20	0.40
1:D:382:ILE:CG1	2:T:140:PRO:HB2	2.51	0.40
1:C:2:ASN:O	1:C:6:LEU:HD13	2.22	0.40
1:C:379:LYS:HB3	1:C:416:MET:HE1	2.02	0.40
1:D:173:ARG:HD2	1:D:302:GLY:HA2	2.03	0.40
1:E:158:THR:HA	1:E:356:PRO:HG3	2.03	0.40
1:E:2:ASN:O	1:E:6:LEU:HD13	2.21	0.40
1:G:402:LYS:HB3	1:G:412:PHE:HE1	1.85	0.40
1:H:349:ILE:HB	1:H:357:ALA:HB1	2.03	0.40
1:J:382:ILE:HG21	1:J:382:ILE:HD13	1.88	0.40
1:A:178:ALA:HB3	1:A:184:LYS:CG	2.51	0.40
1:A:2:ASN:O	1:A:6:LEU:HD13	2.20	0.40
1:B:178:ALA:HB3	1:B:184:LYS:CG	2.51	0.40
1:B:402:LYS:HD3	1:B:402:LYS:HA	1.34	0.40
1:C:158:THR:HA	1:C:356:PRO:HG3	2.04	0.40
1:C:289:VAL:HG22	1:C:327:MET:HE2	2.02	0.40
1:C:5:GLU:O	1:C:9:THR:HG23	2.21	0.40
1:E:178:ALA:HB1	1:E:182:ALA:HB3	2.03	0.40
1:G:178:ALA:HB3	1:G:184:LYS:CG	2.52	0.40
2:U:175:PHE:N	2:U:175:PHE:CD1	2.88	0.40
2:W:175:PHE:CD1	2:W:175:PHE:N	2.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	410/422 (97%)	403 (98%)	7 (2%)	0	100	100
1	B	405/422 (96%)	398 (98%)	7 (2%)	0	100	100
1	C	410/422 (97%)	403 (98%)	7 (2%)	0	100	100
1	D	405/422 (96%)	398 (98%)	7 (2%)	0	100	100
1	E	410/422 (97%)	403 (98%)	7 (2%)	0	100	100
1	F	405/422 (96%)	398 (98%)	7 (2%)	0	100	100
1	G	410/422 (97%)	403 (98%)	7 (2%)	0	100	100
1	H	405/422 (96%)	398 (98%)	7 (2%)	0	100	100
1	I	410/422 (97%)	403 (98%)	7 (2%)	0	100	100
1	J	405/422 (96%)	398 (98%)	7 (2%)	0	100	100
1	K	410/422 (97%)	403 (98%)	7 (2%)	0	100	100
1	L	405/422 (96%)	398 (98%)	7 (2%)	0	100	100
2	M	39/60 (65%)	38 (97%)	1 (3%)	0	100	100
2	N	39/60 (65%)	38 (97%)	1 (3%)	0	100	100
2	O	39/60 (65%)	38 (97%)	1 (3%)	0	100	100
2	P	39/60 (65%)	38 (97%)	1 (3%)	0	100	100
2	Q	39/60 (65%)	38 (97%)	1 (3%)	0	100	100
2	R	39/60 (65%)	38 (97%)	1 (3%)	0	100	100
2	S	39/60 (65%)	38 (97%)	1 (3%)	0	100	100
2	T	39/60 (65%)	37 (95%)	2 (5%)	0	100	100
2	U	39/60 (65%)	37 (95%)	2 (5%)	0	100	100
2	V	39/60 (65%)	38 (97%)	1 (3%)	0	100	100
2	W	39/60 (65%)	37 (95%)	2 (5%)	0	100	100
2	X	39/60 (65%)	38 (97%)	1 (3%)	0	100	100
All	All	5358/5784 (93%)	5259 (98%)	99 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	348/361 (96%)	344 (99%)	4 (1%)	73	85
1	B	348/361 (96%)	345 (99%)	3 (1%)	78	88
1	C	348/361 (96%)	344 (99%)	4 (1%)	73	85
1	D	348/361 (96%)	345 (99%)	3 (1%)	78	88
1	E	348/361 (96%)	344 (99%)	4 (1%)	73	85
1	F	348/361 (96%)	345 (99%)	3 (1%)	78	88
1	G	348/361 (96%)	345 (99%)	3 (1%)	78	88
1	H	348/361 (96%)	345 (99%)	3 (1%)	78	88
1	I	348/361 (96%)	344 (99%)	4 (1%)	73	85
1	J	348/361 (96%)	345 (99%)	3 (1%)	78	88
1	K	348/361 (96%)	344 (99%)	4 (1%)	73	85
1	L	348/361 (96%)	345 (99%)	3 (1%)	78	88
2	M	35/52 (67%)	35 (100%)	0	100	100
2	N	35/52 (67%)	35 (100%)	0	100	100
2	O	35/52 (67%)	35 (100%)	0	100	100
2	P	35/52 (67%)	35 (100%)	0	100	100
2	Q	35/52 (67%)	35 (100%)	0	100	100
2	R	35/52 (67%)	35 (100%)	0	100	100
2	S	35/52 (67%)	35 (100%)	0	100	100
2	T	35/52 (67%)	35 (100%)	0	100	100
2	U	35/52 (67%)	35 (100%)	0	100	100
2	V	35/52 (67%)	35 (100%)	0	100	100
2	W	34/52 (65%)	34 (100%)	0	100	100
2	X	34/52 (65%)	34 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	4594/4956 (93%)	4553 (99%)	41 (1%)	78	88

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	217	THR
1	L	353	ARG
1	L	406	THR
1	A	217	THR
1	A	232	PHE
1	A	353	ARG
1	A	406	THR
1	G	217	THR
1	G	353	ARG
1	G	406	THR
1	B	217	THR
1	B	353	ARG
1	B	406	THR
1	H	217	THR
1	H	353	ARG
1	H	406	THR
1	C	217	THR
1	C	232	PHE
1	C	353	ARG
1	C	406	THR
1	I	217	THR
1	I	232	PHE
1	I	353	ARG
1	I	406	THR
1	D	217	THR
1	D	353	ARG
1	D	406	THR
1	K	217	THR
1	K	232	PHE
1	K	353	ARG
1	K	406	THR
1	F	217	THR
1	F	353	ARG
1	F	406	THR
1	J	217	THR
1	J	353	ARG
1	J	406	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	217	THR
1	E	232	PHE
1	E	353	ARG
1	E	406	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	Y	0/12	-	-
3	Z	0/12	-	-
All	All	0/24	-	-

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 12 are monoatomic - leaving 24 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
4	ADP	L	1000	5,6	24,29,29	0.96	1 (4%)	29,45,45	1.44	6 (20%)
4	ADP	A	1000	5,6	24,29,29	0.94	1 (4%)	29,45,45	1.39	6 (20%)
6	BEF	H	1002	4	0,3,3	0.00	-	-	-	-
4	ADP	E	1000	5,6	24,29,29	0.95	1 (4%)	29,45,45	1.42	5 (17%)
4	ADP	H	1000	5,6	24,29,29	0.96	1 (4%)	29,45,45	1.46	6 (20%)
4	ADP	G	1000	5,6	24,29,29	0.95	1 (4%)	29,45,45	1.40	6 (20%)
6	BEF	F	1002	4	0,3,3	0.00	-	-	-	-
4	ADP	B	1000	5,6	24,29,29	0.96	1 (4%)	29,45,45	1.45	6 (20%)
4	ADP	J	1000	5,6	24,29,29	0.96	1 (4%)	29,45,45	1.43	6 (20%)
6	BEF	K	1002	4	0,3,3	0.00	-	-	-	-
6	BEF	A	1002	4	0,3,3	0.00	-	-	-	-
6	BEF	C	1002	4	0,3,3	0.00	-	-	-	-
6	BEF	G	1002	4	0,3,3	0.00	-	-	-	-
6	BEF	J	1002	4	0,3,3	0.00	-	-	-	-
6	BEF	I	1002	4	0,3,3	0.00	-	-	-	-
6	BEF	B	1002	4	0,3,3	0.00	-	-	-	-
6	BEF	E	1002	4	0,3,3	0.00	-	-	-	-
6	BEF	D	1002	4	0,3,3	0.00	-	-	-	-
4	ADP	C	1000	5,6	24,29,29	0.96	1 (4%)	29,45,45	1.40	6 (20%)
6	BEF	L	1002	4	0,3,3	0.00	-	-	-	-
4	ADP	I	1000	5,6	24,29,29	0.95	1 (4%)	29,45,45	1.44	6 (20%)
4	ADP	K	1000	5,6	24,29,29	0.94	1 (4%)	29,45,45	1.42	6 (20%)
4	ADP	D	1000	5,6	24,29,29	0.96	1 (4%)	29,45,45	1.44	6 (20%)
4	ADP	F	1000	5,6	24,29,29	0.96	1 (4%)	29,45,45	1.45	6 (20%)

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
4	ADP	L	1000	5,6	-	0/12/32/32	0/3/3/3
4	ADP	A	1000	5,6	-	0/12/32/32	0/3/3/3
4	ADP	C	1000	5,6	-	0/12/32/32	0/3/3/3
4	ADP	E	1000	5,6	-	0/12/32/32	0/3/3/3
4	ADP	H	1000	5,6	-	0/12/32/32	0/3/3/3
4	ADP	G	1000	5,6	-	0/12/32/32	0/3/3/3
4	ADP	I	1000	5,6	-	0/12/32/32	0/3/3/3
4	ADP	K	1000	5,6	-	0/12/32/32	0/3/3/3
4	ADP	B	1000	5,6	-	0/12/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	D	1000	5,6	-	0/12/32/32	0/3/3/3
4	ADP	F	1000	5,6	-	0/12/32/32	0/3/3/3
4	ADP	J	1000	5,6	-	0/12/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	1000	ADP	C5-C4	2.47	1.47	1.40
4	E	1000	ADP	C5-C4	2.47	1.47	1.40
4	G	1000	ADP	C5-C4	2.45	1.47	1.40
4	C	1000	ADP	C5-C4	2.44	1.47	1.40
4	K	1000	ADP	C5-C4	2.43	1.47	1.40
4	J	1000	ADP	C5-C4	2.40	1.47	1.40
4	A	1000	ADP	C5-C4	2.40	1.47	1.40
4	F	1000	ADP	C5-C4	2.40	1.47	1.40
4	D	1000	ADP	C5-C4	2.36	1.47	1.40
4	L	1000	ADP	C5-C4	2.35	1.47	1.40
4	H	1000	ADP	C5-C4	2.35	1.47	1.40
4	B	1000	ADP	C5-C4	2.34	1.47	1.40

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1000	ADP	N3-C2-N1	-3.38	123.40	128.68
4	H	1000	ADP	PA-O3A-PB	-3.35	121.31	132.83
4	K	1000	ADP	N3-C2-N1	-3.34	123.46	128.68
4	G	1000	ADP	N3-C2-N1	-3.33	123.48	128.68
4	E	1000	ADP	N3-C2-N1	-3.32	123.49	128.68
4	B	1000	ADP	PA-O3A-PB	-3.28	121.56	132.83
4	I	1000	ADP	N3-C2-N1	-3.26	123.59	128.68
4	A	1000	ADP	N3-C2-N1	-3.25	123.60	128.68
4	L	1000	ADP	PA-O3A-PB	-3.22	121.77	132.83
4	F	1000	ADP	PA-O3A-PB	-3.22	121.79	132.83
4	L	1000	ADP	N3-C2-N1	-3.21	123.67	128.68
4	J	1000	ADP	PA-O3A-PB	-3.20	121.83	132.83
4	H	1000	ADP	N3-C2-N1	-3.20	123.68	128.68
4	D	1000	ADP	N3-C2-N1	-3.19	123.69	128.68
4	B	1000	ADP	N3-C2-N1	-3.19	123.70	128.68
4	D	1000	ADP	C4-C5-N7	-3.16	106.11	109.40
4	F	1000	ADP	N3-C2-N1	-3.15	123.75	128.68
4	J	1000	ADP	N3-C2-N1	-3.15	123.76	128.68
4	F	1000	ADP	C4-C5-N7	-3.12	106.14	109.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	1000	ADP	C4-C5-N7	-3.12	106.15	109.40
4	D	1000	ADP	PA-O3A-PB	-3.10	122.20	132.83
4	B	1000	ADP	C4-C5-N7	-3.07	106.20	109.40
4	H	1000	ADP	C4-C5-N7	-3.06	106.21	109.40
4	I	1000	ADP	C4-C5-N7	-3.04	106.23	109.40
4	E	1000	ADP	C4-C5-N7	-3.03	106.25	109.40
4	L	1000	ADP	C4-C5-N7	-2.98	106.29	109.40
4	I	1000	ADP	PA-O3A-PB	-2.89	122.90	132.83
4	K	1000	ADP	C4-C5-N7	-2.87	106.41	109.40
4	A	1000	ADP	C4-C5-N7	-2.84	106.44	109.40
4	G	1000	ADP	C4-C5-N7	-2.84	106.44	109.40
4	A	1000	ADP	PA-O3A-PB	-2.83	123.12	132.83
4	C	1000	ADP	PA-O3A-PB	-2.82	123.15	132.83
4	C	1000	ADP	C4-C5-N7	-2.82	106.46	109.40
4	I	1000	ADP	C3'-C2'-C1'	2.80	105.20	100.98
4	G	1000	ADP	PA-O3A-PB	-2.78	123.28	132.83
4	E	1000	ADP	PA-O3A-PB	-2.77	123.32	132.83
4	E	1000	ADP	C3'-C2'-C1'	2.76	105.13	100.98
4	K	1000	ADP	PA-O3A-PB	-2.69	123.58	132.83
4	K	1000	ADP	C3'-C2'-C1'	2.65	104.97	100.98
4	G	1000	ADP	C3'-C2'-C1'	2.59	104.87	100.98
4	A	1000	ADP	C3'-C2'-C1'	2.58	104.86	100.98
4	C	1000	ADP	C3'-C2'-C1'	2.57	104.84	100.98
4	H	1000	ADP	C3'-C2'-C1'	2.33	104.49	100.98
4	F	1000	ADP	C3'-C2'-C1'	2.32	104.47	100.98
4	L	1000	ADP	C3'-C2'-C1'	2.31	104.46	100.98
4	B	1000	ADP	C3'-C2'-C1'	2.27	104.39	100.98
4	J	1000	ADP	C3'-C2'-C1'	2.21	104.30	100.98
4	B	1000	ADP	O3B-PB-O2B	2.19	115.99	107.64
4	L	1000	ADP	O3B-PB-O2B	2.17	115.94	107.64
4	D	1000	ADP	C3'-C2'-C1'	2.16	104.23	100.98
4	J	1000	ADP	O3B-PB-O2B	2.14	115.82	107.64
4	H	1000	ADP	O3B-PB-O2B	2.13	115.79	107.64
4	C	1000	ADP	O2A-PA-O1A	2.12	122.72	112.24
4	I	1000	ADP	O2A-PA-O1A	2.12	122.70	112.24
4	L	1000	ADP	O2A-PA-O1A	2.11	122.68	112.24
4	F	1000	ADP	O3B-PB-O2B	2.10	115.66	107.64
4	F	1000	ADP	O2A-PA-O1A	2.09	122.59	112.24
4	I	1000	ADP	O3B-PB-O2B	2.08	115.60	107.64
4	H	1000	ADP	O2A-PA-O1A	2.08	122.50	112.24
4	D	1000	ADP	O2A-PA-O1A	2.07	122.47	112.24
4	B	1000	ADP	O2A-PA-O1A	2.06	122.43	112.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1000	ADP	O2A-PA-O1A	2.06	122.41	112.24
4	A	1000	ADP	O3B-PB-O2B	2.06	115.50	107.64
4	K	1000	ADP	O2A-PA-O1A	2.05	122.40	112.24
4	J	1000	ADP	O2A-PA-O1A	2.05	122.39	112.24
4	G	1000	ADP	O2A-PA-O1A	2.03	122.30	112.24
4	D	1000	ADP	O3B-PB-O2B	2.03	115.40	107.64
4	K	1000	ADP	C2-N1-C6	2.03	122.22	118.75
4	A	1000	ADP	O2A-PA-O1A	2.02	122.23	112.24
4	C	1000	ADP	O3B-PB-O2B	2.01	115.33	107.64
4	G	1000	ADP	O3B-PB-O2B	2.00	115.29	107.64

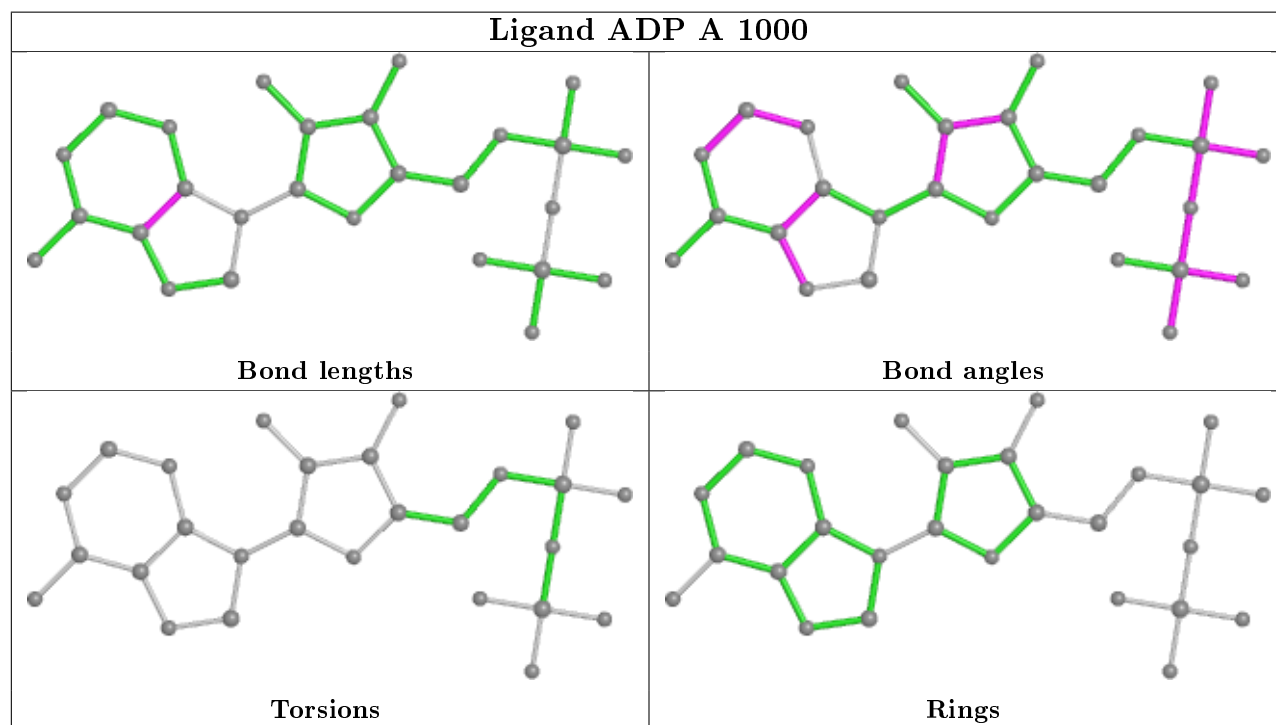
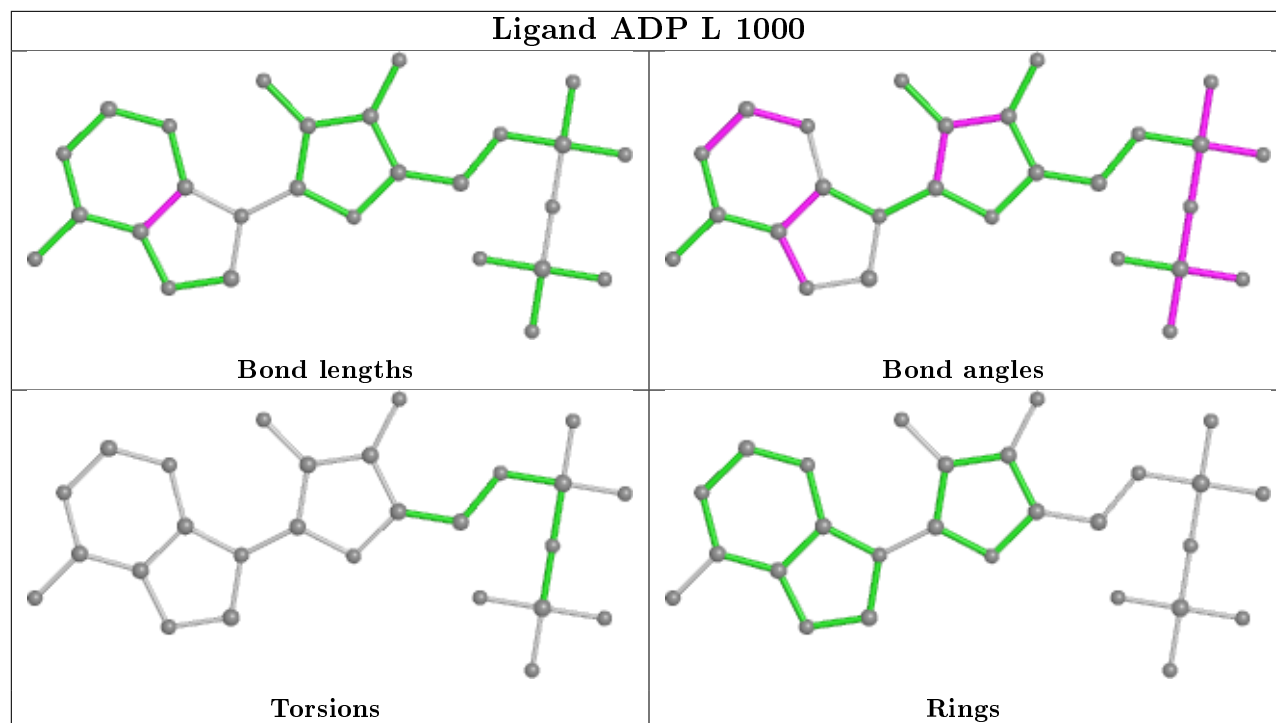
There are no chirality outliers.

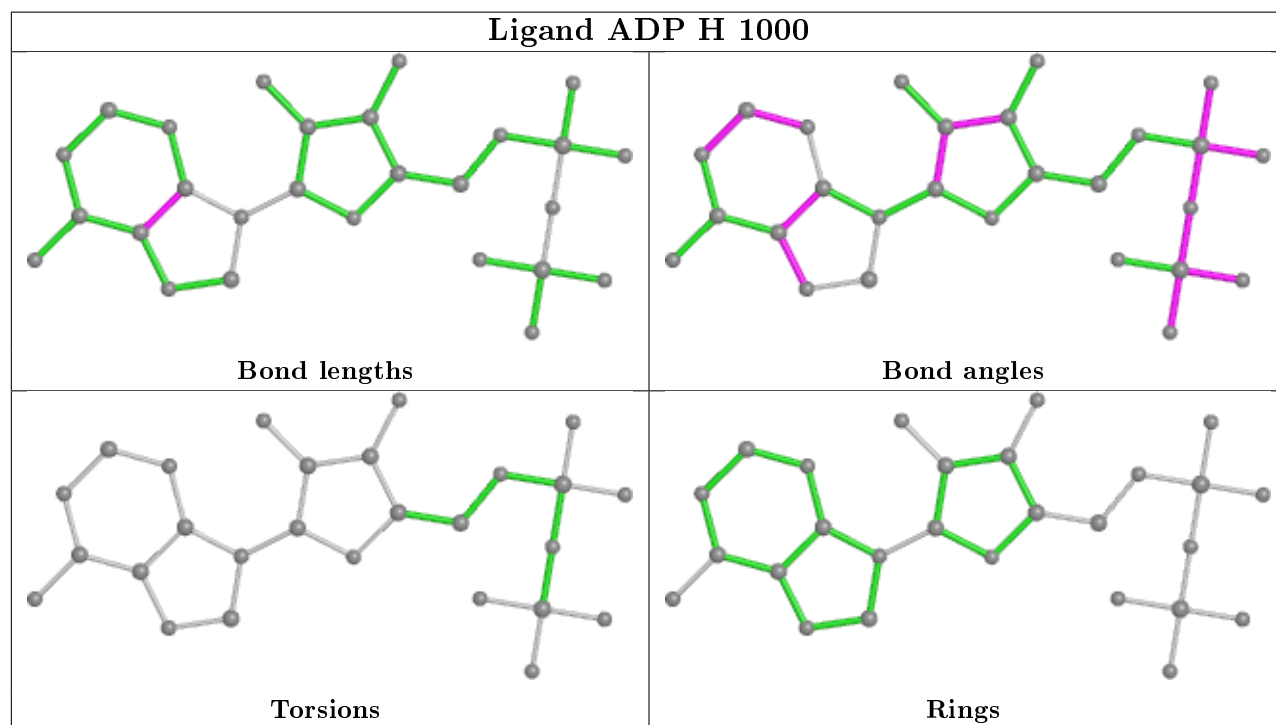
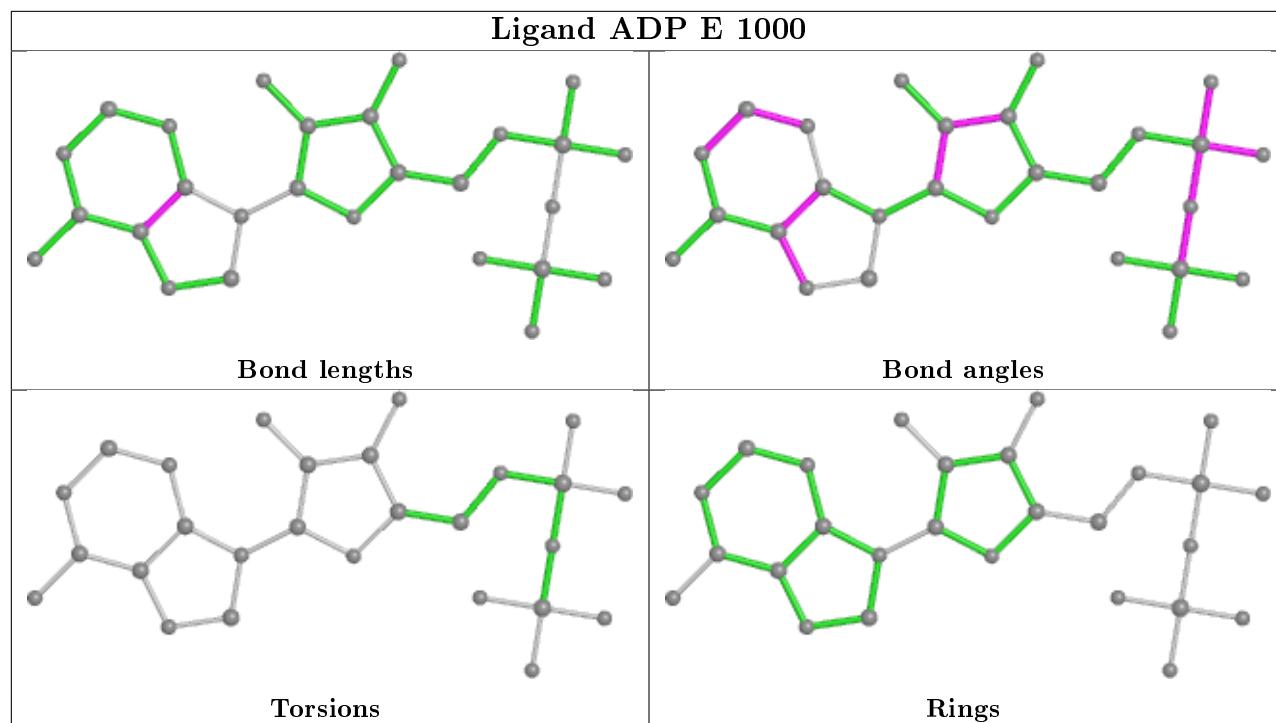
There are no torsion outliers.

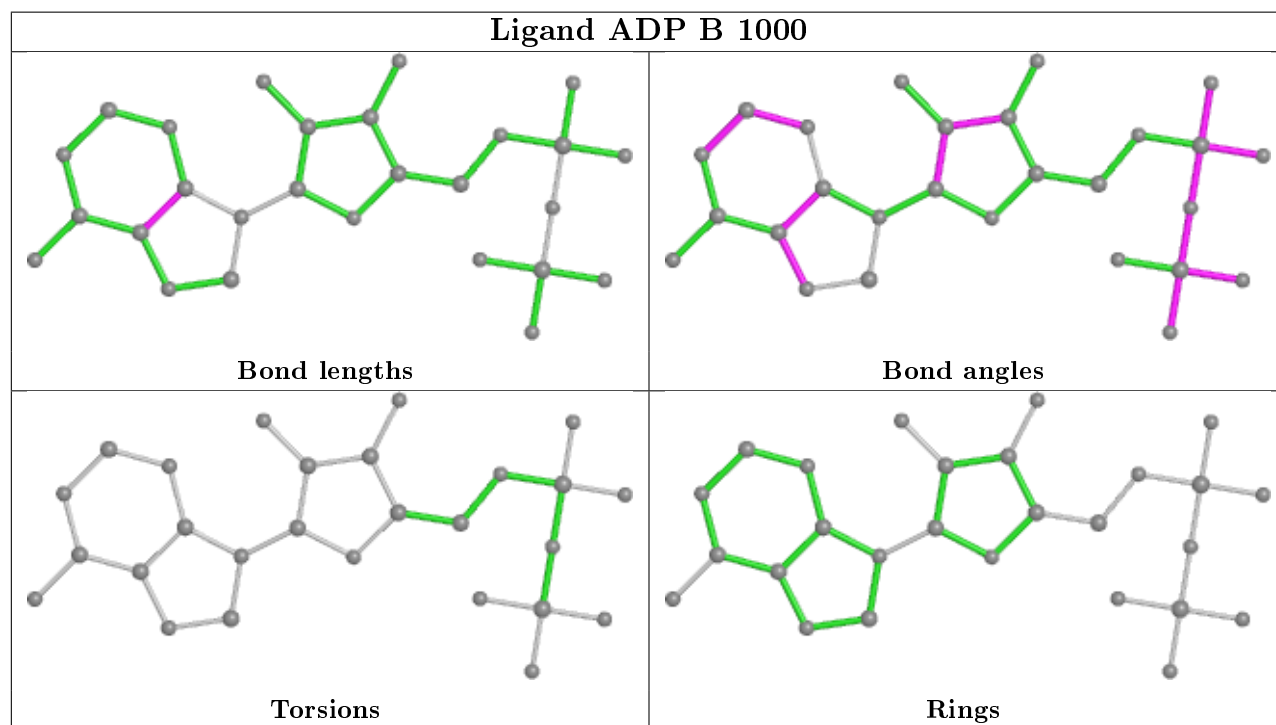
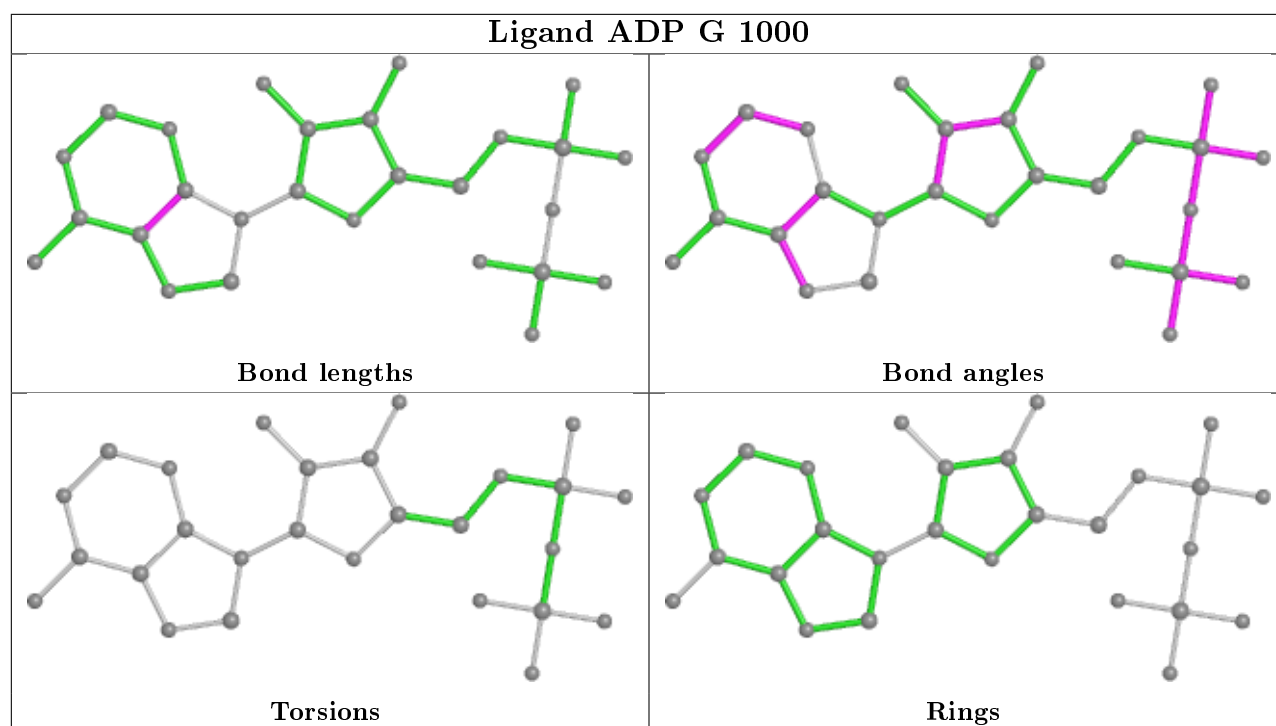
There are no ring outliers.

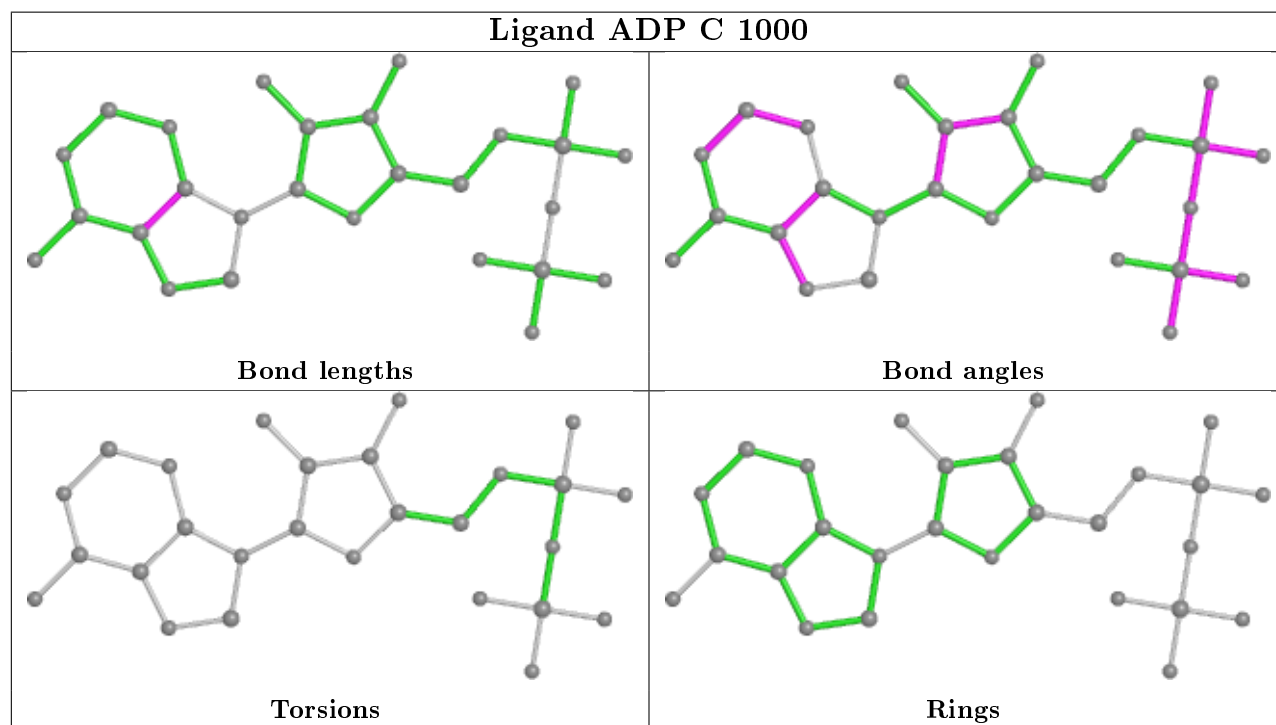
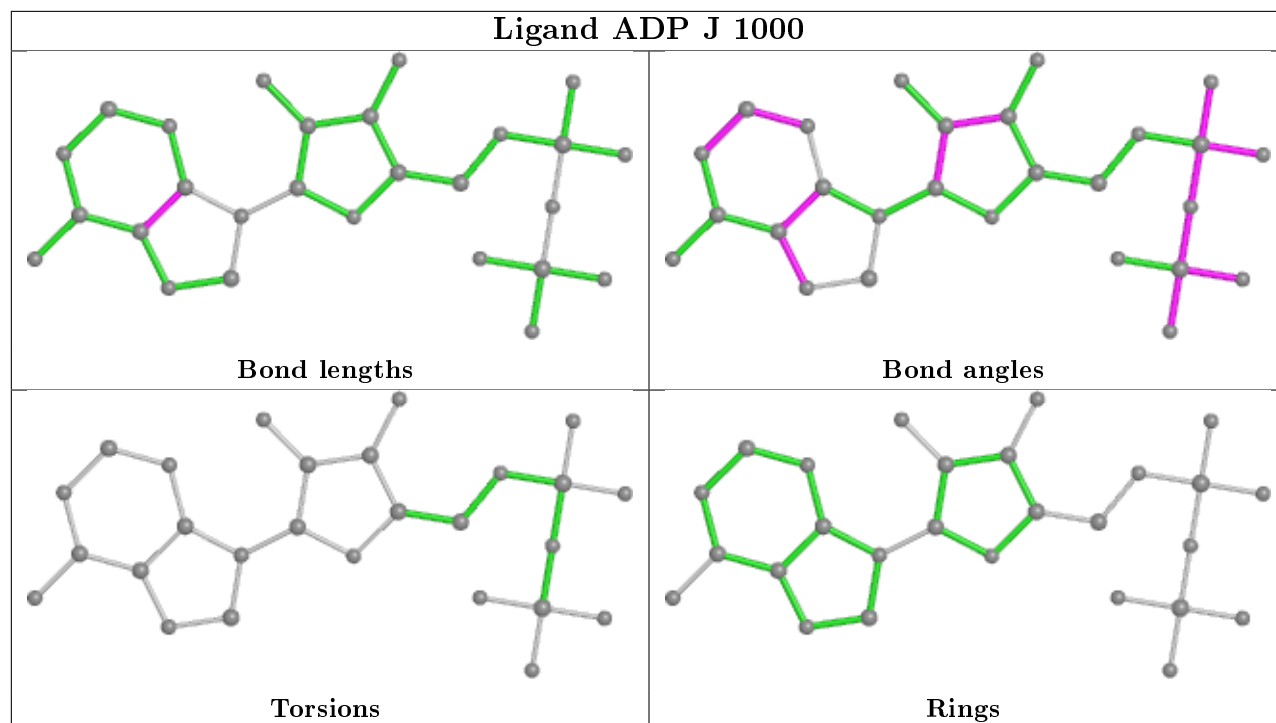
No monomer is involved in short contacts.

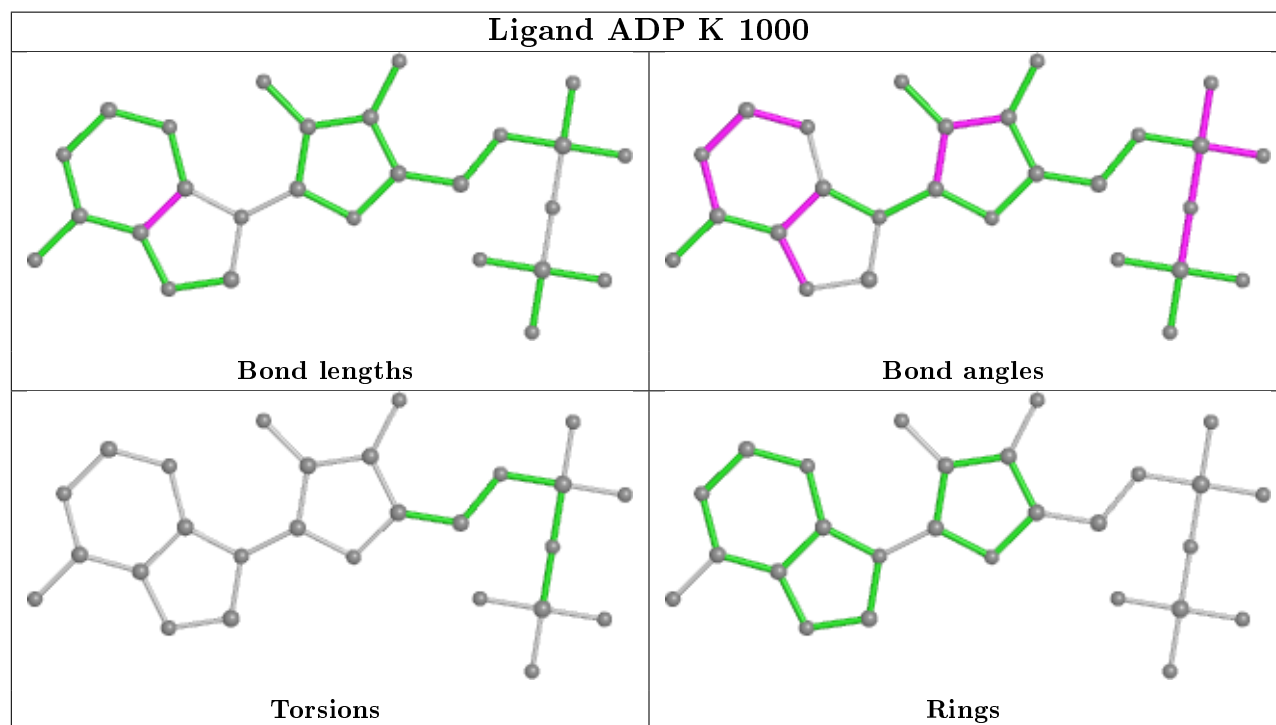
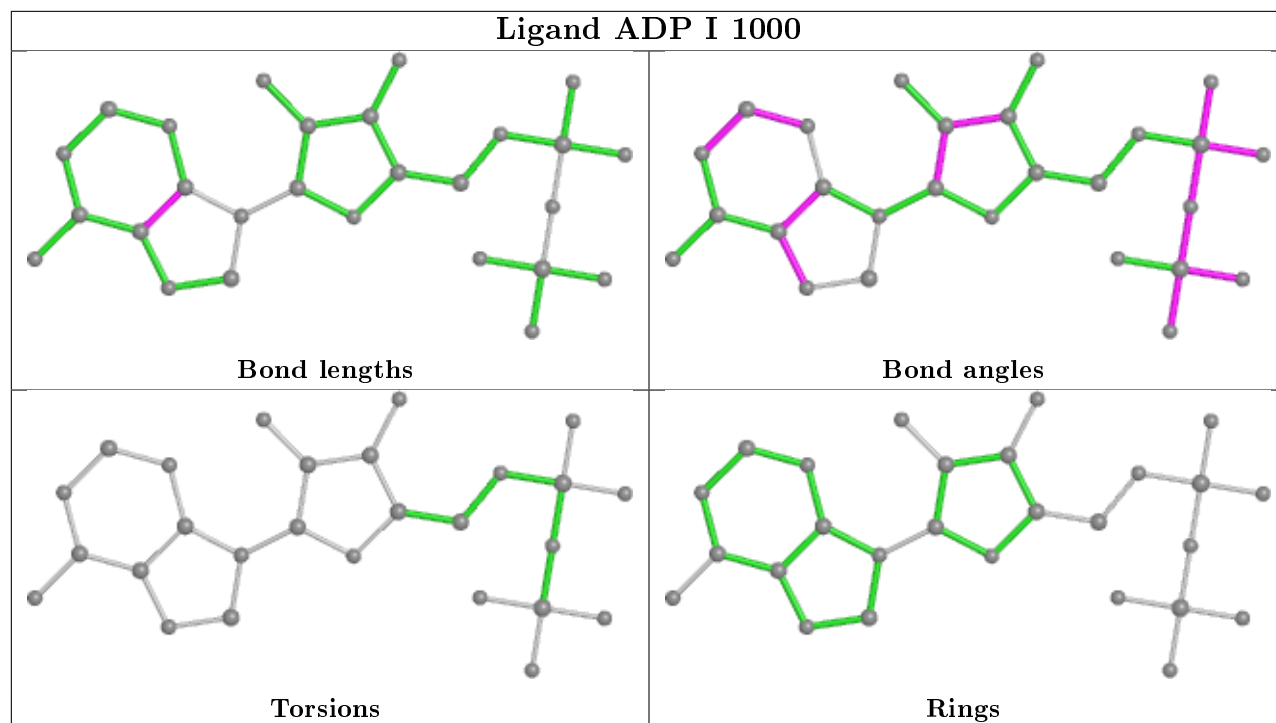
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

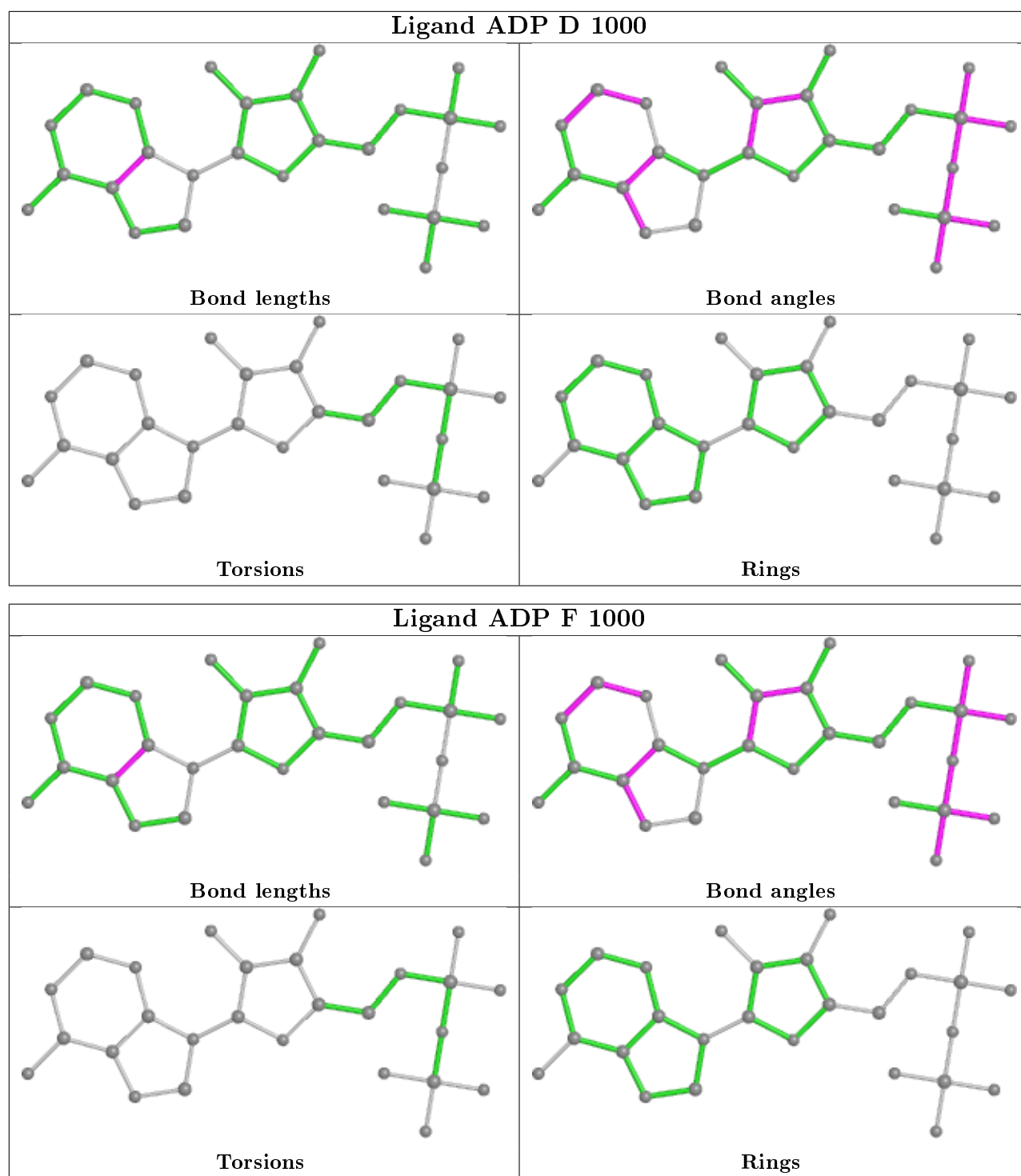












5.7 Other polymers ⓘ

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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	414/422 (98%)	0.07	20 (4%) 30 22	156, 200, 267, 301	0
1	B	409/422 (96%)	0.04	12 (2%) 51 39	110, 167, 245, 283	0
1	C	414/422 (98%)	-0.03	23 (5%) 24 17	141, 196, 260, 300	0
1	D	409/422 (96%)	-0.03	11 (2%) 54 42	119, 174, 249, 295	0
1	E	414/422 (98%)	0.16	30 (7%) 15 11	130, 219, 294, 330	0
1	F	409/422 (96%)	-0.12	11 (2%) 54 42	109, 170, 236, 273	0
1	G	414/422 (98%)	0.13	20 (4%) 30 22	158, 197, 262, 289	0
1	H	409/422 (96%)	-0.06	12 (2%) 51 39	116, 170, 252, 287	0
1	I	414/422 (98%)	0.19	31 (7%) 14 10	143, 210, 277, 312	0
1	J	409/422 (96%)	0.02	13 (3%) 47 35	114, 177, 243, 285	0
1	K	414/422 (98%)	-0.02	20 (4%) 30 22	143, 208, 271, 300	0
1	L	409/422 (96%)	0.00	10 (2%) 59 47	113, 169, 248, 293	0
2	M	43/60 (71%)	0.84	11 (25%) 0 0	219, 281, 308, 314	0
2	N	43/60 (71%)	1.11	12 (27%) 0 0	220, 291, 337, 346	0
2	O	43/60 (71%)	0.56	6 (13%) 2 3	233, 304, 350, 362	0
2	P	43/60 (71%)	0.99	11 (25%) 0 0	228, 287, 334, 351	0
2	Q	43/60 (71%)	1.36	14 (32%) 0 0	217, 305, 355, 367	0
2	R	43/60 (71%)	1.13	11 (25%) 0 0	233, 299, 356, 372	0
2	S	43/60 (71%)	0.72	7 (16%) 1 1	287, 329, 349, 357	0
2	T	43/60 (71%)	1.06	10 (23%) 0 0	303, 322, 348, 354	0
2	U	43/60 (71%)	1.43	16 (37%) 0 0	323, 350, 360, 363	0
2	V	43/60 (71%)	1.62	20 (46%) 0 0	309, 337, 364, 373	0
2	W	43/60 (71%)	1.74	10 (23%) 0 0	318, 340, 356, 363	0
2	X	43/60 (71%)	0.61	9 (20%) 1 0	335, 355, 374, 376	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	Y	6/12 (50%)	1.34	1 (16%) 1 1	50, 59, 70, 70	0
3	Z	6/12 (50%)	1.22	1 (16%) 1 1	50, 57, 60, 65	0
All	All	5466/5808 (94%)	0.13	352 (6%) 19 13	50, 193, 323, 376	0

All (352) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	W	161	SER	11.6
2	Q	150	GLU	9.9
2	U	181	ALA	9.5
2	W	150	GLU	9.2
2	R	150	GLU	9.1
2	W	157	ARG	8.7
2	N	150	GLU	8.5
1	I	293	ALA	8.1
2	O	150	GLU	8.0
1	J	281	SER	7.2
2	Q	175	PHE	7.0
2	P	150	GLU	6.9
1	E	330	VAL	6.9
1	E	331	ILE	6.8
1	D	286	THR	6.8
2	W	159	LYS	6.8
2	R	181	ALA	6.5
2	W	160	VAL	6.4
2	R	158	LEU	6.4
2	P	176	SER	6.3
2	W	181	ALA	6.2
1	B	289	VAL	6.1
2	X	181	ALA	6.0
2	T	150	GLU	6.0
2	Q	181	ALA	5.9
1	E	281	SER	5.9
2	M	181	ALA	5.8
2	T	161	SER	5.8
2	P	175	PHE	5.6
1	I	282	GLY	5.6
1	B	49	ILE	5.6
2	T	159	LYS	5.5
1	D	281	SER	5.5
2	V	176	SER	5.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	V	147	VAL	5.4
1	E	77	ASP	5.3
2	N	176	SER	5.3
1	L	165	ALA	5.3
2	S	150	GLU	5.2
1	C	293	ALA	5.1
1	K	330	VAL	5.1
2	U	178	VAL	5.0
2	W	178	VAL	5.0
1	I	281	SER	5.0
1	H	286	THR	4.9
1	F	45	SER	4.9
1	D	287	GLY	4.9
2	R	133	MET	4.9
2	T	181	ALA	4.9
2	T	160	VAL	4.9
1	B	14	LEU	4.8
2	N	158	LEU	4.8
2	V	175	PHE	4.8
1	H	291	ALA	4.8
2	V	159	LYS	4.8
1	A	165	ALA	4.7
1	A	356	PRO	4.7
1	I	335	PHE	4.7
1	I	151	ASN	4.6
2	R	134	VAL	4.6
1	G	286	THR	4.6
1	K	195	ILE	4.6
2	R	160	VAL	4.5
1	G	14	LEU	4.5
2	V	180	LYS	4.5
2	V	181	ALA	4.5
2	W	170	PRO	4.5
2	Q	174	ASP	4.4
2	V	171	VAL	4.4
2	S	176	SER	4.4
2	Q	180	LYS	4.4
1	G	176	ILE	4.4
1	I	127	ALA	4.4
2	M	160	VAL	4.4
1	J	49	ILE	4.4
2	T	148	VAL	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	293	ALA	4.2
2	M	169	THR	4.1
2	Q	179	GLU	4.1
1	G	28	ARG	4.1
2	U	133	MET	4.1
2	V	148	VAL	4.1
1	K	403	LEU	4.0
1	A	151	ASN	4.0
1	D	89	PHE	4.0
1	G	289	VAL	4.0
1	L	320	LEU	4.0
1	E	176	ILE	4.0
2	X	171	VAL	4.0
2	U	158	LEU	3.9
1	G	315	ILE	3.9
1	E	28	ARG	3.9
1	A	26	LEU	3.9
2	P	180	LYS	3.8
2	P	160	VAL	3.8
1	A	62	PHE	3.8
1	D	164	LEU	3.7
2	R	148	VAL	3.7
1	K	356	PRO	3.7
1	G	175	LEU	3.7
2	V	170	PRO	3.7
1	I	294	LEU	3.7
1	G	358	ILE	3.6
1	C	402	LYS	3.6
2	S	159	LYS	3.6
2	T	178	VAL	3.6
2	V	161	SER	3.6
2	O	181	ALA	3.6
1	C	28	ARG	3.5
1	C	356	PRO	3.5
2	M	150	GLU	3.5
1	G	293	ALA	3.5
2	M	175	PHE	3.5
1	K	188	LEU	3.5
1	J	176	ILE	3.5
2	P	169	THR	3.5
2	U	173	LEU	3.5
1	H	44	LYS	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	49	ILE	3.5
2	N	159	LYS	3.5
2	V	133	MET	3.4
2	U	165	PHE	3.4
2	N	133	MET	3.4
1	L	14	LEU	3.4
1	E	291	ALA	3.4
1	E	76	PRO	3.4
1	A	403	LEU	3.4
1	G	291	ALA	3.4
1	E	315	ILE	3.4
2	X	170	PRO	3.4
2	T	179	GLU	3.4
2	N	181	ALA	3.4
1	A	168	ILE	3.3
2	P	181	ALA	3.3
2	Q	141	PHE	3.3
2	T	177	GLN	3.3
2	X	161	SER	3.3
1	I	291	ALA	3.3
1	I	229	ALA	3.3
2	T	165	PHE	3.3
1	I	275	ASN	3.3
2	M	161	SER	3.3
1	A	138	PRO	3.3
1	E	413	PHE	3.3
2	U	157	ARG	3.2
1	J	286	THR	3.2
2	N	148	VAL	3.2
1	E	282	GLY	3.2
2	S	181	ALA	3.2
1	E	335	PHE	3.1
2	V	179	GLU	3.1
2	Q	161	SER	3.1
2	Q	133	MET	3.1
1	K	119	VAL	3.1
2	W	158	LEU	3.1
1	K	335	PHE	3.1
1	I	413	PHE	3.1
1	K	377	LEU	3.0
2	P	179	GLU	3.0
1	G	140	HIS	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	15	ILE	3.0
1	C	229	ALA	3.0
2	U	161	SER	3.0
1	D	193	GLN	3.0
2	N	134	VAL	3.0
2	O	169	THR	3.0
1	A	399	LEU	3.0
2	V	149	GLU	3.0
1	H	402	LYS	3.0
1	J	395	ALA	3.0
1	C	294	LEU	3.0
2	O	157	ARG	3.0
3	Y	6[A]	U	3.0
1	B	164	LEU	3.0
1	B	291	ALA	3.0
1	E	175	LEU	3.0
1	G	281	SER	2.9
1	B	275	ASN	2.9
1	J	164	LEU	2.9
1	J	56	GLU	2.9
1	K	399	LEU	2.9
1	L	138	PRO	2.9
2	U	180	LYS	2.9
2	X	178	VAL	2.9
2	R	157	ARG	2.9
2	N	149	GLU	2.9
1	E	357	ALA	2.9
2	S	178	VAL	2.9
2	M	133	MET	2.9
2	Q	149	GLU	2.8
1	F	220	GLN	2.8
1	A	330	VAL	2.8
1	J	413	PHE	2.8
1	E	274	TYR	2.8
1	A	106	GLU	2.8
1	I	403	LEU	2.8
2	V	163	SER	2.8
1	C	176	ILE	2.8
1	C	403	LEU	2.8
1	J	292	ASN	2.8
2	S	171	VAL	2.8
1	A	313	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	328	ASP	2.7
1	C	387	ILE	2.7
1	E	262	ILE	2.7
1	C	207	LEU	2.7
1	C	109	ARG	2.7
1	D	320	LEU	2.7
1	E	289	VAL	2.7
1	C	285	LEU	2.7
2	N	141	PHE	2.7
2	V	162	VAL	2.7
1	K	91	LEU	2.6
2	M	179	GLU	2.6
1	K	328	ASP	2.6
1	F	330	VAL	2.6
1	A	97	ILE	2.6
1	C	263	LEU	2.6
2	N	160	VAL	2.6
2	U	170	PRO	2.6
1	I	399	LEU	2.6
1	E	332	TYR	2.6
2	U	164	ILE	2.6
2	V	169	THR	2.6
1	D	61	GLY	2.5
1	E	290	ASP	2.5
1	F	399	LEU	2.5
2	Q	176	SER	2.5
2	R	169	THR	2.5
1	H	285	LEU	2.5
1	I	316	ILE	2.5
1	D	263	LEU	2.5
2	P	159	LYS	2.5
1	I	331	ILE	2.5
1	F	91	LEU	2.5
2	Q	177	GLN	2.5
1	C	343	LEU	2.5
1	I	303	ALA	2.5
2	V	164	ILE	2.5
1	I	150	GLY	2.5
1	K	380	MET	2.5
1	L	149	ARG	2.5
1	C	282	GLY	2.5
1	B	281	SER	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	V	178	VAL	2.5
2	U	172	GLU	2.4
1	F	324	GLY	2.4
2	X	159	LYS	2.4
2	V	150	GLU	2.4
1	A	61	GLY	2.4
1	A	63	GLY	2.4
1	E	270	LEU	2.4
2	M	176	SER	2.4
1	C	383	LEU	2.4
1	K	264	LEU	2.4
1	H	360	TYR	2.4
1	I	402	LYS	2.4
1	A	291	ALA	2.4
1	B	345	LEU	2.4
1	L	289	VAL	2.4
2	Q	148	VAL	2.4
2	R	141	PHE	2.4
2	X	177	GLN	2.3
2	W	145	ASN	2.3
1	K	383	LEU	2.3
1	I	165	ALA	2.3
2	Q	178	VAL	2.3
2	P	174	ASP	2.3
1	L	151	ASN	2.3
1	I	58	LEU	2.3
1	J	175	LEU	2.3
1	E	106	GLU	2.3
1	I	405	MET	2.3
3	Z	6[A]	U	2.3
2	U	145	ASN	2.3
1	E	416	MET	2.3
1	B	316	ILE	2.3
1	G	116	VAL	2.3
1	J	279	PRO	2.3
1	I	101	ILE	2.3
1	K	331	ILE	2.3
1	I	169	GLY	2.3
1	G	331	ILE	2.3
2	M	177	GLN	2.3
1	F	39	LEU	2.3
2	O	136	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	140	HIS	2.3
1	L	169	GLY	2.2
1	G	335	PHE	2.2
1	C	157	LEU	2.2
1	F	188	LEU	2.2
1	A	149	ARG	2.2
1	E	316	ILE	2.2
1	D	335	PHE	2.2
1	E	292	ASN	2.2
1	C	264	LEU	2.2
2	R	149	GLU	2.2
1	I	170	ARG	2.2
1	I	113	LEU	2.2
2	N	174	ASP	2.2
1	C	291	ALA	2.2
1	C	91	LEU	2.2
1	C	150	GLY	2.2
1	A	169	GLY	2.2
1	G	240	VAL	2.2
1	E	360	TYR	2.2
2	X	138	ASP	2.1
1	H	343	LEU	2.1
1	L	291	ALA	2.1
1	I	356	PRO	2.1
2	X	133	MET	2.1
1	E	399	LEU	2.1
1	C	247	ILE	2.1
1	F	176	ILE	2.1
1	B	288	GLY	2.1
1	J	106	GLU	2.1
1	C	187	LEU	2.1
1	E	329	GLU	2.1
1	H	294	LEU	2.1
1	G	316	ILE	2.1
1	A	320	LEU	2.1
2	M	178	VAL	2.1
2	O	158	LEU	2.1
1	B	413	PHE	2.1
1	D	49	ILE	2.1
1	E	358	ILE	2.1
1	K	168	ILE	2.1
2	U	174	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	174	GLY	2.1
1	I	100	LYS	2.1
2	V	177	GLN	2.1
1	F	281	SER	2.1
1	H	131	ILE	2.1
1	I	49	ILE	2.1
1	J	308	GLU	2.1
1	H	247	ILE	2.1
1	K	176	ILE	2.1
1	G	354	VAL	2.1
1	I	164	LEU	2.1
1	I	187	LEU	2.1
1	G	164	LEU	2.0
1	H	289	VAL	2.0
2	S	177	GLN	2.0
2	U	159	LYS	2.0
1	K	317	ALA	2.0
1	L	97	ILE	2.0
1	K	175	LEU	2.0
2	U	171	VAL	2.0
1	H	248	GLU	2.0
1	F	161	VAL	2.0
2	P	148	VAL	2.0
1	K	279	PRO	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](#)

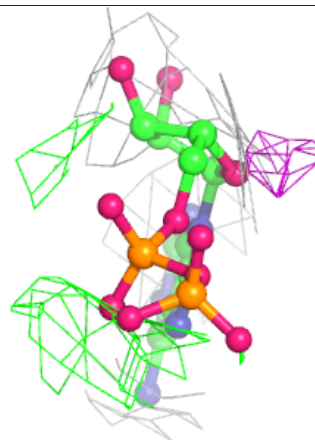
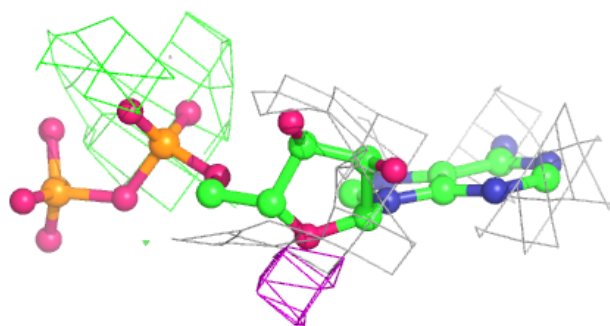
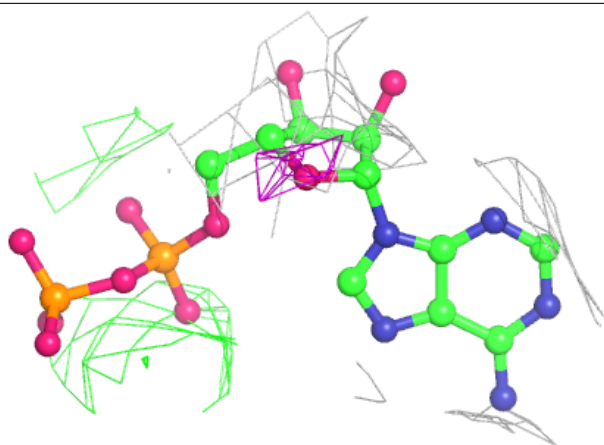
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	BEF	E	1002	4/4	0.67	0.20	162,178,182,194	0
6	BEF	I	1002	4/4	0.79	0.26	158,158,163,176	0
6	BEF	C	1002	4/4	0.83	0.25	151,152,156,160	0
6	BEF	G	1002	4/4	0.84	0.24	157,164,172,177	0
4	ADP	E	1000	27/27	0.87	0.20	162,186,230,258	0
6	BEF	A	1002	4/4	0.89	0.24	156,172,179,191	0
4	ADP	K	1000	27/27	0.91	0.25	155,176,228,246	0
6	BEF	L	1002	4/4	0.92	0.28	142,142,142,152	0
4	ADP	J	1000	27/27	0.92	0.23	142,147,173,190	0
5	MG	D	1001	1/1	0.92	0.23	132,132,132,132	0
6	BEF	K	1002	4/4	0.93	0.17	155,172,183,192	0
4	ADP	G	1000	27/27	0.93	0.23	157,174,210,230	0
4	ADP	C	1000	27/27	0.93	0.26	151,165,204,232	0
4	ADP	I	1000	27/27	0.94	0.17	158,175,215,221	0
6	BEF	J	1002	4/4	0.94	0.16	142,142,142,142	0
4	ADP	F	1000	27/27	0.94	0.23	142,147,170,189	0
4	ADP	B	1000	27/27	0.94	0.25	133,133,154,177	0
4	ADP	L	1000	27/27	0.95	0.23	142,144,165,188	0
4	ADP	A	1000	27/27	0.95	0.20	156,171,210,235	0
6	BEF	B	1002	4/4	0.95	0.27	133,133,133,133	0
4	ADP	D	1000	27/27	0.95	0.22	132,132,157,181	0
6	BEF	H	1002	4/4	0.95	0.30	134,134,134,135	0
4	ADP	H	1000	27/27	0.95	0.25	134,135,156,193	0
5	MG	E	1001	1/1	0.97	0.29	162,162,162,162	0
5	MG	I	1001	1/1	0.97	0.28	158,158,158,158	0
6	BEF	D	1002	4/4	0.97	0.27	132,132,132,132	0
5	MG	G	1001	1/1	0.97	0.34	157,157,157,157	0
5	MG	K	1001	1/1	0.97	0.16	155,155,155,155	0
5	MG	F	1001	1/1	0.98	0.18	142,142,142,142	0
5	MG	H	1001	1/1	0.98	0.34	134,134,134,134	0
5	MG	A	1001	1/1	0.99	0.25	156,156,156,156	0
5	MG	C	1001	1/1	0.99	0.33	151,151,151,151	0
5	MG	J	1001	1/1	0.99	0.23	142,142,142,142	0
6	BEF	F	1002	4/4	0.99	0.17	142,142,142,142	0
5	MG	L	1001	1/1	0.99	0.30	142,142,142,142	0
5	MG	B	1001	1/1	0.99	0.33	133,133,133,133	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.

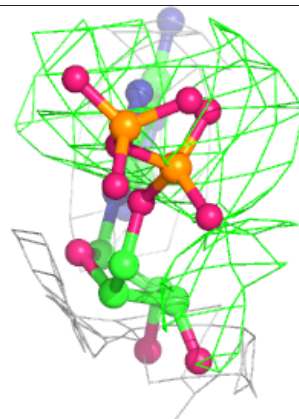
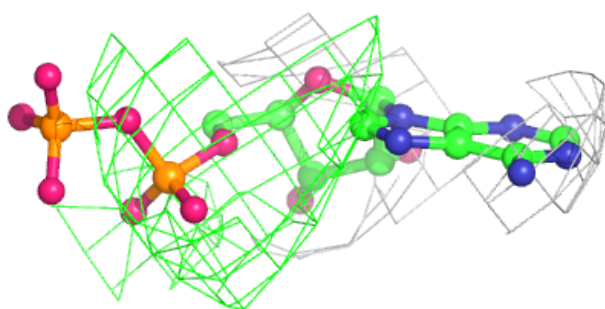
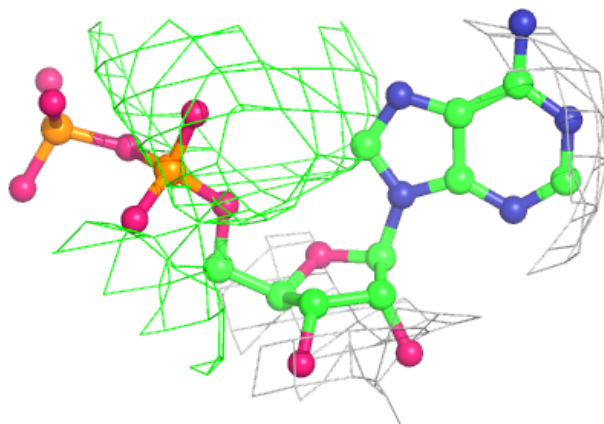
Electron density around ADP E 1000:

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



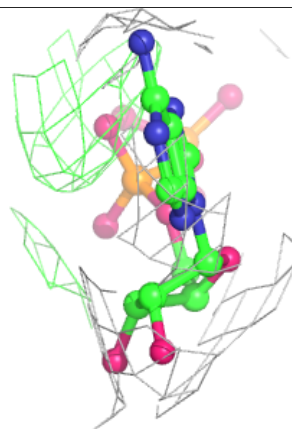
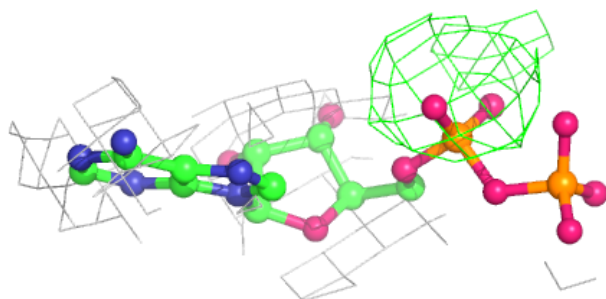
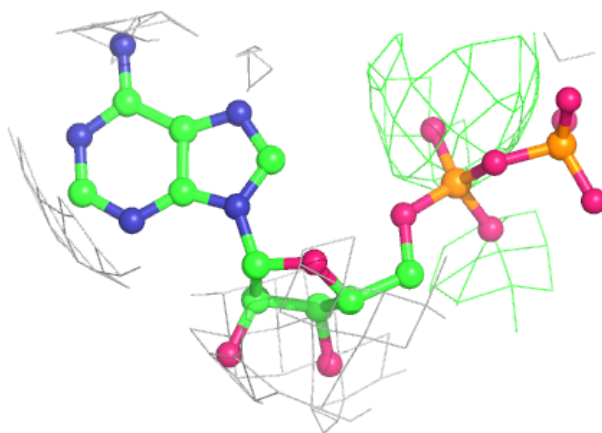
Electron density around ADP K 1000:

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

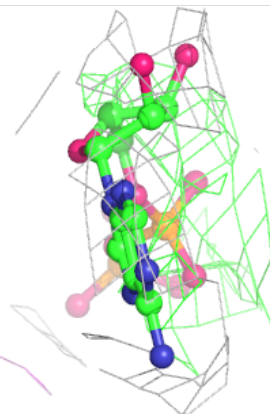
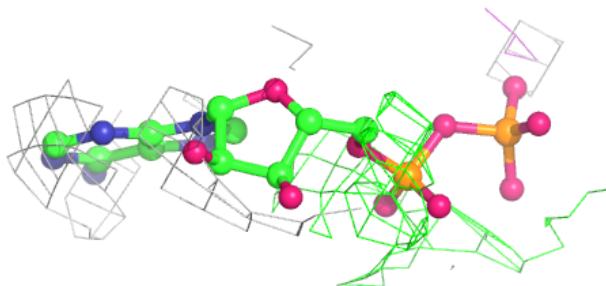
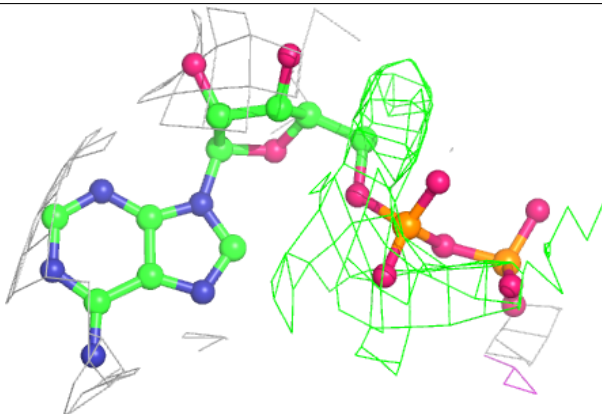


Electron density around ADP J 1000:

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

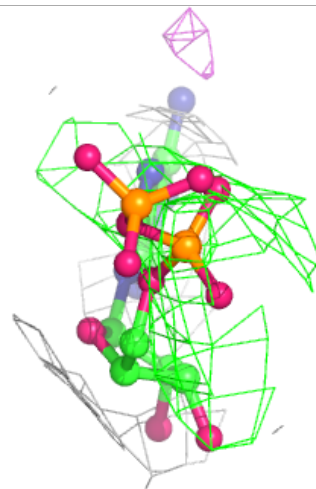
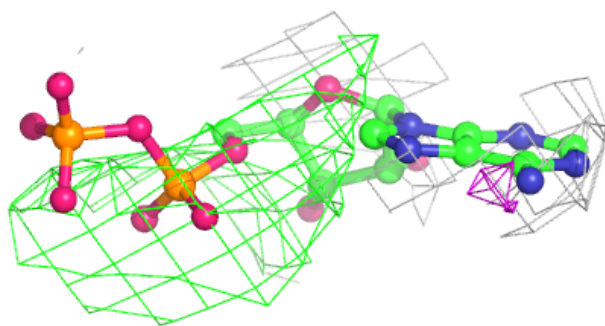
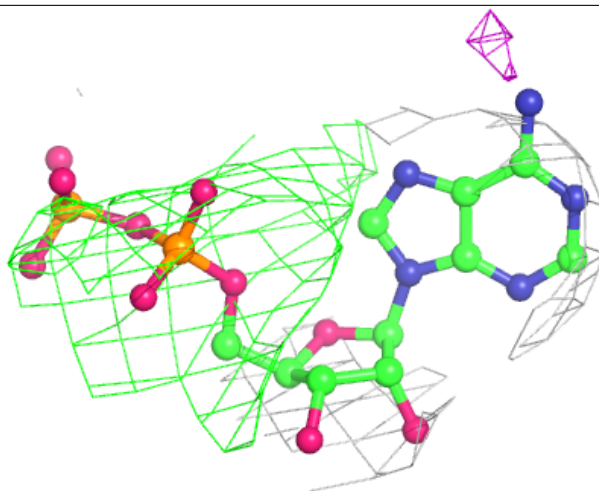
**Electron density around ADP G 1000:**

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



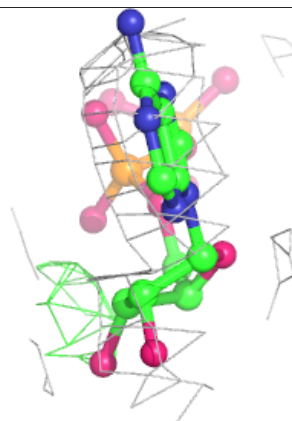
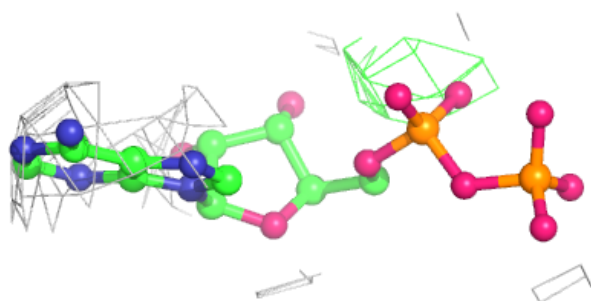
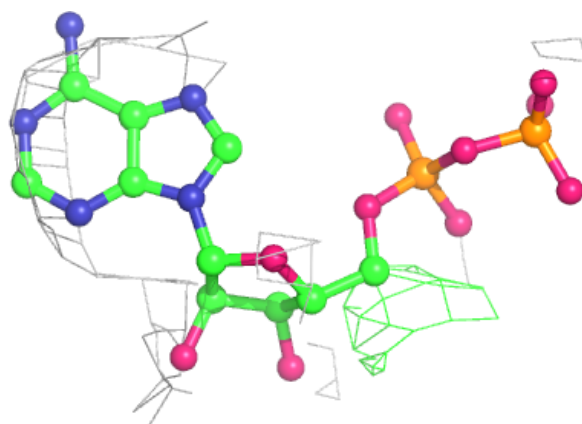
Electron density around ADP C 1000:

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



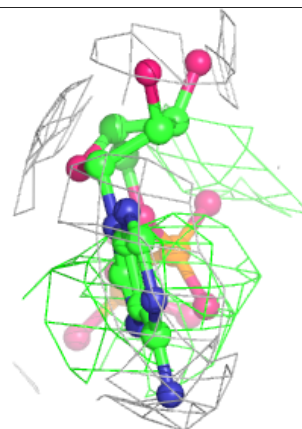
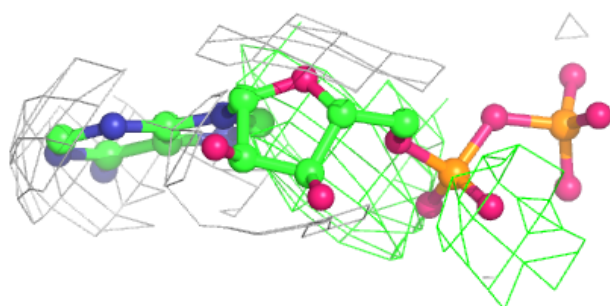
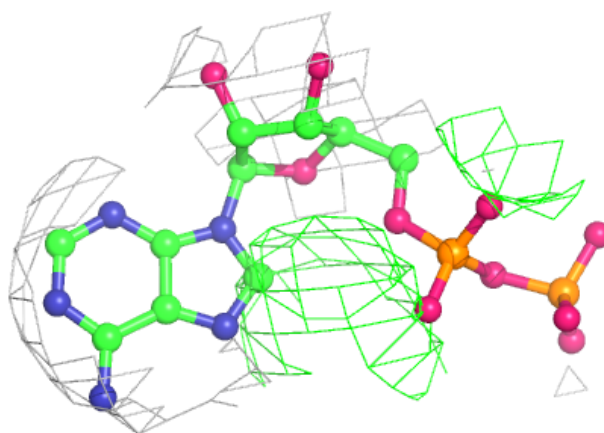
Electron density around ADP I 1000:

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

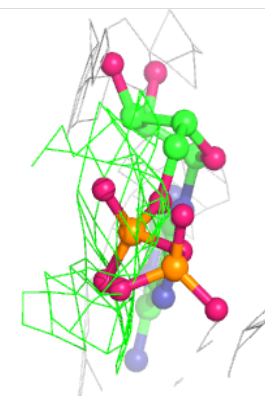
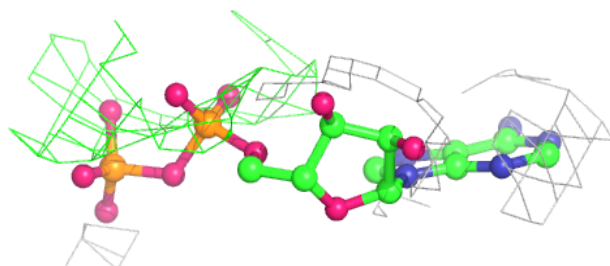
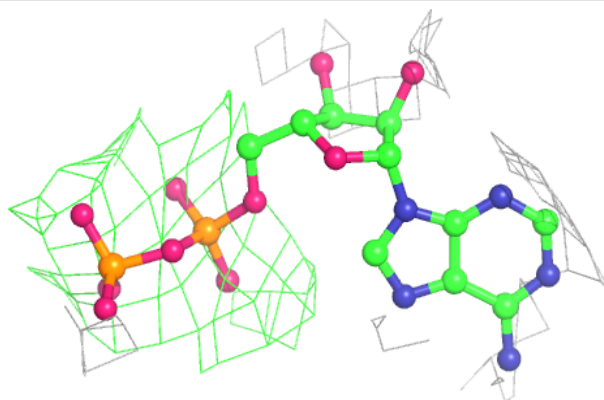


Electron density around ADP F 1000:

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

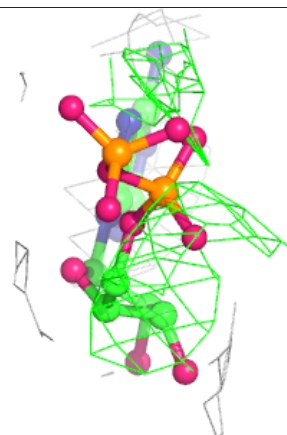
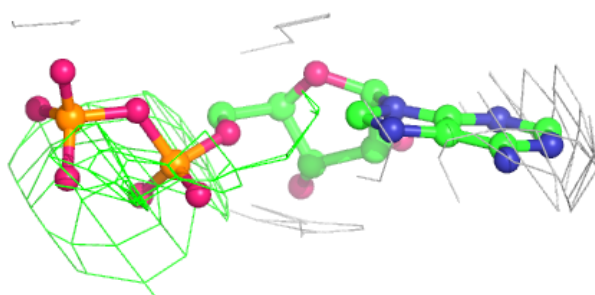
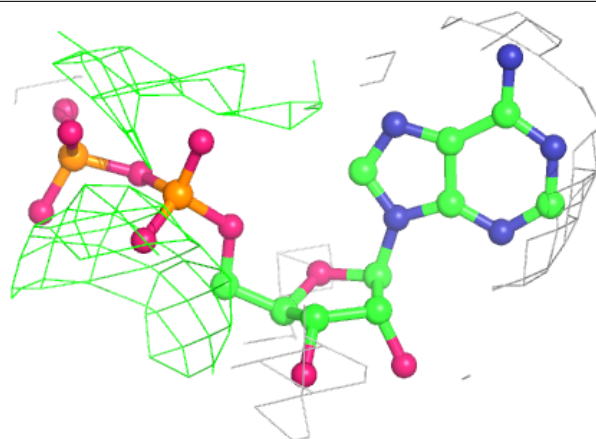
**Electron density around ADP B 1000:**

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



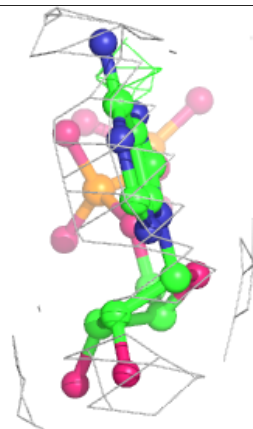
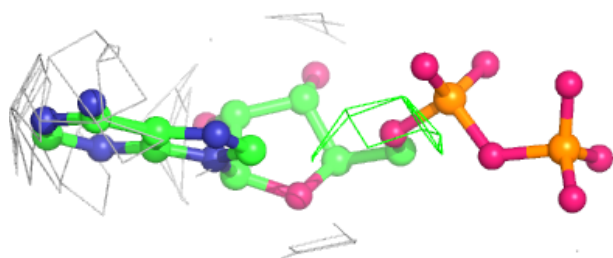
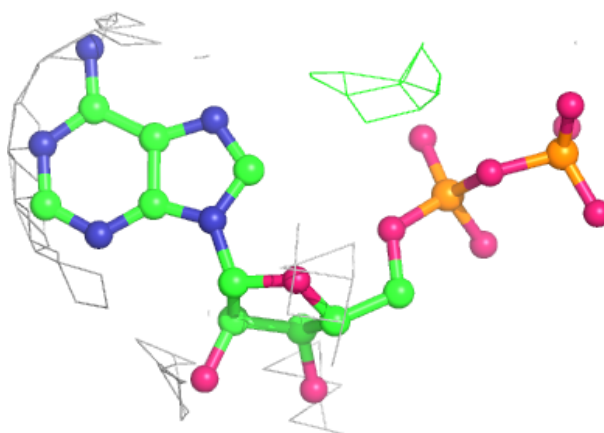
Electron density around ADP L 1000:

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

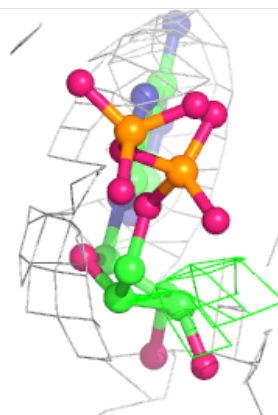
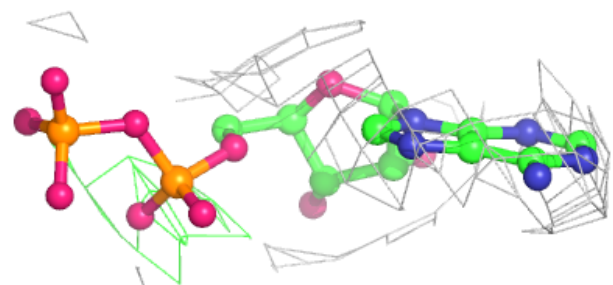
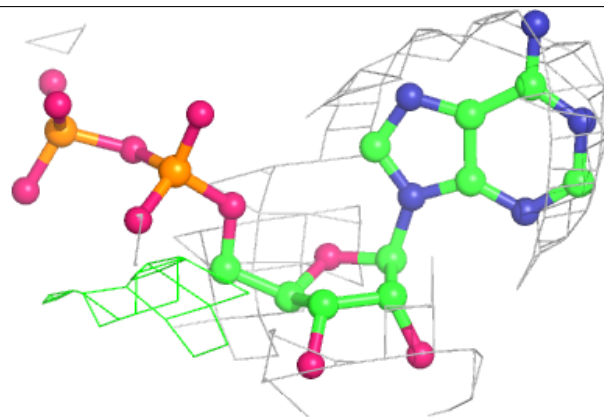


Electron density around ADP A 1000:

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

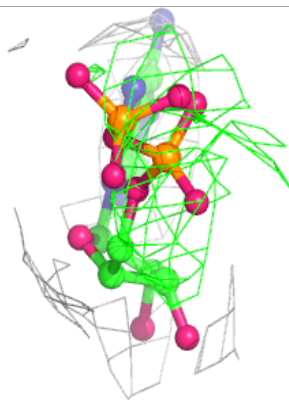
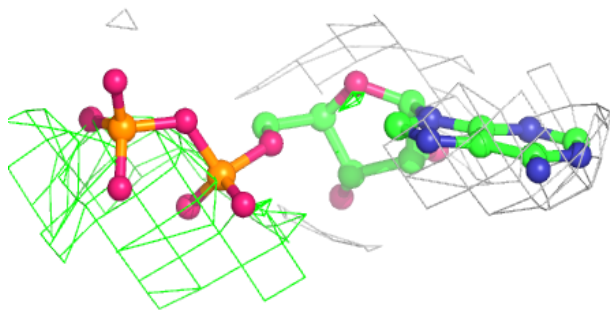
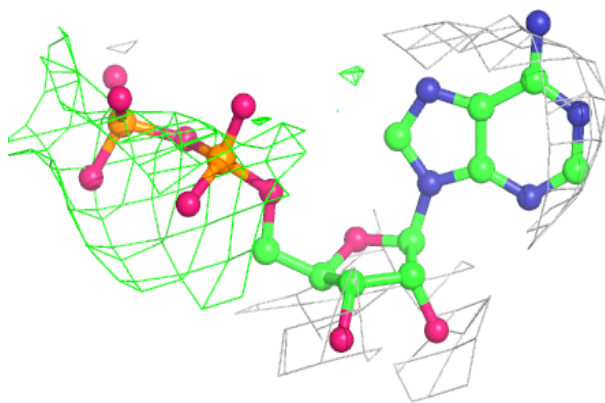
**Electron density around ADP D 1000:**

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



Electron density around ADP H 1000:

$2mF_o - DF_c$ (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.