



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:37 PM UTC

PDB ID : 3KQU / pdb_00003kqu
Title : Three Conformational Snapshots of the Hepatitis C Virus NS3 Helicase Reveal a Ratchet Translocation Mechanism
Authors : Gu, M.; Rice, C.M.
Deposited on : 2009-11-17
Resolution : 2.40 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 types of validation reports are described at

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

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

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

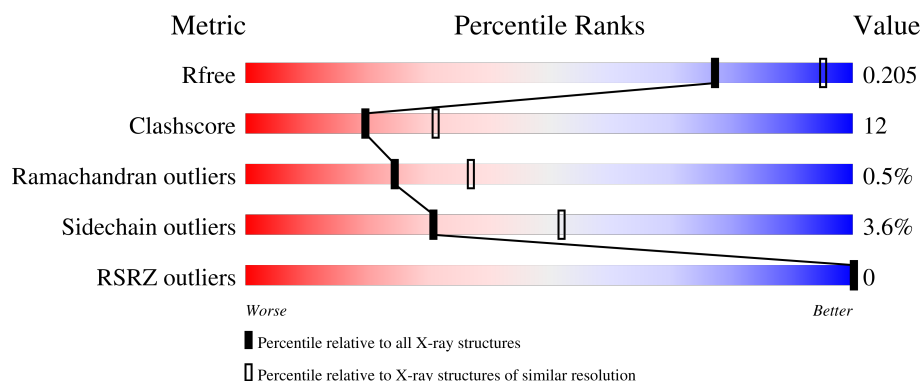
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	437	 74% 24% .
1	B	437	 75% 23% .
1	C	437	 73% 25% .
1	D	437	 72% 26% .
1	E	437	 74% 24% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	437	 74% 24% •
2	M	19	 53% 21% 21% 5%
2	N	19	 53% 26% 16% 5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23155 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 Serine protease/NTPase/helicase NS3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3280	2077	556	626	21			
1	B	437	Total	C	N	O	S	0	0	0
			3280	2077	556	626	21			
1	C	437	Total	C	N	O	S	0	0	0
			3280	2077	556	626	21			
1	D	437	Total	C	N	O	S	0	0	0
			3280	2077	556	626	21			
1	E	437	Total	C	N	O	S	0	0	0
			3280	2077	556	626	21			
1	F	437	Total	C	N	O	S	0	0	0
			3280	2077	556	626	21			

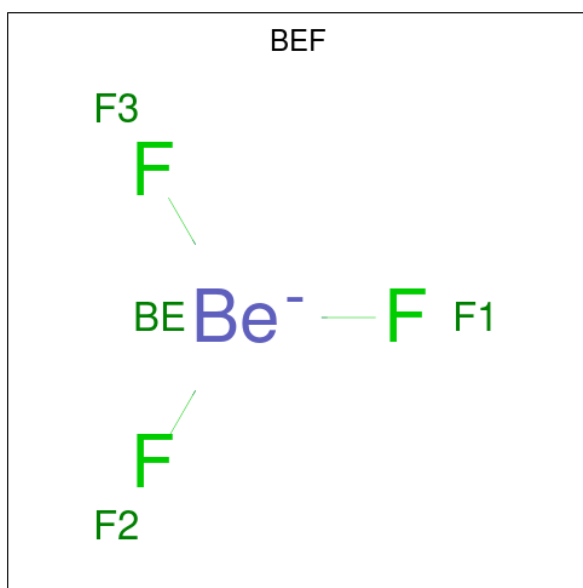
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	625	ALA	-	expression tag	UNP Q9WMX2
B	625	ALA	-	expression tag	UNP Q9WMX2
C	625	ALA	-	expression tag	UNP Q9WMX2
D	625	ALA	-	expression tag	UNP Q9WMX2
E	625	ALA	-	expression tag	UNP Q9WMX2
F	625	ALA	-	expression tag	UNP Q9WMX2

- Molecule 2 is a DNA chain called 5'-D(*T*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	18	Total	C	N	O	P	0	18	0
			1428	720	144	496	68			
2	N	18	Total	C	N	O	P	0	18	0
			1428	720	144	496	68			

- Molecule 3 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3).



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

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	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	C	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	E	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		

- Molecule 5 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mn	0	0
			1	1		
5	B	1	Total	Mn	0	0
			1	1		
5	C	1	Total	Mn	0	0
			1	1		
5	D	1	Total	Mn	0	0
			1	1		
5	E	1	Total	Mn	0	0
			1	1		
5	F	1	Total	Mn	0	0
			1	1		

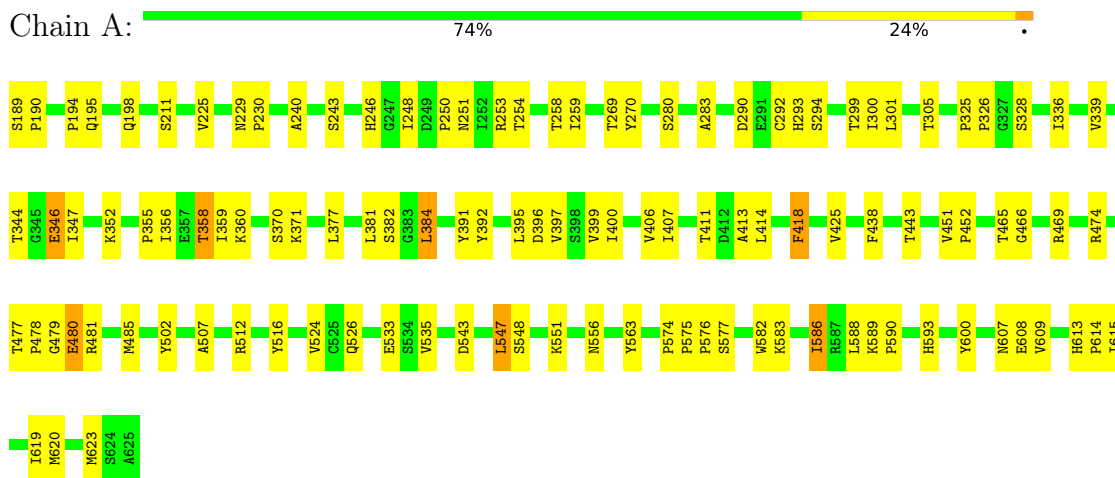
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	72	Total 72	O 72	0	0
6	B	70	Total 70	O 70	0	0
6	C	63	Total 63	O 63	0	0
6	D	71	Total 71	O 71	0	0
6	E	66	Total 66	O 66	0	0
6	F	63	Total 63	O 63	0	0
6	M	9	Total 9	O 9	0	0
6	N	13	Total 13	O 13	0	0

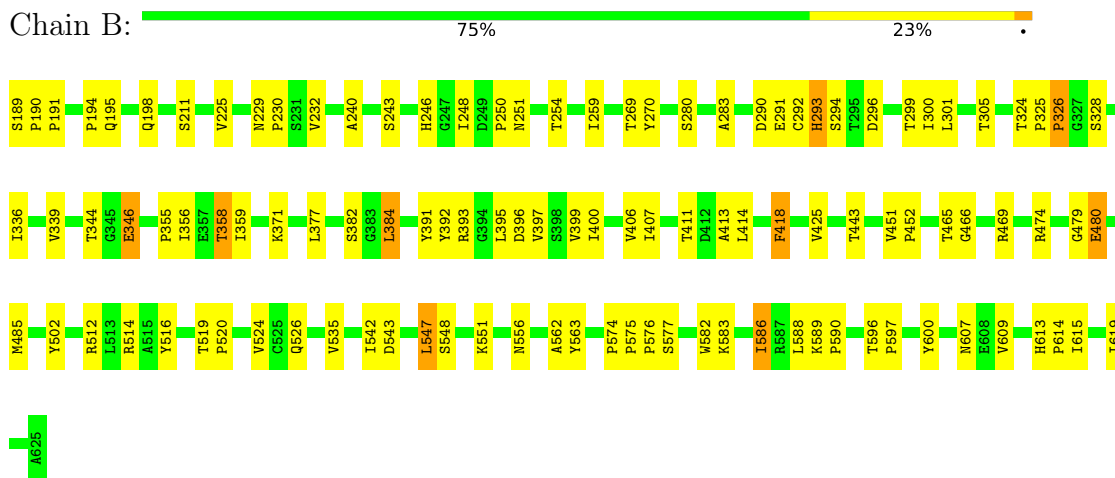
3 Residue-property plots

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

• Molecule 1: Serine protease/NTPase/helicase NS3

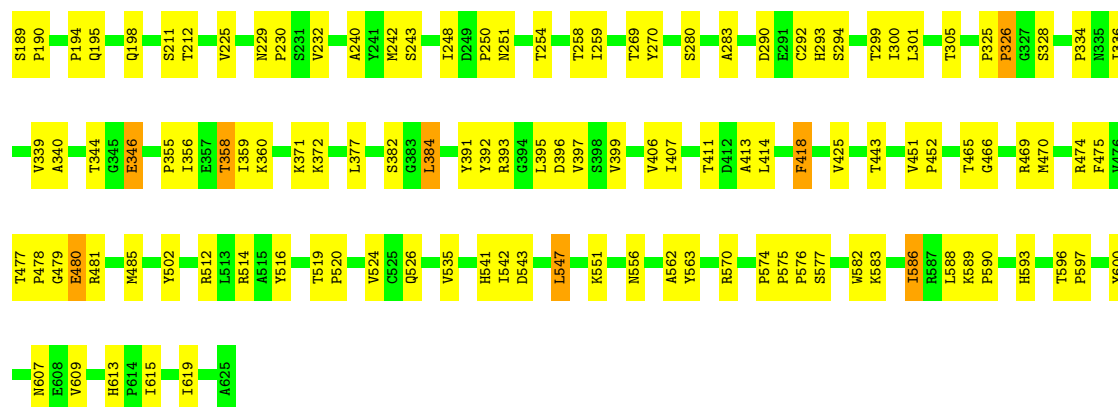


• Molecule 1: Serine protease/NTPase/helicase NS3



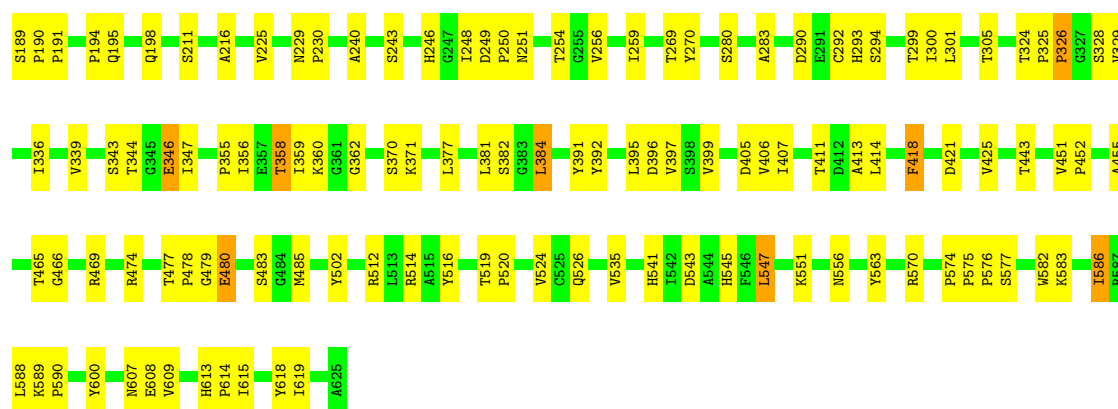
• Molecule 1: Serine protease/NTPase/helicase NS3





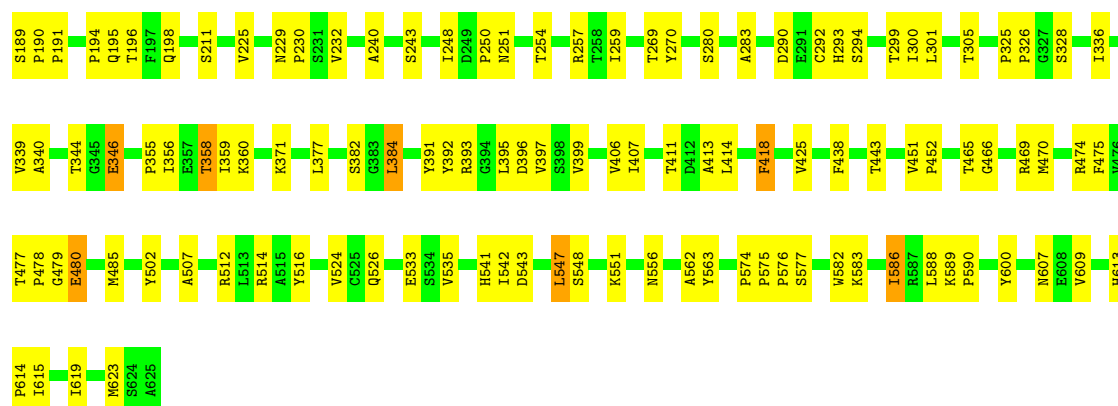
- Molecule 1: Serine protease/NTPase/helicase NS3

Chain D: 72% 26%



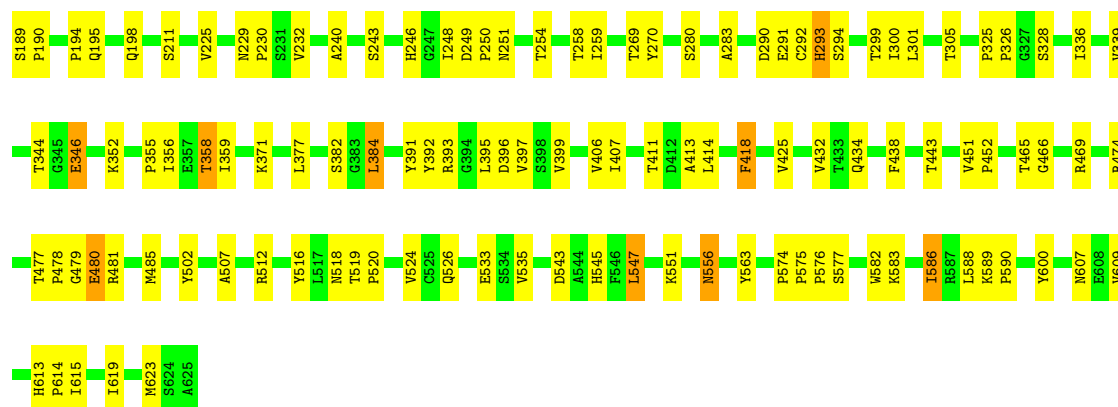
- Molecule 1: Serine protease/NTPase/helicase NS3

Chain E: 74% 24%



- Molecule 1: Serine protease/NTPase/helicase NS3

Chain F: 74% 24%



- Molecule 2: 5'-D(*T*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP)-3'



- Molecule 2: 5'-D(*T*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	116.53Å 116.47Å 71.11Å 90.00° 90.00° 119.97°	Depositor
Resolution (Å)	50.00 – 2.40 50.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	87.2 (50.00-2.40) 87.5 (50.00-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.197 , 0.215 0.188 , 0.205	Depositor DCC
R_{free} test set	5511 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	38.0	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 21.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.467 for -k,h+k,l 0.467 for h+k,-h,l 0.460 for -h-k,h,l 0.460 for k,-h-k,l 0.468 for -h,-k,l 0.048 for -h-k,k,-l 0.048 for h,-h-k,-l 0.051 for k,h,-l 0.049 for -k,-h,-l 0.048 for h+k,-k,-l 0.048 for -h,h+k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	23155	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, 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	0.49	0/3361	0.93	8/4592 (0.2%)
1	B	0.49	0/3361	0.94	10/4592 (0.2%)
1	C	0.48	0/3361	0.94	7/4592 (0.2%)
1	D	0.49	0/3361	0.94	9/4592 (0.2%)
1	E	0.49	0/3361	0.94	7/4592 (0.2%)
1	F	0.48	0/3361	0.94	7/4592 (0.2%)
2	M	0.41	0/1568	1.16	28/2416 (1.2%)
2	N	0.40	0/1568	1.15	28/2416 (1.2%)
All	All	0.48	0/23302	0.97	104/32384 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	M	0	1

There are no bond length outliers.

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	336	ILE	N-CA-C	8.03	119.47	107.75
1	A	336	ILE	N-CA-C	7.90	119.28	107.75
1	F	336	ILE	N-CA-C	7.79	119.13	107.75
1	C	336	ILE	N-CA-C	7.75	119.07	107.75
1	B	336	ILE	N-CA-C	7.73	119.03	107.75
1	E	336	ILE	N-CA-C	7.71	119.01	107.75
2	N	32[A]	DT	C2'-C3'-O3'	-6.89	101.16	111.50
2	N	32[B]	DT	C2'-C3'-O3'	-6.89	101.16	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	32[C]	DT	C2'-C3'-O3'	-6.89	101.16	111.50
2	N	32[D]	DT	C2'-C3'-O3'	-6.89	101.16	111.50
2	M	12[A]	DT	C2'-C3'-O3'	-6.71	101.44	111.50
2	M	12[B]	DT	C2'-C3'-O3'	-6.71	101.44	111.50
2	M	12[C]	DT	C2'-C3'-O3'	-6.71	101.44	111.50
2	M	12[D]	DT	C2'-C3'-O3'	-6.71	101.44	111.50
2	M	13[A]	DT	C2'-C3'-O3'	-6.64	101.54	111.50
2	M	13[B]	DT	C2'-C3'-O3'	-6.64	101.54	111.50
2	M	13[C]	DT	C2'-C3'-O3'	-6.64	101.54	111.50
2	M	13[D]	DT	C2'-C3'-O3'	-6.64	101.54	111.50
1	E	293	HIS	N-CA-C	-6.60	105.38	113.50
1	B	293	HIS	N-CA-C	-6.60	105.39	113.50
2	N	33[A]	DT	C2'-C3'-O3'	-6.56	101.66	111.50
2	N	33[B]	DT	C2'-C3'-O3'	-6.56	101.66	111.50
2	N	33[C]	DT	C2'-C3'-O3'	-6.56	101.66	111.50
2	N	33[D]	DT	C2'-C3'-O3'	-6.56	101.66	111.50
1	A	225	VAL	N-CA-C	6.55	117.29	108.11
2	N	27[A]	DT	C2'-C3'-O3'	-6.54	101.69	111.50
2	N	27[B]	DT	C2'-C3'-O3'	-6.54	101.69	111.50
2	N	27[C]	DT	C2'-C3'-O3'	-6.54	101.69	111.50
2	N	27[D]	DT	C2'-C3'-O3'	-6.54	101.69	111.50
1	A	293	HIS	N-CA-C	-6.46	105.55	113.50
1	C	225	VAL	N-CA-C	6.46	117.15	108.11
1	C	293	HIS	N-CA-C	-6.44	105.58	113.50
2	M	7[A]	DT	C2'-C3'-O3'	-6.41	101.88	111.50
2	M	7[B]	DT	C2'-C3'-O3'	-6.41	101.88	111.50
2	M	7[C]	DT	C2'-C3'-O3'	-6.41	101.88	111.50
2	M	7[D]	DT	C2'-C3'-O3'	-6.41	101.88	111.50
1	F	293	HIS	N-CA-C	-6.40	105.63	113.50
1	F	225	VAL	N-CA-C	6.39	117.06	108.11
1	D	293	HIS	N-CA-C	-6.38	105.65	113.50
1	D	225	VAL	N-CA-C	6.37	117.03	108.11
1	E	225	VAL	N-CA-C	6.37	117.02	108.11
1	B	225	VAL	N-CA-C	6.26	116.88	108.11
2	M	6[A]	DT	C2'-C3'-O3'	-6.15	102.28	111.50
2	M	6[B]	DT	C2'-C3'-O3'	-6.15	102.28	111.50
2	M	6[C]	DT	C2'-C3'-O3'	-6.15	102.28	111.50
2	M	6[D]	DT	C2'-C3'-O3'	-6.15	102.28	111.50
2	N	26[A]	DT	C2'-C3'-O3'	-6.01	102.48	111.50
2	N	26[B]	DT	C2'-C3'-O3'	-6.01	102.48	111.50
2	N	26[C]	DT	C2'-C3'-O3'	-6.01	102.48	111.50
2	N	26[D]	DT	C2'-C3'-O3'	-6.01	102.48	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	22[A]	DT	C2'-C3'-O3'	-5.75	102.87	111.50
2	N	22[B]	DT	C2'-C3'-O3'	-5.75	102.87	111.50
2	N	22[C]	DT	C2'-C3'-O3'	-5.75	102.87	111.50
2	N	22[D]	DT	C2'-C3'-O3'	-5.75	102.87	111.50
1	B	502	TYR	N-CA-C	5.66	119.50	112.59
1	E	502	TYR	N-CA-C	5.57	119.39	112.59
1	F	502	TYR	N-CA-C	5.56	119.37	112.59
1	F	609	VAL	N-CA-C	5.55	116.73	108.46
1	D	502	TYR	N-CA-C	5.52	119.32	112.59
1	B	418	PHE	N-CA-C	5.50	118.42	110.28
1	D	418	PHE	N-CA-C	5.50	118.41	110.28
1	C	502	TYR	N-CA-C	5.49	119.28	112.59
1	F	418	PHE	N-CA-C	5.48	118.39	110.28
1	A	418	PHE	N-CA-C	5.47	118.38	110.28
1	A	502	TYR	N-CA-C	5.46	119.25	112.59
1	B	556	ASN	N-CA-C	-5.39	102.50	110.48
1	D	609	VAL	N-CA-C	5.36	116.44	108.46
1	C	418	PHE	N-CA-C	5.34	118.18	110.28
2	M	2[A]	DT	C2'-C3'-O3'	-5.33	103.51	111.50
2	M	2[B]	DT	C2'-C3'-O3'	-5.33	103.51	111.50
2	M	2[C]	DT	C2'-C3'-O3'	-5.33	103.51	111.50
2	M	2[D]	DT	C2'-C3'-O3'	-5.33	103.51	111.50
1	E	556	ASN	N-CA-C	-5.32	102.60	110.48
1	A	556	ASN	N-CA-C	-5.25	102.71	110.48
1	C	609	VAL	N-CA-C	5.23	116.25	108.46
1	C	556	ASN	N-CA-C	-5.21	102.77	110.48
1	A	609	VAL	N-CA-C	5.21	116.22	108.46
1	B	609	VAL	N-CA-C	5.17	116.17	108.46
1	E	418	PHE	N-CA-C	5.17	117.93	110.28
1	F	556	ASN	N-CA-C	-5.15	102.86	110.48
2	M	6[A]	DT	N1-C1'-C2'	5.14	121.20	113.50
2	M	6[B]	DT	N1-C1'-C2'	5.14	121.20	113.50
2	M	6[C]	DT	N1-C1'-C2'	5.14	121.20	113.50
2	M	6[D]	DT	N1-C1'-C2'	5.14	121.20	113.50
2	N	32[A]	DT	N1-C1'-C2'	5.13	121.19	113.50
2	N	32[B]	DT	N1-C1'-C2'	5.13	121.19	113.50
2	N	32[C]	DT	N1-C1'-C2'	5.13	121.19	113.50
2	N	32[D]	DT	N1-C1'-C2'	5.13	121.19	113.50
1	B	324	THR	CA-C-N	5.12	123.40	119.66
1	B	324	THR	C-N-CA	5.12	123.40	119.66
1	E	609	VAL	N-CA-C	5.11	116.08	108.46
1	B	400	ILE	N-CA-C	5.08	112.19	107.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	324	THR	CA-C-N	5.08	123.36	119.66
1	D	324	THR	C-N-CA	5.08	123.36	119.66
1	D	556	ASN	N-CA-C	-5.07	102.98	110.48
2	M	12[A]	DT	N1-C1'-C2'	5.06	121.09	113.50
2	M	12[B]	DT	N1-C1'-C2'	5.06	121.09	113.50
2	M	12[C]	DT	N1-C1'-C2'	5.06	121.09	113.50
2	M	12[D]	DT	N1-C1'-C2'	5.06	121.09	113.50
1	A	400	ILE	N-CA-C	5.02	112.12	107.56
2	N	26[A]	DT	N1-C1'-C2'	5.01	121.01	113.50
2	N	26[B]	DT	N1-C1'-C2'	5.01	121.01	113.50
2	N	26[C]	DT	N1-C1'-C2'	5.01	121.01	113.50
2	N	26[D]	DT	N1-C1'-C2'	5.01	121.01	113.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	M	18[A]	DT	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3280	0	3240	73	0
1	B	3280	0	3240	72	0
1	C	3280	0	3240	89	0
1	D	3280	0	3240	84	0
1	E	3280	0	3240	76	0
1	F	3280	0	3240	95	0
2	M	1428	0	872	36	0
2	N	1428	0	872	38	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
3	E	4	0	0	0	0
3	F	4	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	27	0	12	0	0
4	B	27	0	12	1	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	1	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
6	A	72	0	0	14	0
6	B	70	0	0	4	0
6	C	63	0	0	11	0
6	D	71	0	0	24	0
6	E	66	0	0	5	0
6	F	63	0	0	13	0
6	M	9	0	0	1	0
6	N	13	0	0	0	0
All	All	23155	0	21256	506	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 12.

All (506) 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)
2:N:37[C]:DT:H2''	2:N:38[C]:DT:H5'	1.44	0.99
1:F:243:SER:HA	6:F:658:HOH:O	1.63	0.97
1:D:243:SER:HA	6:D:180:HOH:O	1.66	0.96
1:B:232:VAL:HG23	2:M:13[A]:DT:H5''	1.60	0.84
1:C:232:VAL:HG23	2:M:13[B]:DT:H5''	1.59	0.83
1:F:232:VAL:HG23	2:N:33[B]:DT:H5''	1.63	0.81
1:C:393:ARG:CZ	2:M:7[A]:DT:H71	2.11	0.80
1:F:232:VAL:HG23	2:N:27[A]:DT:H5''	1.63	0.80
1:E:232:VAL:HG23	2:N:33[A]:DT:H5''	1.62	0.80
1:B:393:ARG:CZ	2:M:13[A]:DT:H71	2.12	0.79
1:E:393:ARG:CZ	2:N:33[A]:DT:H71	2.12	0.79
1:F:393:ARG:CZ	2:N:27[A]:DT:H71	2.12	0.79
1:C:393:ARG:CZ	2:M:13[B]:DT:H71	2.13	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:393:ARG:CZ	2:N:33[B]:DT:H71	2.11	0.79
1:C:232:VAL:HG23	2:M:7[A]:DT:H5''	1.63	0.79
1:F:393:ARG:NE	2:N:27[A]:DT:H72	1.99	0.78
1:C:393:ARG:NE	2:M:7[A]:DT:H72	1.99	0.78
1:C:393:ARG:NE	2:M:7[A]:DT:C7	2.48	0.77
6:D:659:HOH:O	1:E:583:LYS:HE3	1.83	0.77
1:C:586:ILE:HD13	1:C:586:ILE:O	1.86	0.76
1:F:393:ARG:NE	2:N:33[B]:DT:C7	2.49	0.76
1:F:393:ARG:NE	2:N:27[A]:DT:C7	2.49	0.76
1:F:393:ARG:NE	2:N:33[B]:DT:H72	2.01	0.75
1:D:586:ILE:HD13	1:D:586:ILE:O	1.87	0.75
1:E:393:ARG:NE	2:N:33[A]:DT:C7	2.50	0.75
1:E:393:ARG:NE	2:N:33[A]:DT:H72	2.02	0.75
1:C:393:ARG:NE	2:M:13[B]:DT:H72	2.02	0.74
1:E:586:ILE:HD13	1:E:586:ILE:O	1.87	0.74
1:B:393:ARG:NE	2:M:13[A]:DT:H72	2.03	0.73
1:D:485:MET:HG3	1:D:524:VAL:HG23	1.69	0.73
1:F:586:ILE:O	1:F:586:ILE:HD13	1.87	0.73
1:F:189:SER:HB2	6:F:172:HOH:O	1.87	0.73
1:B:393:ARG:NE	2:M:13[A]:DT:C7	2.51	0.73
1:B:485:MET:HG3	1:B:524:VAL:HG23	1.69	0.73
1:A:485:MET:HG3	1:A:524:VAL:HG23	1.69	0.73
1:F:485:MET:HG3	1:F:524:VAL:HG23	1.70	0.73
1:C:393:ARG:NE	2:M:13[B]:DT:C7	2.50	0.73
1:E:485:MET:HG3	1:E:524:VAL:HG23	1.69	0.73
2:N:37[C]:DT:C2'	2:N:38[C]:DT:H5'	2.18	0.73
1:B:586:ILE:HD13	1:B:586:ILE:O	1.87	0.72
1:C:485:MET:HG3	1:C:524:VAL:HG23	1.70	0.72
1:A:586:ILE:HD13	1:A:586:ILE:O	1.88	0.72
1:F:589:LYS:HE3	6:F:628:HOH:O	1.89	0.71
1:C:212:THR:HB	6:C:629:HOH:O	1.90	0.71
1:C:589:LYS:HE3	6:C:650:HOH:O	1.91	0.71
1:D:455:ALA:HB3	6:D:114:HOH:O	1.91	0.70
1:C:334:PRO:HD3	1:D:618:TYR:CD1	2.27	0.69
1:A:589:LYS:HE3	6:A:658:HOH:O	1.91	0.69
1:B:563:TYR:HE2	1:B:615:ILE:HD13	1.58	0.69
1:F:563:TYR:HE2	1:F:615:ILE:HD13	1.58	0.68
1:D:583:LYS:HE3	6:D:652:HOH:O	1.92	0.68
1:E:194:PRO:HG3	1:E:198:GLN:HB3	1.76	0.68
1:C:563:TYR:HE2	1:C:615:ILE:HD13	1.57	0.68
1:E:563:TYR:HE2	1:E:615:ILE:HD13	1.59	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:THR:HG23	1:B:359:ILE:HG23	1.75	0.68
1:A:194:PRO:HG3	1:A:198:GLN:HB3	1.76	0.68
1:D:280:SER:HB2	1:D:283:ALA:HB2	1.76	0.68
1:A:563:TYR:HE2	1:A:615:ILE:HD13	1.59	0.68
1:C:194:PRO:HG3	1:C:198:GLN:HB3	1.76	0.67
1:D:194:PRO:HG3	1:D:198:GLN:HB3	1.76	0.67
1:A:280:SER:HB2	1:A:283:ALA:HB2	1.76	0.67
1:C:358:THR:HG23	1:C:359:ILE:HG23	1.75	0.67
1:A:397:VAL:HG23	6:A:77:HOH:O	1.95	0.67
1:F:194:PRO:HG3	1:F:198:GLN:HB3	1.76	0.67
1:F:358:THR:HG23	1:F:359:ILE:HG23	1.76	0.67
1:D:358:THR:HG23	1:D:359:ILE:HG23	1.76	0.67
1:B:194:PRO:HG3	1:B:198:GLN:HB3	1.75	0.67
1:D:563:TYR:HE2	1:D:615:ILE:HD13	1.59	0.67
1:B:280:SER:HB2	1:B:283:ALA:HB2	1.77	0.67
1:A:358:THR:HG23	1:A:359:ILE:HG23	1.75	0.66
1:C:280:SER:HB2	1:C:283:ALA:HB2	1.77	0.66
1:D:608:GLU:OE2	1:F:258:THR:HG22	1.95	0.66
1:D:246:HIS:HB3	6:D:634:HOH:O	1.95	0.66
1:D:343:SER:HB3	6:D:626:HOH:O	1.96	0.66
1:E:280:SER:HB2	1:E:283:ALA:HB2	1.77	0.66
1:F:280:SER:HB2	1:F:283:ALA:HB2	1.77	0.66
1:A:608:GLU:OE2	1:C:258:THR:HG22	1.95	0.65
1:E:358:THR:HG23	1:E:359:ILE:HG23	1.76	0.65
1:E:371:LYS:HD3	1:E:392:TYR:CD2	2.31	0.65
1:D:397:VAL:HG23	6:D:627:HOH:O	1.96	0.65
1:A:371:LYS:HD3	1:A:392:TYR:CD2	2.32	0.64
1:A:548:SER:HB2	6:A:183:HOH:O	1.98	0.64
1:D:371:LYS:HD3	1:D:392:TYR:CD2	2.32	0.64
1:F:371:LYS:HD3	1:F:392:TYR:CD2	2.33	0.64
6:D:640:HOH:O	1:E:548:SER:HB2	1.98	0.63
1:F:393:ARG:CD	2:N:33[B]:DT:H72	2.28	0.63
1:B:371:LYS:HD3	1:B:392:TYR:CD2	2.34	0.63
1:C:371:LYS:HD3	1:C:392:TYR:CD2	2.34	0.63
1:E:393:ARG:CD	2:N:33[A]:DT:H72	2.29	0.63
1:C:189:SER:HB2	6:C:634:HOH:O	1.98	0.62
1:A:189:SER:HB2	6:A:653:HOH:O	2.00	0.62
1:B:583:LYS:O	1:B:586:ILE:HG22	2.00	0.61
1:B:589:LYS:HE3	6:B:663:HOH:O	1.98	0.61
1:C:393:ARG:CD	2:M:13[B]:DT:H72	2.30	0.61
1:A:211:SER:OG	1:A:290:ASP:OD1	2.17	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:393:ARG:CD	2:N:27[A]:DT:H72	2.31	0.61
1:C:393:ARG:CD	2:M:7[A]:DT:H72	2.30	0.61
1:B:393:ARG:CD	2:M:13[A]:DT:H72	2.31	0.60
1:D:211:SER:OG	1:D:290:ASP:OD1	2.18	0.60
1:A:229:ASN:O	1:A:269:THR:HA	2.01	0.60
1:B:229:ASN:O	1:B:269:THR:HA	2.02	0.60
1:C:583:LYS:O	1:C:586:ILE:HG22	2.02	0.60
6:D:659:HOH:O	1:E:586:ILE:HG21	2.00	0.60
1:D:229:ASN:O	1:D:269:THR:HA	2.02	0.60
1:F:583:LYS:O	1:F:586:ILE:HG22	2.02	0.60
1:F:229:ASN:O	1:F:269:THR:HA	2.01	0.59
1:D:586:ILE:HG21	6:D:652:HOH:O	2.02	0.59
1:E:229:ASN:O	1:E:269:THR:HA	2.02	0.59
1:C:229:ASN:O	1:C:269:THR:HA	2.03	0.58
1:D:583:LYS:O	1:D:586:ILE:HG22	2.03	0.58
1:B:589:LYS:HB3	1:B:590:PRO:HD3	1.86	0.58
1:F:211:SER:OG	1:F:290:ASP:OD1	2.21	0.58
1:C:294:SER:HB2	1:C:299:THR:HG21	1.85	0.58
1:A:583:LYS:O	1:A:586:ILE:HG22	2.03	0.58
1:C:211:SER:OG	1:C:290:ASP:OD1	2.21	0.58
1:E:211:SER:OG	1:E:290:ASP:OD1	2.22	0.58
2:N:37[A]:DT:H2''	2:N:38[A]:DT:O5'	2.03	0.58
1:B:280:SER:HB2	1:B:283:ALA:CB	2.34	0.58
1:C:280:SER:HB2	1:C:283:ALA:CB	2.33	0.58
1:F:589:LYS:HB3	1:F:590:PRO:HD3	1.86	0.58
1:E:280:SER:HB2	1:E:283:ALA:CB	2.34	0.57
1:F:280:SER:HB2	1:F:283:ALA:CB	2.33	0.57
1:B:391:TYR:HA	1:B:395:LEU:HD12	1.86	0.57
1:A:589:LYS:HB3	1:A:590:PRO:HD3	1.85	0.57
1:C:586:ILE:HD13	1:C:586:ILE:C	2.29	0.57
1:D:294:SER:HB2	1:D:299:THR:HG21	1.85	0.57
1:B:294:SER:HB2	1:B:299:THR:HG21	1.85	0.57
1:E:583:LYS:O	1:E:586:ILE:HG22	2.04	0.57
1:E:586:ILE:HD13	1:E:586:ILE:C	2.29	0.57
1:B:586:ILE:HD13	1:B:586:ILE:C	2.29	0.57
1:C:574:PRO:HG2	1:C:607:ASN:ND2	2.20	0.57
1:D:280:SER:HB2	1:D:283:ALA:CB	2.34	0.57
1:D:589:LYS:HB3	1:D:590:PRO:HD3	1.86	0.57
1:A:280:SER:HB2	1:A:283:ALA:CB	2.34	0.57
1:D:586:ILE:HD13	1:D:586:ILE:C	2.29	0.57
1:F:391:TYR:HA	1:F:395:LEU:HD12	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:391:TYR:HA	1:D:395:LEU:HD12	1.86	0.57
1:F:586:ILE:HD13	1:F:586:ILE:C	2.30	0.57
1:E:294:SER:HB2	1:E:299:THR:HG21	1.85	0.57
1:E:574:PRO:HG2	1:E:607:ASN:ND2	2.19	0.57
1:C:589:LYS:HB3	1:C:590:PRO:HD3	1.86	0.56
1:A:586:ILE:HD13	1:A:586:ILE:C	2.30	0.56
1:F:574:PRO:HG2	1:F:607:ASN:ND2	2.20	0.56
1:A:620:MET:HE3	6:A:659:HOH:O	2.04	0.56
1:D:425:VAL:HG23	1:D:465:THR:HB	1.88	0.56
1:A:391:TYR:HA	1:A:395:LEU:HD12	1.87	0.56
1:B:358:THR:CG2	1:B:359:ILE:HG23	2.36	0.56
1:F:294:SER:HB2	1:F:299:THR:HG21	1.87	0.56
1:A:574:PRO:HG2	1:A:607:ASN:ND2	2.20	0.56
1:C:391:TYR:HA	1:C:395:LEU:HD12	1.87	0.56
1:E:391:TYR:HA	1:E:395:LEU:HD12	1.87	0.56
1:F:254:THR:HG22	1:F:269:THR:HG23	1.88	0.56
1:A:254:THR:HG22	1:A:269:THR:HG23	1.88	0.56
1:D:574:PRO:HG2	1:D:607:ASN:ND2	2.21	0.56
1:E:589:LYS:HB3	1:E:590:PRO:HD3	1.86	0.56
2:M:1[C]:DT:H5''	2:M:2[C]:DT:N3	2.21	0.56
1:E:254:THR:HG22	1:E:269:THR:HG23	1.87	0.56
1:E:393:ARG:CZ	2:N:33[A]:DT:C7	2.84	0.56
1:D:411:THR:C	1:D:413:ALA:H	2.14	0.56
1:D:254:THR:HG22	1:D:269:THR:HG23	1.87	0.55
1:F:425:VAL:HG23	1:F:465:THR:HB	1.88	0.55
1:A:294:SER:HB2	1:A:299:THR:HG21	1.87	0.55
1:B:254:THR:HG22	1:B:269:THR:HG23	1.88	0.55
1:B:425:VAL:HG23	1:B:465:THR:HB	1.89	0.55
1:E:393:ARG:NE	2:N:33[A]:DT:H71	2.20	0.55
1:B:211:SER:OG	1:B:290:ASP:OD1	2.24	0.55
1:B:574:PRO:HG2	1:B:607:ASN:ND2	2.22	0.55
1:C:305:THR:OG1	1:C:512:ARG:HD3	2.06	0.55
2:M:17[A]:DT:H2''	2:M:18[A]:DT:O5'	2.05	0.55
1:A:358:THR:CG2	1:A:359:ILE:HG23	2.37	0.55
1:F:358:THR:CG2	1:F:359:ILE:HG23	2.36	0.55
1:C:393:ARG:CZ	2:M:7[A]:DT:C7	2.82	0.55
1:C:358:THR:CG2	1:C:359:ILE:HG23	2.36	0.55
1:D:305:THR:OG1	1:D:512:ARG:HD3	2.06	0.54
1:D:358:THR:CG2	1:D:359:ILE:HG23	2.36	0.54
1:C:254:THR:HG22	1:C:269:THR:HG23	1.88	0.54
1:E:358:THR:CG2	1:E:359:ILE:HG23	2.37	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:393:ARG:NH2	2:M:7[A]:DT:H71	2.22	0.54
2:M:17[D]:DT:H2'	2:M:18[D]:DT:H71	1.90	0.54
2:N:21[D]:DT:H72	2:N:22[D]:DT:O4	2.08	0.54
1:A:425:VAL:HG23	1:A:465:THR:HB	1.88	0.54
1:C:242:MET:SD	6:C:629:HOH:O	2.59	0.54
1:F:305:THR:OG1	1:F:512:ARG:HD3	2.08	0.54
1:A:339:VAL:O	1:A:474:ARG:HA	2.08	0.54
1:D:370:SER:HB2	2:N:37[A]:DT:OP1	2.08	0.54
1:E:355:PRO:O	1:E:358:THR:HG22	2.08	0.54
1:B:393:ARG:CZ	2:M:13[A]:DT:C7	2.84	0.53
1:B:393:ARG:NE	2:M:13[A]:DT:H71	2.21	0.53
1:B:397:VAL:HG23	6:B:635:HOH:O	2.07	0.53
1:A:355:PRO:O	1:A:358:THR:HG22	2.09	0.53
1:A:370:SER:HB2	2:M:17[A]:DT:OP1	2.09	0.53
1:F:393:ARG:NH2	2:N:27[A]:DT:H71	2.22	0.53
1:A:305:THR:OG1	1:A:512:ARG:HD3	2.09	0.53
1:E:425:VAL:HG23	1:E:465:THR:HB	1.89	0.53
1:C:339:VAL:O	1:C:474:ARG:HA	2.09	0.53
1:D:339:VAL:O	1:D:474:ARG:HA	2.09	0.53
1:C:411:THR:C	1:C:413:ALA:H	2.17	0.53
1:F:189:SER:HB3	1:F:190:PRO:HD3	1.91	0.53
1:B:189:SER:HB3	1:B:190:PRO:HD3	1.91	0.53
1:D:248:ILE:C	6:D:180:HOH:O	2.52	0.53
1:F:249:ASP:N	6:F:658:HOH:O	2.42	0.53
1:F:451:VAL:HB	6:F:141:HOH:O	2.08	0.53
1:C:425:VAL:HG23	1:C:465:THR:HB	1.90	0.53
1:D:189:SER:HB3	1:D:190:PRO:HD3	1.91	0.53
1:F:248:ILE:C	6:F:658:HOH:O	2.51	0.53
1:B:305:THR:OG1	1:B:512:ARG:HD3	2.09	0.52
1:B:355:PRO:O	1:B:358:THR:HG22	2.10	0.52
1:A:189:SER:HB3	1:A:190:PRO:HD3	1.91	0.52
1:F:339:VAL:O	1:F:474:ARG:HA	2.09	0.52
1:A:588:LEU:HD12	1:A:588:LEU:N	2.25	0.52
1:E:305:THR:OG1	1:E:512:ARG:HD3	2.09	0.52
1:E:411:THR:C	1:E:413:ALA:H	2.17	0.52
1:C:189:SER:HB3	1:C:190:PRO:HD3	1.91	0.52
1:E:360:LYS:HD3	6:E:166:HOH:O	2.09	0.52
1:A:253:ARG:CZ	6:A:666:HOH:O	2.57	0.52
1:A:411:THR:C	1:A:413:ALA:H	2.16	0.52
1:C:355:PRO:O	1:C:358:THR:HG22	2.09	0.52
1:C:588:LEU:HD12	1:C:588:LEU:N	2.25	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:393:ARG:CZ	2:N:27[A]:DT:C7	2.82	0.51
1:F:411:THR:C	1:F:413:ALA:H	2.17	0.51
1:E:479:GLY:C	1:E:480:GLU:HG3	2.34	0.51
1:A:352:LYS:NZ	6:A:646:HOH:O	2.41	0.51
1:C:479:GLY:C	1:C:480:GLU:HG3	2.35	0.51
1:D:355:PRO:O	1:D:358:THR:HG22	2.10	0.51
1:E:189:SER:HB3	1:E:190:PRO:HD3	1.92	0.51
1:F:479:GLY:C	1:F:480:GLU:HG3	2.35	0.51
1:B:393:ARG:NH2	2:M:13[A]:DT:H71	2.26	0.51
1:A:479:GLY:C	1:A:480:GLU:HG3	2.35	0.51
1:E:588:LEU:N	1:E:588:LEU:HD12	2.26	0.51
1:C:393:ARG:NE	2:M:13[B]:DT:H71	2.20	0.51
1:D:479:GLY:C	1:D:480:GLU:HG3	2.35	0.51
1:D:483:SER:HB3	6:D:114:HOH:O	2.11	0.51
1:F:588:LEU:HD12	1:F:588:LEU:N	2.26	0.51
1:F:355:PRO:O	1:F:358:THR:HG22	2.10	0.51
2:N:21[C]:DT:H72	2:N:22[C]:DT:H72	1.91	0.51
1:B:588:LEU:N	1:B:588:LEU:HD12	2.26	0.50
6:D:662:HOH:O	1:E:586:ILE:HG22	2.11	0.50
1:C:393:ARG:NE	2:M:7[A]:DT:H71	2.18	0.50
1:D:451:VAL:HB	1:D:452:PRO:CD	2.42	0.50
1:D:483:SER:N	6:D:114:HOH:O	2.45	0.50
1:B:339:VAL:O	1:B:474:ARG:HA	2.12	0.50
1:B:411:THR:C	1:B:413:ALA:H	2.17	0.50
1:E:339:VAL:O	1:E:474:ARG:HA	2.11	0.50
1:F:393:ARG:CZ	2:N:33[B]:DT:C7	2.83	0.50
1:D:588:LEU:N	1:D:588:LEU:HD12	2.26	0.50
2:N:37[B]:DT:H2''	2:N:38[B]:DT:O5'	2.10	0.50
1:F:393:ARG:NH2	2:N:33[B]:DT:H71	2.26	0.50
1:E:535:VAL:HG13	1:E:619:ILE:HD12	1.93	0.50
1:F:481:ARG:HD3	6:F:141:HOH:O	2.11	0.50
1:B:535:VAL:HG13	1:B:619:ILE:HD12	1.94	0.49
1:C:481:ARG:HD3	6:C:661:HOH:O	2.12	0.49
1:C:535:VAL:HG13	1:C:619:ILE:HD12	1.94	0.49
1:A:360:LYS:HB3	6:A:656:HOH:O	2.12	0.49
1:B:479:GLY:C	1:B:480:GLU:HG3	2.36	0.49
1:C:393:ARG:NH2	2:M:13[B]:DT:H71	2.27	0.49
1:A:593:HIS:HE1	6:A:652:HOH:O	1.95	0.49
1:C:443:THR:HG21	1:C:619:ILE:HB	1.95	0.49
1:C:372:LYS:HG3	6:C:627:HOH:O	2.12	0.49
2:M:17[A]:DT:H1'	2:M:18[A]:DT:H5'	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:VAL:HG13	1:A:619:ILE:HD12	1.95	0.48
1:E:257:ARG:HD3	6:E:640:HOH:O	2.13	0.48
1:F:434:GLN:HE22	2:N:38[C]:DT:H71	1.78	0.48
1:D:443:THR:HG21	1:D:619:ILE:HB	1.95	0.48
1:F:451:VAL:HB	1:F:452:PRO:CD	2.43	0.48
2:N:37[A]:DT:H1'	2:N:38[A]:DT:H5'	1.95	0.48
1:C:451:VAL:HB	1:C:452:PRO:CD	2.43	0.48
1:A:451:VAL:HB	1:A:452:PRO:CD	2.43	0.48
1:E:393:ARG:NH2	2:N:33[A]:DT:H71	2.27	0.48
1:C:360:LYS:HB3	6:C:648:HOH:O	2.13	0.48
1:F:466:GLY:HA2	1:F:469:ARG:O	2.13	0.48
4:B:2:ADP:H3'	6:B:633:HOH:O	2.12	0.48
1:D:466:GLY:HA2	1:D:469:ARG:O	2.14	0.48
1:E:451:VAL:HB	1:E:452:PRO:CD	2.44	0.47
2:N:21[C]:DT:H5''	2:N:22[C]:DT:N3	2.28	0.47
1:D:535:VAL:HG13	1:D:619:ILE:HD12	1.95	0.47
1:F:535:VAL:HG13	1:F:619:ILE:HD12	1.95	0.47
1:D:256:VAL:HG21	6:D:660:HOH:O	2.12	0.47
1:E:443:THR:HG21	1:E:619:ILE:HB	1.96	0.47
1:B:443:THR:HG21	1:B:619:ILE:HB	1.95	0.47
1:D:483:SER:CB	6:D:114:HOH:O	2.63	0.47
1:E:466:GLY:HA2	1:E:469:ARG:O	2.15	0.47
2:M:2[B]:DT:O2	2:M:2[B]:DT:H2'	2.14	0.47
1:A:466:GLY:HA2	1:A:469:ARG:O	2.14	0.47
1:C:397:VAL:HG12	1:C:397:VAL:O	2.15	0.47
1:D:216:ALA:HB1	6:D:634:HOH:O	2.14	0.47
1:F:397:VAL:HG23	6:F:636:HOH:O	2.14	0.47
1:B:451:VAL:HB	1:B:452:PRO:CD	2.44	0.47
1:C:406:VAL:HG22	1:C:407:ILE:N	2.28	0.47
1:D:249:ASP:N	6:D:180:HOH:O	2.48	0.47
1:F:576:PRO:HD2	1:F:582:TRP:CE2	2.50	0.47
1:F:613:HIS:CE1	1:F:615:ILE:HD12	2.50	0.47
1:A:325:PRO:HG2	1:A:328:SER:HB3	1.96	0.47
1:D:360:LYS:HB3	6:D:656:HOH:O	2.13	0.47
1:F:397:VAL:O	1:F:397:VAL:HG12	2.15	0.47
1:F:443:THR:HG21	1:F:619:ILE:HB	1.95	0.47
1:A:443:THR:HG21	1:A:619:ILE:HB	1.96	0.47
1:B:230:PRO:HD3	1:B:270:TYR:HE2	1.79	0.47
1:F:556:ASN:HD21	2:N:37[C]:DT:H73	1.79	0.47
1:C:372:LYS:HB2	6:M:415:HOH:O	2.15	0.47
1:C:593:HIS:HE1	6:C:656:HOH:O	1.98	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:248:ILE:O	1:F:250:PRO:HD3	2.15	0.47
1:A:230:PRO:HD3	1:A:270:TYR:HE2	1.80	0.46
1:A:451:VAL:HB	6:A:630:HOH:O	2.14	0.46
1:D:248:ILE:O	1:D:250:PRO:HD3	2.15	0.46
1:B:397:VAL:HG12	1:B:397:VAL:O	2.15	0.46
1:C:466:GLY:HA2	1:C:469:ARG:O	2.15	0.46
1:F:240:ALA:O	1:F:243:SER:HB3	2.15	0.46
1:D:216:ALA:CB	6:D:634:HOH:O	2.62	0.46
1:D:576:PRO:HD2	1:D:582:TRP:CE2	2.50	0.46
1:E:230:PRO:HD3	1:E:270:TYR:HE2	1.79	0.46
1:E:576:PRO:HD2	1:E:582:TRP:CE2	2.50	0.46
1:D:406:VAL:HG22	1:D:407:ILE:N	2.31	0.46
1:E:397:VAL:HG12	1:E:397:VAL:O	2.16	0.46
1:F:406:VAL:HG22	1:F:407:ILE:N	2.30	0.46
1:B:466:GLY:HA2	1:B:469:ARG:O	2.16	0.46
1:D:240:ALA:O	1:D:243:SER:HB3	2.16	0.46
1:E:406:VAL:HG22	1:E:407:ILE:N	2.31	0.46
1:B:406:VAL:HG22	1:B:407:ILE:N	2.30	0.46
1:E:325:PRO:HG2	1:E:328:SER:HB3	1.97	0.46
1:F:325:PRO:HG2	1:F:328:SER:HB3	1.97	0.46
1:F:563:TYR:CE2	1:F:615:ILE:HD13	2.47	0.46
1:A:248:ILE:O	1:A:250:PRO:HD3	2.16	0.46
1:A:406:VAL:HG22	1:A:407:ILE:N	2.30	0.46
1:B:576:PRO:HD2	1:B:582:TRP:CE2	2.51	0.46
1:C:576:PRO:HD2	1:C:582:TRP:CE2	2.50	0.46
1:A:382:SER:C	1:A:384:LEU:H	2.24	0.46
1:A:396:ASP:O	1:A:399:VAL:HG13	2.16	0.46
1:F:352:LYS:NZ	6:F:650:HOH:O	2.48	0.46
1:F:434:GLN:HG3	2:N:37[C]:DT:O4	2.16	0.46
1:A:575:PRO:HG2	1:A:577:SER:O	2.16	0.46
1:D:575:PRO:HG2	1:D:577:SER:O	2.16	0.46
1:A:481:ARG:HD3	6:A:630:HOH:O	2.16	0.45
1:B:382:SER:C	1:B:384:LEU:H	2.24	0.45
1:B:613:HIS:CE1	1:B:615:ILE:HD12	2.51	0.45
1:D:421:ASP:HB2	6:D:657:HOH:O	2.15	0.45
4:F:2:ADP:H3'	6:F:642:HOH:O	2.16	0.45
2:M:2[B]:DT:O2	2:M:2[B]:DT:C2'	2.64	0.45
1:B:248:ILE:O	1:B:250:PRO:HD3	2.16	0.45
1:C:382:SER:C	1:C:384:LEU:H	2.24	0.45
1:F:382:SER:C	1:F:384:LEU:H	2.24	0.45
1:A:576:PRO:HD2	1:A:582:TRP:CE2	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:PRO:HD3	1:C:270:TYR:HE2	1.80	0.45
1:C:248:ILE:O	1:C:250:PRO:HD3	2.16	0.45
1:C:240:ALA:O	1:C:243:SER:HB3	2.16	0.45
1:E:360:LYS:HB3	6:E:166:HOH:O	2.16	0.45
1:A:613:HIS:ND1	1:A:614:PRO:HD2	2.32	0.45
1:B:414:LEU:HD22	1:B:418:PHE:CD2	2.52	0.45
1:C:325:PRO:HG2	1:C:328:SER:HB3	1.98	0.45
1:D:613:HIS:CE1	1:D:615:ILE:HD12	2.52	0.45
1:D:613:HIS:ND1	1:D:614:PRO:HD2	2.32	0.45
1:E:190:PRO:HA	1:E:191:PRO:HD3	1.90	0.45
1:E:240:ALA:O	1:E:243:SER:HB3	2.16	0.45
1:E:382:SER:C	1:E:384:LEU:H	2.25	0.45
1:F:230:PRO:HD3	1:F:270:TYR:HE2	1.82	0.45
1:A:258:THR:HG23	6:A:666:HOH:O	2.16	0.45
1:B:575:PRO:HG2	1:B:577:SER:O	2.17	0.45
1:D:382:SER:C	1:D:384:LEU:H	2.24	0.45
1:E:414:LEU:HD22	1:E:418:PHE:CD2	2.52	0.45
1:B:240:ALA:O	1:B:243:SER:HB3	2.17	0.44
1:C:613:HIS:CE1	1:C:615:ILE:HD12	2.53	0.44
1:C:615:ILE:O	1:C:619:ILE:HG12	2.16	0.44
1:D:545:HIS:CG	6:D:169:HOH:O	2.70	0.44
1:D:230:PRO:HD3	1:D:270:TYR:HE2	1.80	0.44
1:D:397:VAL:HG12	1:D:397:VAL:O	2.16	0.44
1:D:411:THR:C	1:D:413:ALA:N	2.75	0.44
1:A:240:ALA:O	1:A:243:SER:HB3	2.18	0.44
1:E:575:PRO:HG2	1:E:577:SER:O	2.18	0.44
1:E:613:HIS:CE1	1:E:615:ILE:HD12	2.51	0.44
1:F:249:ASP:CA	6:F:658:HOH:O	2.64	0.44
1:B:514:ARG:HA	1:B:514:ARG:HD2	1.85	0.44
1:E:396:ASP:O	1:E:399:VAL:HG13	2.17	0.44
1:E:514:ARG:HD2	1:E:514:ARG:HA	1.85	0.44
1:B:325:PRO:HG2	1:B:328:SER:HB3	1.98	0.44
1:B:519:THR:HA	1:B:520:PRO:HD3	1.86	0.44
1:C:393:ARG:CZ	2:M:13[B]:DT:C7	2.85	0.44
1:C:575:PRO:HG2	1:C:577:SER:O	2.18	0.44
1:A:563:TYR:CE2	1:A:615:ILE:HD13	2.47	0.44
1:F:396:ASP:O	1:F:399:VAL:HG13	2.17	0.44
1:A:397:VAL:O	1:A:397:VAL:HG12	2.17	0.44
1:A:411:THR:C	1:A:413:ALA:N	2.76	0.44
1:C:451:VAL:HB	6:C:661:HOH:O	2.17	0.44
1:D:346:GLU:HG3	1:D:356:ILE:HD12	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:613:HIS:ND1	1:E:614:PRO:HD2	2.33	0.44
1:F:547:LEU:O	1:F:551:LYS:HG3	2.17	0.44
2:M:17[D]:DT:H2'	2:M:18[D]:DT:C7	2.47	0.44
1:D:325:PRO:HG2	1:D:328:SER:HB3	1.98	0.44
1:A:547:LEU:O	1:A:551:LYS:HG3	2.18	0.43
1:B:542:ILE:HG22	6:B:651:HOH:O	2.17	0.43
1:D:190:PRO:HA	1:D:191:PRO:HD3	1.89	0.43
1:D:563:TYR:CE2	1:D:615:ILE:HD13	2.47	0.43
1:E:248:ILE:O	1:E:250:PRO:HD3	2.18	0.43
1:C:563:TYR:CE2	1:C:615:ILE:HD13	2.45	0.43
1:F:575:PRO:HG2	1:F:577:SER:O	2.18	0.43
1:F:615:ILE:O	1:F:619:ILE:HG12	2.18	0.43
1:B:296:ASP:HB3	2:M:18[B]:DT:O2	2.18	0.43
1:B:613:HIS:ND1	1:B:614:PRO:HD2	2.34	0.43
1:B:615:ILE:O	1:B:619:ILE:HG12	2.18	0.43
1:C:514:ARG:HA	1:C:514:ARG:HD2	1.85	0.43
1:D:396:ASP:O	1:D:399:VAL:HG13	2.17	0.43
1:E:543:ASP:OD2	1:E:543:ASP:C	2.62	0.43
1:F:613:HIS:HE1	1:F:615:ILE:HD12	1.82	0.43
1:D:346:GLU:HG3	1:D:356:ILE:CD1	2.49	0.43
1:A:414:LEU:HD22	1:A:418:PHE:CD2	2.54	0.43
1:A:613:HIS:CE1	1:A:615:ILE:HD12	2.54	0.43
1:C:212:THR:C	6:C:629:HOH:O	2.62	0.43
1:C:547:LEU:O	1:C:551:LYS:HG3	2.19	0.43
1:F:249:ASP:HA	6:F:658:HOH:O	2.19	0.43
1:F:411:THR:C	1:F:413:ALA:N	2.77	0.43
1:C:414:LEU:HD22	1:C:418:PHE:CD2	2.54	0.43
1:F:519:THR:HA	1:F:520:PRO:HD3	1.86	0.43
1:B:396:ASP:O	1:B:399:VAL:HG13	2.19	0.43
1:C:396:ASP:O	1:C:399:VAL:HG13	2.18	0.43
1:D:615:ILE:O	1:D:619:ILE:HG12	2.18	0.43
1:E:196:THR:N	6:E:93:HOH:O	2.51	0.42
1:F:543:ASP:C	1:F:543:ASP:OD2	2.61	0.42
1:A:346:GLU:HG3	1:A:356:ILE:HD12	2.00	0.42
1:D:514:ARG:HD2	1:D:514:ARG:HA	1.84	0.42
1:B:251:ASN:HA	1:B:259:ILE:O	2.19	0.42
1:B:547:LEU:O	1:B:551:LYS:HG3	2.19	0.42
1:C:542:ILE:HD11	1:C:562:ALA:HB3	2.01	0.42
1:A:251:ASN:HA	1:A:259:ILE:O	2.20	0.42
1:B:563:TYR:CE2	1:B:615:ILE:HD13	2.47	0.42
1:C:251:ASN:HA	1:C:259:ILE:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:360:LYS:HD3	6:D:656:HOH:O	2.19	0.42
1:D:414:LEU:HD22	1:D:418:PHE:CD2	2.54	0.42
1:E:547:LEU:O	1:E:551:LYS:HG3	2.20	0.42
1:A:346:GLU:HG3	1:A:356:ILE:CD1	2.49	0.42
1:A:360:LYS:HD3	6:A:656:HOH:O	2.19	0.42
1:A:477:THR:HG22	1:A:478:PRO:O	2.20	0.42
1:E:563:TYR:CE2	1:E:615:ILE:HD13	2.47	0.42
1:F:300:ILE:HD12	1:F:516:TYR:CZ	2.54	0.42
1:F:346:GLU:HG3	1:F:356:ILE:HD12	2.01	0.42
1:F:438:PHE:CD1	1:F:623:MET:HE3	2.54	0.42
1:D:519:THR:HA	1:D:520:PRO:HD3	1.86	0.42
1:E:251:ASN:HA	1:E:259:ILE:O	2.20	0.42
1:F:251:ASN:HA	1:F:259:ILE:O	2.20	0.42
1:F:393:ARG:HD2	2:N:38[C]:DT:H3'	2.02	0.42
1:F:545:HIS:CG	6:F:648:HOH:O	2.72	0.42
1:D:251:ASN:HA	1:D:259:ILE:O	2.20	0.42
1:E:411:THR:C	1:E:413:ALA:N	2.77	0.42
1:F:414:LEU:HD22	1:F:418:PHE:CD2	2.55	0.42
1:A:615:ILE:O	1:A:619:ILE:HG12	2.19	0.41
1:C:300:ILE:HD12	1:C:516:TYR:CZ	2.54	0.41
1:D:300:ILE:HD12	1:D:516:TYR:CZ	2.55	0.41
1:D:329:VAL:HB	6:D:182:HOH:O	2.19	0.41
2:M:1[C]:DT:H3'	2:M:2[C]:DT:C2	2.55	0.41
1:C:613:HIS:HE1	1:C:615:ILE:HD12	1.85	0.41
1:D:547:LEU:O	1:D:551:LYS:HG3	2.20	0.41
1:F:346:GLU:HG3	1:F:356:ILE:CD1	2.50	0.41
1:F:556:ASN:ND2	2:N:37[C]:DT:H73	2.36	0.41
1:A:347:ILE:HD13	1:A:381:LEU:CD2	2.51	0.41
1:C:397:VAL:HG23	6:C:626:HOH:O	2.19	0.41
1:E:340:ALA:HB2	1:E:475:PHE:CZ	2.55	0.41
2:M:1[C]:DT:H72	2:M:2[C]:DT:H72	2.03	0.41
2:M:17[D]:DT:C2'	2:M:18[D]:DT:H71	2.49	0.41
1:C:543:ASP:OD2	1:C:543:ASP:C	2.62	0.41
1:A:300:ILE:HD12	1:A:516:TYR:CZ	2.56	0.41
1:B:300:ILE:HD12	1:B:516:TYR:CZ	2.55	0.41
1:B:346:GLU:HG3	1:B:356:ILE:HD12	2.03	0.41
1:A:543:ASP:OD2	1:A:543:ASP:C	2.63	0.41
1:E:346:GLU:HG3	1:E:356:ILE:CD1	2.50	0.41
1:E:541:HIS:HD2	6:E:642:HOH:O	2.03	0.41
1:F:371:LYS:HD3	1:F:392:TYR:CE2	2.55	0.41
1:F:477:THR:HG22	1:F:478:PRO:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:HIS:O	1:A:248:ILE:HG22	2.21	0.41
1:C:346:GLU:HG3	1:C:356:ILE:HD12	2.01	0.41
1:C:541:HIS:O	1:C:570:ARG:NH2	2.53	0.41
1:E:346:GLU:HG3	1:E:356:ILE:HD12	2.01	0.41
1:E:371:LYS:HD3	1:E:392:TYR:CE2	2.55	0.41
1:E:477:THR:HG22	1:E:478:PRO:O	2.21	0.41
1:A:438:PHE:CD1	1:A:623:MET:HE3	2.55	0.41
1:E:542:ILE:HD11	1:E:562:ALA:HB3	2.02	0.41
1:B:542:ILE:HD11	1:B:562:ALA:HB3	2.02	0.41
1:B:543:ASP:OD2	1:B:543:ASP:C	2.62	0.41
1:B:613:HIS:HE1	1:B:615:ILE:HD12	1.86	0.41
1:C:477:THR:HG22	1:C:478:PRO:O	2.20	0.41
1:D:347:ILE:HD13	1:D:381:LEU:CD2	2.50	0.41
1:E:300:ILE:HD12	1:E:516:TYR:CZ	2.56	0.41
1:E:438:PHE:CD1	1:E:623:MET:HE3	2.56	0.41
1:F:246:HIS:O	1:F:248:ILE:HG22	2.21	0.41
1:B:291:GLU:C	1:B:293:HIS:H	2.29	0.41
6:A:164:HOH:O	1:B:548:SER:HB2	2.21	0.40
1:D:246:HIS:O	1:D:248:ILE:HG22	2.20	0.40
1:D:543:ASP:OD2	1:D:543:ASP:C	2.63	0.40
1:F:393:ARG:HB2	2:N:27[A]:DT:OP2	2.21	0.40
1:F:432:VAL:HG21	2:N:37[C]:DT:H5"	2.02	0.40
1:A:507:ALA:HA	1:A:533:GLU:OE2	2.21	0.40
1:D:541:HIS:O	1:D:570:ARG:NH2	2.54	0.40
1:C:519:THR:HA	1:C:520:PRO:HD3	1.86	0.40
1:D:477:THR:HG22	1:D:478:PRO:O	2.20	0.40
1:F:291:GLU:C	1:F:293:HIS:H	2.30	0.40
1:F:518:ASN:HD22	1:F:518:ASN:HA	1.71	0.40
1:A:371:LYS:HD3	1:A:392:TYR:CE2	2.56	0.40
1:B:346:GLU:HG3	1:B:356:ILE:CD1	2.52	0.40
1:C:596:THR:HA	1:C:597:PRO:HD3	1.92	0.40
1:E:507:ALA:HA	1:E:533:GLU:OE2	2.21	0.40
1:F:507:ALA:HA	1:F:533:GLU:OE2	2.21	0.40
1:B:190:PRO:HA	1:B:191:PRO:HD3	1.89	0.40
1:B:246:HIS:O	1:B:248:ILE:HG22	2.22	0.40
1:B:596:THR:HA	1:B:597:PRO:HD3	1.93	0.40
1:C:340:ALA:HB2	1:C:475:PHE:CZ	2.56	0.40
1:C:346:GLU:HG3	1:C:356:ILE:CD1	2.51	0.40
1:C:411:THR:C	1:C:413:ALA:N	2.77	0.40
1:D:362:GLY:H	1:D:405:ASP:CG	2.30	0.40
1:D:613:HIS:HE1	1:D:615:ILE:HD12	1.87	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:613:HIS:ND1	1:F:614:PRO:HD2	2.36	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	435/437 (100%)	407 (94%)	26 (6%)	2 (0%)	24	37
1	B	435/437 (100%)	407 (94%)	26 (6%)	2 (0%)	24	37
1	C	435/437 (100%)	408 (94%)	25 (6%)	2 (0%)	24	37
1	D	435/437 (100%)	408 (94%)	25 (6%)	2 (0%)	24	37
1	E	435/437 (100%)	408 (94%)	25 (6%)	2 (0%)	24	37
1	F	435/437 (100%)	408 (94%)	25 (6%)	2 (0%)	24	37
All	All	2610/2622 (100%)	2446 (94%)	152 (6%)	12 (0%)	24	37

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	292	CYS
1	E	292	CYS
1	A	292	CYS
1	B	326	PRO
1	C	292	CYS
1	D	292	CYS
1	D	326	PRO
1	E	326	PRO
1	F	292	CYS
1	A	326	PRO
1	C	326	PRO
1	F	326	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	356/356 (100%)	344 (97%)	12 (3%)	32	54
1	B	356/356 (100%)	343 (96%)	13 (4%)	30	51
1	C	356/356 (100%)	342 (96%)	14 (4%)	28	48
1	D	356/356 (100%)	343 (96%)	13 (4%)	30	51
1	E	356/356 (100%)	343 (96%)	13 (4%)	30	51
1	F	356/356 (100%)	344 (97%)	12 (3%)	32	54
All	All	2136/2136 (100%)	2059 (96%)	77 (4%)	31	52

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	195	GLN
1	A	301	LEU
1	A	344	THR
1	A	346	GLU
1	A	358	THR
1	A	377	LEU
1	A	384	LEU
1	A	480	GLU
1	A	526	GLN
1	A	547	LEU
1	A	586	ILE
1	A	600	TYR
1	B	195	GLN
1	B	301	LEU
1	B	326	PRO
1	B	344	THR
1	B	346	GLU
1	B	358	THR
1	B	377	LEU
1	B	384	LEU
1	B	480	GLU
1	B	526	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	547	LEU
1	B	586	ILE
1	B	600	TYR
1	C	195	GLN
1	C	301	LEU
1	C	326	PRO
1	C	344	THR
1	C	346	GLU
1	C	358	THR
1	C	377	LEU
1	C	384	LEU
1	C	470	MET
1	C	480	GLU
1	C	526	GLN
1	C	547	LEU
1	C	586	ILE
1	C	600	TYR
1	D	195	GLN
1	D	301	LEU
1	D	326	PRO
1	D	344	THR
1	D	346	GLU
1	D	358	THR
1	D	377	LEU
1	D	384	LEU
1	D	480	GLU
1	D	526	GLN
1	D	547	LEU
1	D	586	ILE
1	D	600	TYR
1	E	195	GLN
1	E	301	LEU
1	E	344	THR
1	E	346	GLU
1	E	358	THR
1	E	377	LEU
1	E	384	LEU
1	E	470	MET
1	E	480	GLU
1	E	526	GLN
1	E	547	LEU
1	E	586	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	600	TYR
1	F	195	GLN
1	F	301	LEU
1	F	344	THR
1	F	346	GLU
1	F	358	THR
1	F	377	LEU
1	F	384	LEU
1	F	480	GLU
1	F	526	GLN
1	F	547	LEU
1	F	586	ILE
1	F	600	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	HIS
1	A	335	ASN
1	A	434	GLN
1	A	518	ASN
1	A	526	GLN
1	A	549	GLN
1	A	552	GLN
1	B	201	HIS
1	B	221	GLN
1	B	335	ASN
1	B	434	GLN
1	B	518	ASN
1	B	526	GLN
1	B	545	HIS
1	B	549	GLN
1	C	201	HIS
1	C	221	GLN
1	C	335	ASN
1	C	434	GLN
1	C	518	ASN
1	C	545	HIS
1	C	549	GLN
1	D	201	HIS
1	D	221	GLN
1	D	335	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	434	GLN
1	D	518	ASN
1	D	541	HIS
1	D	552	GLN
1	E	201	HIS
1	E	335	ASN
1	E	434	GLN
1	E	518	ASN
1	E	526	GLN
1	E	545	HIS
1	E	549	GLN
1	F	201	HIS
1	F	335	ASN
1	F	434	GLN
1	F	518	ASN
1	F	545	HIS
1	F	549	GLN
1	F	556	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	BEF	F	1	5,4	0,3,3	-	-	-		
4	ADP	B	2	5,3	28,29,29	1.37	3 (10%)	43,45,45	2.00	9 (20%)
3	BEF	A	1	5,4	0,3,3	-	-	-		
4	ADP	E	2	5,3	28,29,29	1.36	2 (7%)	43,45,45	2.00	9 (20%)
4	ADP	F	2	5,3	28,29,29	1.42	3 (10%)	43,45,45	2.00	9 (20%)
3	BEF	C	1	5,4	0,3,3	-	-	-		
3	BEF	E	1	5,4	0,3,3	-	-	-		
3	BEF	B	1	5,4	0,3,3	-	-	-		
4	ADP	A	2	5,3	28,29,29	1.34	2 (7%)	43,45,45	2.02	10 (23%)
4	ADP	D	2	5,3	28,29,29	1.35	2 (7%)	43,45,45	2.02	10 (23%)
4	ADP	C	2	5,3	28,29,29	1.42	2 (7%)	43,45,45	1.98	9 (20%)
3	BEF	D	1	5,4	0,3,3	-	-	-		

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	B	2	5,3	-	2/16/32/32	0/3/3/3
4	ADP	F	2	5,3	-	2/16/32/32	0/3/3/3
4	ADP	E	2	5,3	-	2/16/32/32	0/3/3/3
4	ADP	A	2	5,3	-	2/16/32/32	0/3/3/3
4	ADP	D	2	5,3	-	2/16/32/32	0/3/3/3
4	ADP	C	2	5,3	-	2/16/32/32	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	2	ADP	C5-N7	-4.54	1.30	1.39
4	C	2	ADP	C5-N7	-4.44	1.31	1.39
4	E	2	ADP	C5-N7	-4.29	1.31	1.39
4	B	2	ADP	C5-N7	-4.16	1.31	1.39
4	A	2	ADP	C5-N7	-3.92	1.31	1.39
4	D	2	ADP	C5-N7	-3.91	1.31	1.39
4	C	2	ADP	C4-N9	-2.39	1.32	1.37
4	E	2	ADP	C4-N9	-2.33	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2	ADP	C4-N9	-2.30	1.32	1.37
4	F	2	ADP	C4-N9	-2.28	1.32	1.37
4	D	2	ADP	C4-N9	-2.27	1.33	1.37
4	A	2	ADP	C4-N9	-2.22	1.33	1.37
4	B	2	ADP	C5-C4	2.07	1.42	1.39
4	F	2	ADP	C5-C4	2.02	1.42	1.39

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2	ADP	N3-C2-N1	-6.59	118.61	128.58
4	A	2	ADP	N3-C2-N1	-6.57	118.64	128.58
4	F	2	ADP	N3-C2-N1	-6.53	118.69	128.58
4	C	2	ADP	N3-C2-N1	-6.52	118.72	128.58
4	B	2	ADP	N3-C2-N1	-6.51	118.73	128.58
4	E	2	ADP	N3-C2-N1	-6.44	118.83	128.58
4	E	2	ADP	C5-C4-N3	-5.48	119.17	126.72
4	B	2	ADP	C5-C4-N3	-5.46	119.19	126.72
4	F	2	ADP	C5-C4-N3	-5.38	119.31	126.72
4	D	2	ADP	C5-C4-N3	-5.36	119.33	126.72
4	A	2	ADP	C5-C4-N3	-5.33	119.37	126.72
4	C	2	ADP	C5-C4-N3	-5.33	119.38	126.72
4	E	2	ADP	C2-N3-C4	4.56	122.97	111.83
4	D	2	ADP	C2-N3-C4	4.50	122.83	111.83
4	A	2	ADP	C2-N3-C4	4.48	122.78	111.83
4	B	2	ADP	C2-N3-C4	4.47	122.76	111.83
4	F	2	ADP	C2-N3-C4	4.45	122.69	111.83
4	C	2	ADP	C2-N3-C4	4.44	122.68	111.83
4	A	2	ADP	N3-C4-N9	3.94	133.86	127.17
4	D	2	ADP	N3-C4-N9	3.91	133.82	127.17
4	E	2	ADP	N3-C4-N9	3.90	133.80	127.17
4	B	2	ADP	N3-C4-N9	3.87	133.76	127.17
4	F	2	ADP	N3-C4-N9	3.83	133.68	127.17
4	C	2	ADP	N3-C4-N9	3.81	133.65	127.17
4	A	2	ADP	C5-N7-C8	3.35	108.72	103.45
4	F	2	ADP	C5-N7-C8	3.27	108.59	103.45
4	D	2	ADP	C5-N7-C8	3.25	108.55	103.45
4	E	2	ADP	C5-N7-C8	3.21	108.50	103.45
4	C	2	ADP	C5-N7-C8	3.21	108.49	103.45
4	A	2	ADP	N9-C8-N7	-3.17	109.44	113.94
4	A	2	ADP	C4-C5-N7	-3.15	106.98	110.58
4	D	2	ADP	N9-C8-N7	-3.14	109.48	113.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2	ADP	C5-N7-C8	3.10	108.32	103.45
4	F	2	ADP	C4-C5-N7	-3.08	107.06	110.58
4	C	2	ADP	N9-C8-N7	-3.07	109.58	113.94
4	E	2	ADP	C4-C5-N7	-3.06	107.08	110.58
4	E	2	ADP	N9-C8-N7	-3.03	109.64	113.94
4	F	2	ADP	N9-C8-N7	-3.02	109.65	113.94
4	D	2	ADP	C4-C5-N7	-3.01	107.14	110.58
4	C	2	ADP	C4-C5-N7	-2.99	107.16	110.58
4	B	2	ADP	N9-C8-N7	-2.98	109.71	113.94
4	B	2	ADP	C4-C5-N7	-2.93	107.23	110.58
4	F	2	ADP	O4'-C1'-N9	2.51	112.91	108.09
4	E	2	ADP	O4'-C1'-N9	2.49	112.88	108.09
4	A	2	ADP	O4'-C1'-N9	2.41	112.72	108.09
4	C	2	ADP	O4'-C1'-N9	2.40	112.71	108.09
4	D	2	ADP	O4'-C1'-N9	2.39	112.68	108.09
4	B	2	ADP	O4'-C1'-N9	2.38	112.66	108.09
4	F	2	ADP	O3B-PB-O3A	2.28	112.27	104.64
4	D	2	ADP	O3B-PB-O3A	2.27	112.26	104.64
4	A	2	ADP	O3B-PB-O3A	2.24	112.16	104.64
4	C	2	ADP	O3B-PB-O3A	2.24	112.15	104.64
4	A	2	ADP	C4-N9-C8	2.23	108.08	105.74
4	B	2	ADP	O3B-PB-O3A	2.16	111.88	104.64
4	E	2	ADP	O3B-PB-O3A	2.14	111.81	104.64
4	D	2	ADP	C4-N9-C8	2.13	107.97	105.74

There are no chirality outliers.

All (12) torsion outliers are listed below:

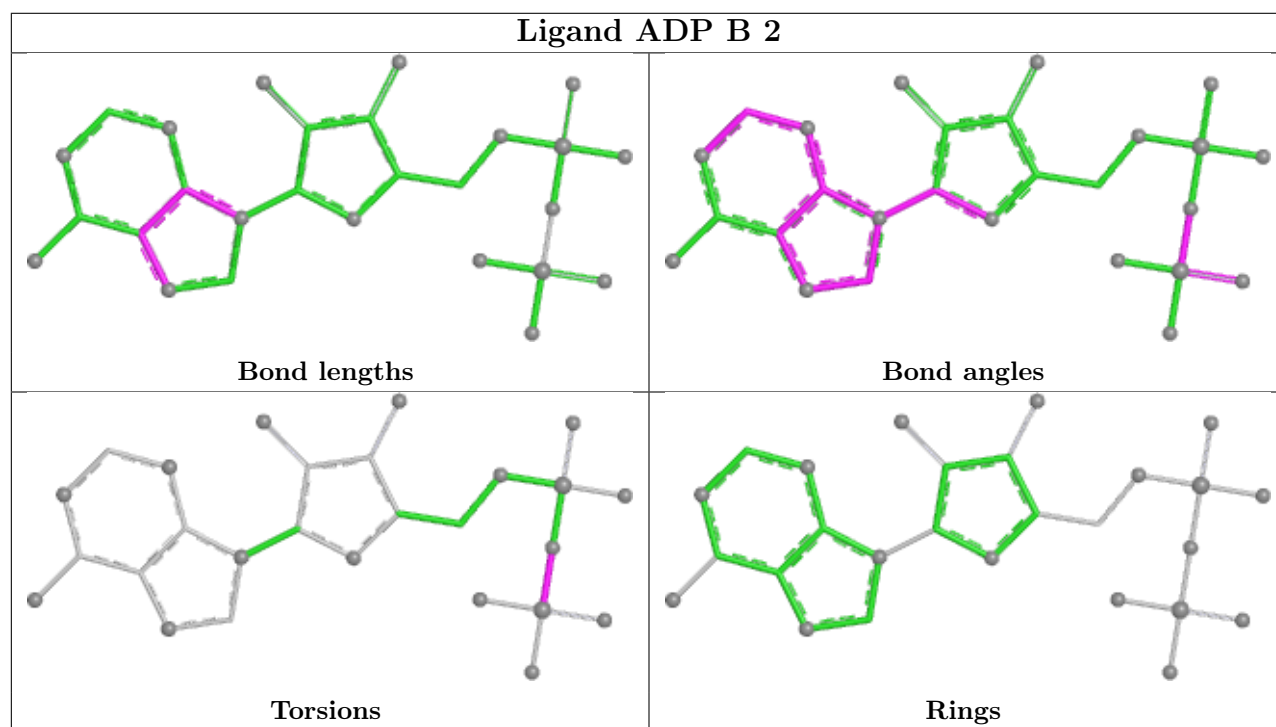
Mol	Chain	Res	Type	Atoms
4	A	2	ADP	PA-O3A-PB-O3B
4	B	2	ADP	PA-O3A-PB-O3B
4	C	2	ADP	PA-O3A-PB-O3B
4	D	2	ADP	PA-O3A-PB-O3B
4	E	2	ADP	PA-O3A-PB-O3B
4	F	2	ADP	PA-O3A-PB-O3B
4	A	2	ADP	PA-O3A-PB-O2B
4	B	2	ADP	PA-O3A-PB-O2B
4	C	2	ADP	PA-O3A-PB-O2B
4	D	2	ADP	PA-O3A-PB-O2B
4	E	2	ADP	PA-O3A-PB-O2B
4	F	2	ADP	PA-O3A-PB-O2B

There are no ring outliers.

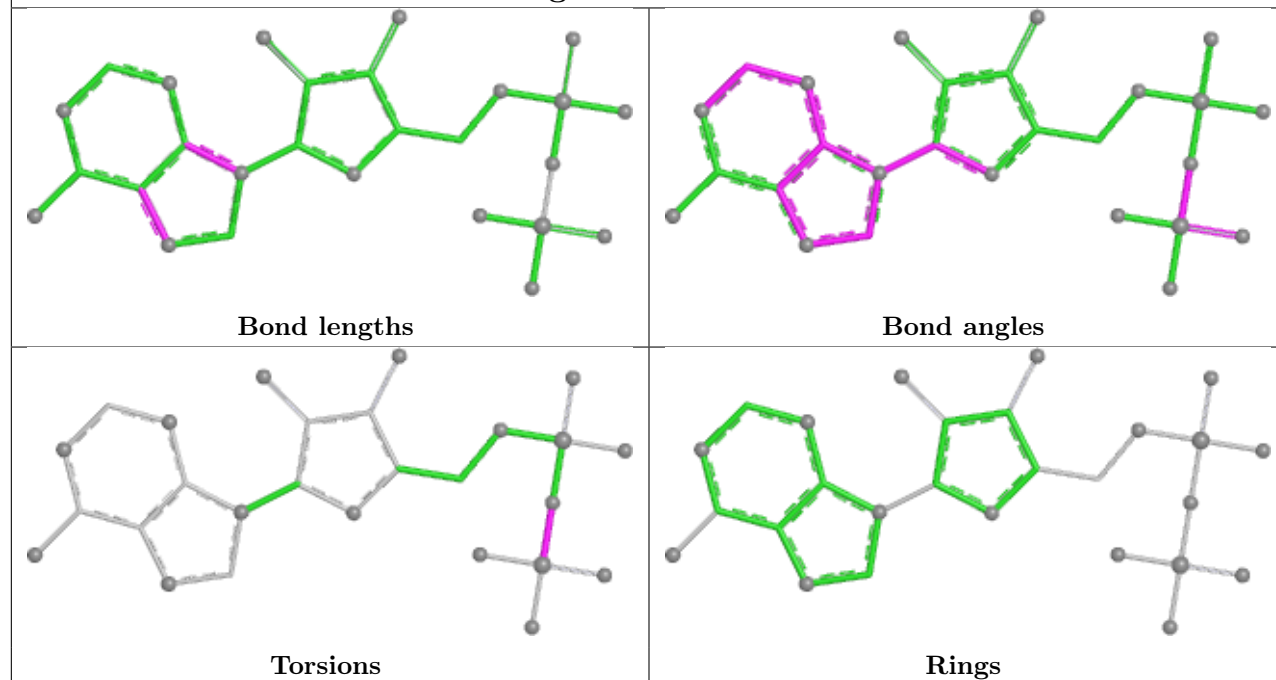
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2	ADP	1	0
4	F	2	ADP	1	0

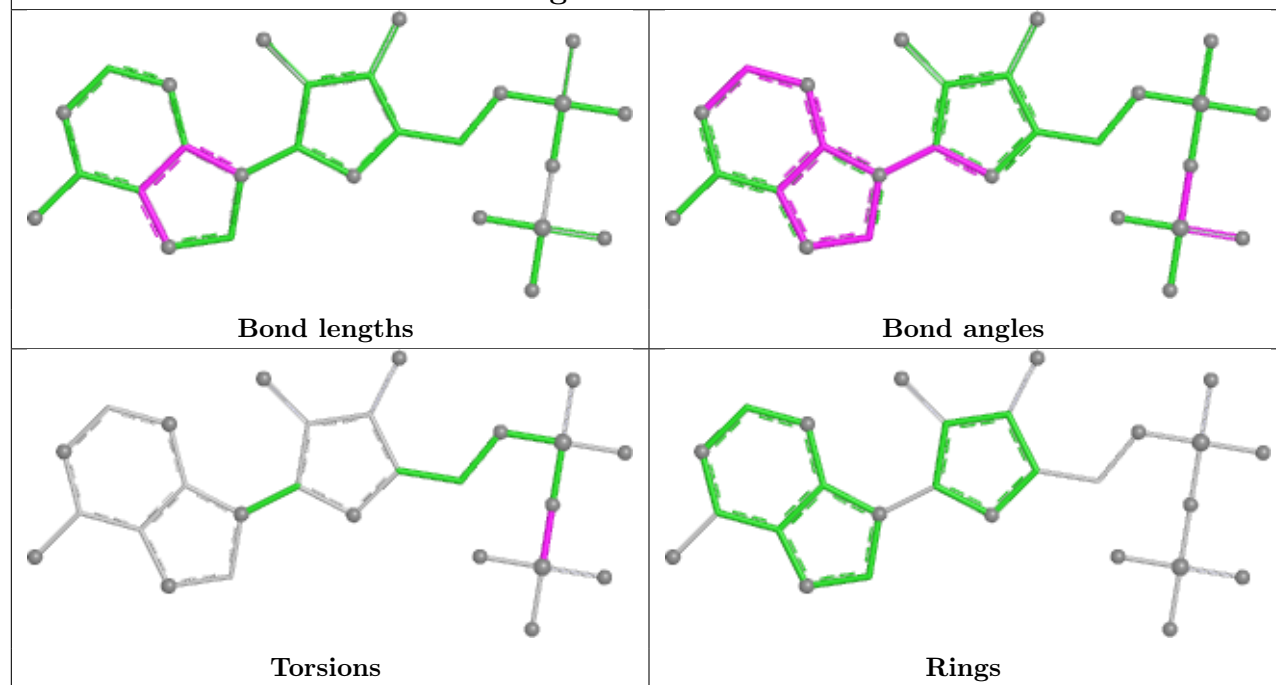
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



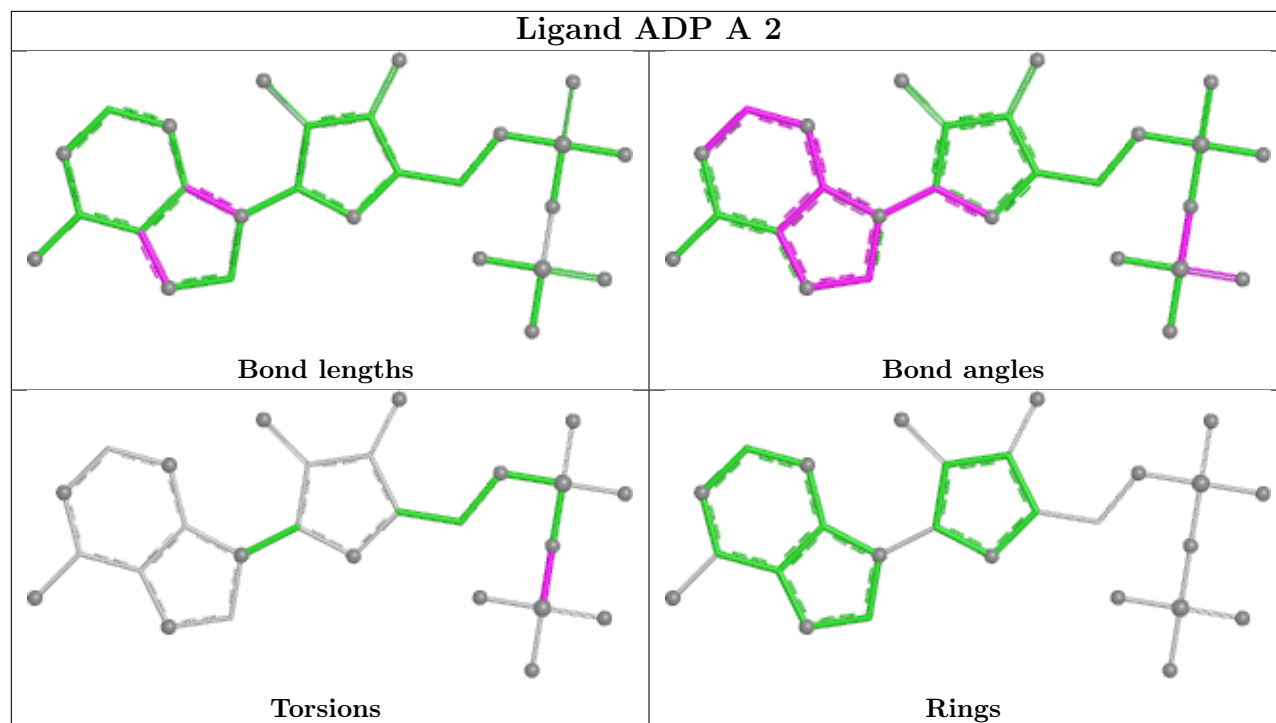
Ligand ADP E 2



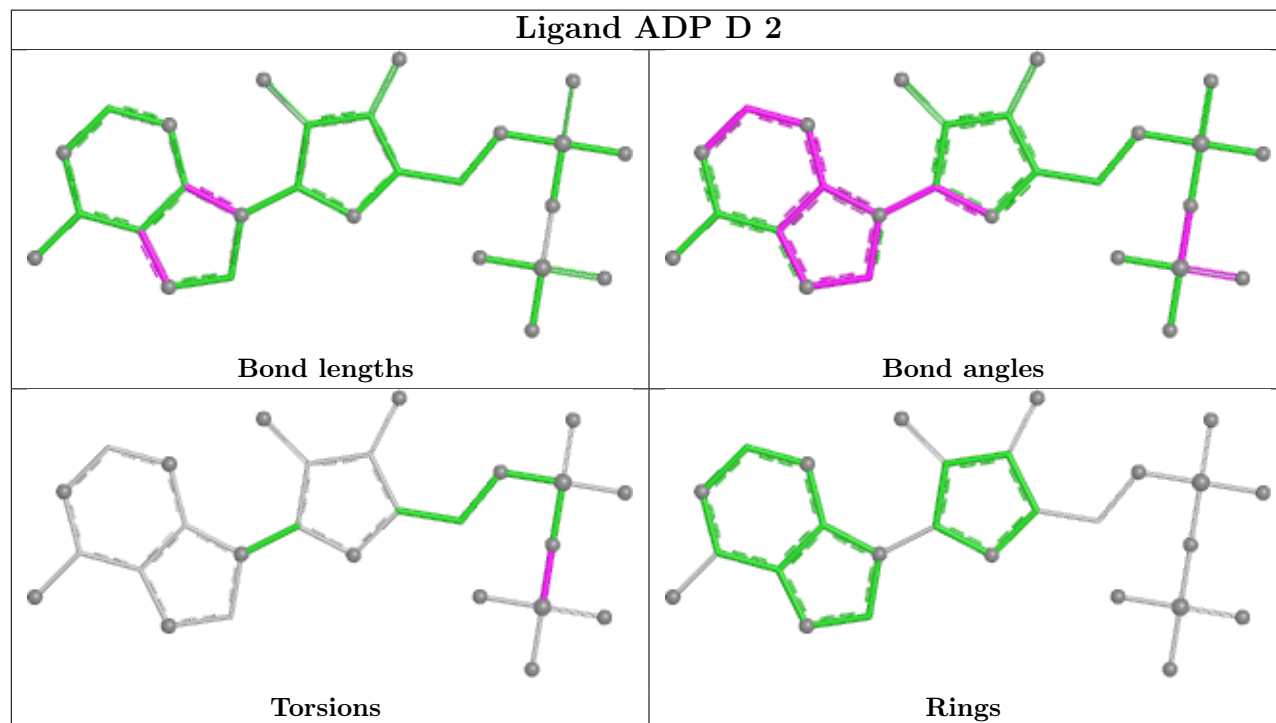
Ligand ADP F 2

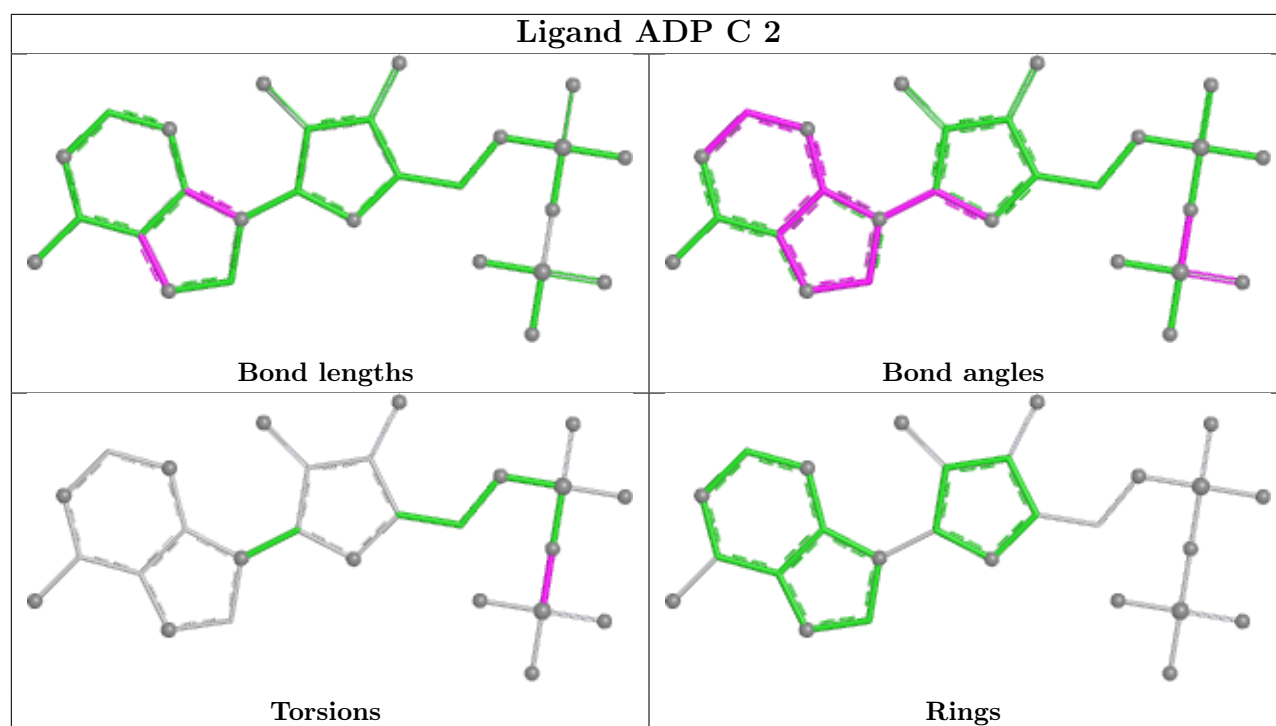


Ligand ADP A 2



Ligand ADP D 2





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	437/437 (100%)	-1.50	0 100 100	20, 38, 56, 67	0
1	B	437/437 (100%)	-1.49	0 100 100	19, 38, 56, 67	0
1	C	437/437 (100%)	-1.50	0 100 100	18, 38, 57, 67	0
1	D	437/437 (100%)	-1.49	0 100 100	20, 38, 56, 67	0
1	E	437/437 (100%)	-1.49	0 100 100	19, 38, 57, 68	0
1	F	437/437 (100%)	-1.50	0 100 100	18, 38, 57, 67	0
2	M	18/19 (94%)	-1.51	0 100 100	5, 12, 14, 14	18 (100%)
2	N	18/19 (94%)	-1.50	0 100 100	5, 12, 14, 14	18 (100%)
All	All	2658/2660 (99%)	-1.50	0 100 100	5, 38, 57, 68	36 (1%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

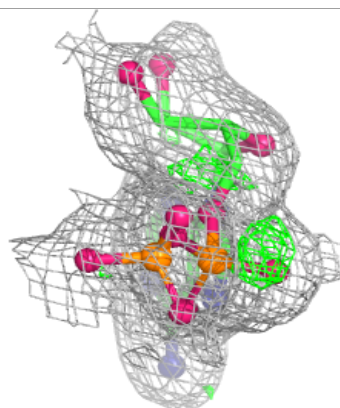
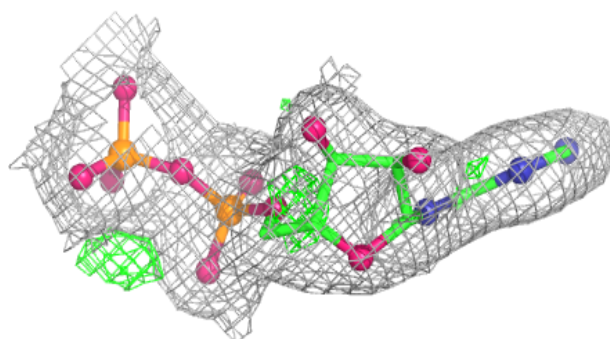
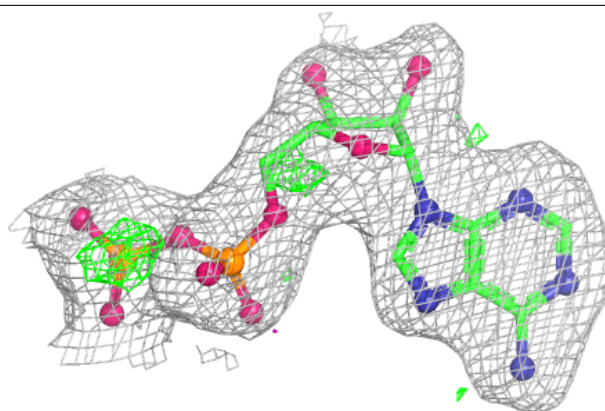
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BEF	C	1	4/4	0.99	0.03	25,26,27,31	0
3	BEF	B	1	4/4	1.00	0.02	22,24,25,28	0
3	BEF	A	1	4/4	1.00	0.01	23,25,27,28	0
3	BEF	D	1	4/4	1.00	0.02	23,24,26,28	0
3	BEF	E	1	4/4	1.00	0.02	23,23,25,27	0
3	BEF	F	1	4/4	1.00	0.03	27,27,30,33	0
4	ADP	A	2	27/27	1.00	0.03	23,33,37,40	0
4	ADP	B	2	27/27	1.00	0.03	23,34,37,40	0
4	ADP	C	2	27/27	1.00	0.03	22,33,37,39	0
4	ADP	D	2	27/27	1.00	0.02	23,33,37,39	0
4	ADP	E	2	27/27	1.00	0.02	23,33,37,40	0
4	ADP	F	2	27/27	1.00	0.03	21,33,37,40	0
5	MN	A	3	1/1	1.00	0.01	25,25,25,25	0
5	MN	B	3	1/1	1.00	0.01	23,23,23,23	0
5	MN	C	3	1/1	1.00	0.01	25,25,25,25	0
5	MN	D	3	1/1	1.00	0.01	24,24,24,24	0
5	MN	E	3	1/1	1.00	0.01	23,23,23,23	0
5	MN	F	3	1/1	1.00	0.01	26,26,26,26	0

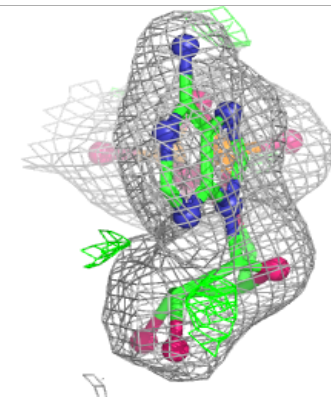
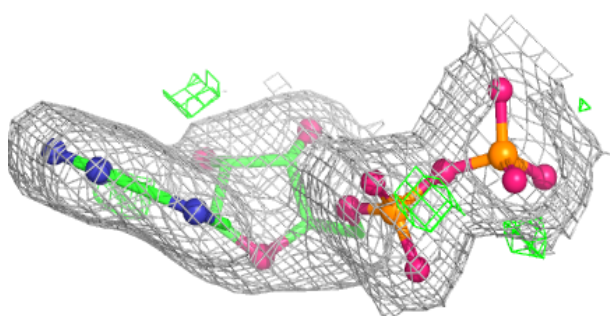
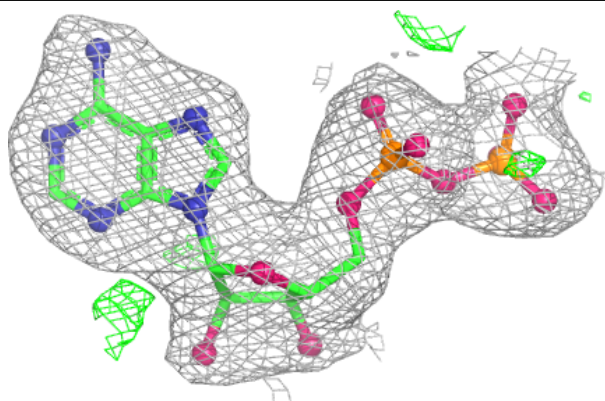
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP A 2:

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

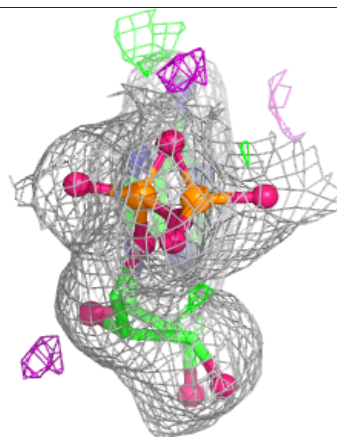
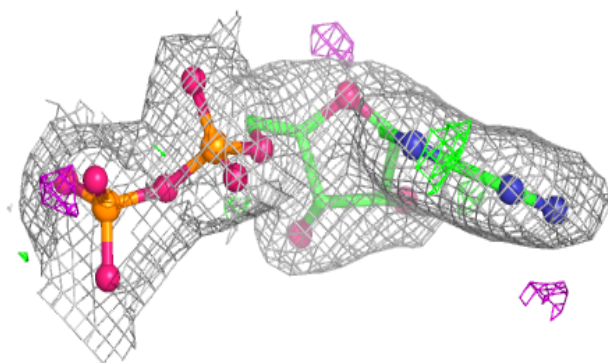
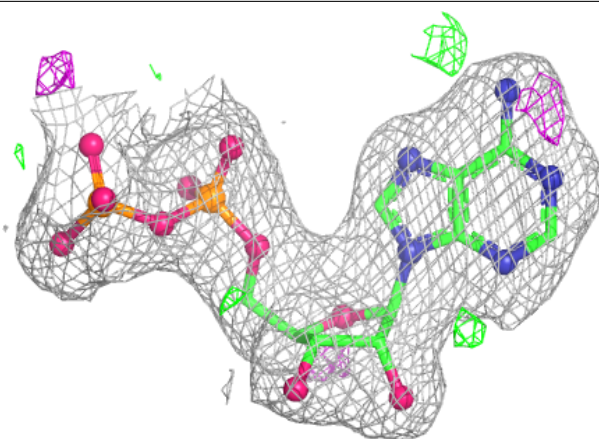
**Electron density around ADP B 2:**

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



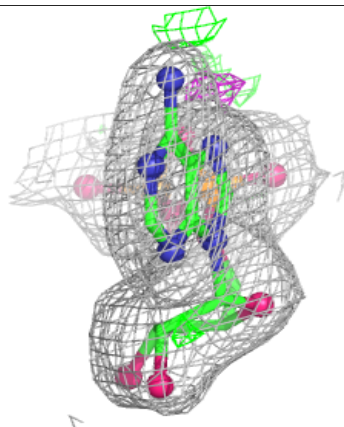
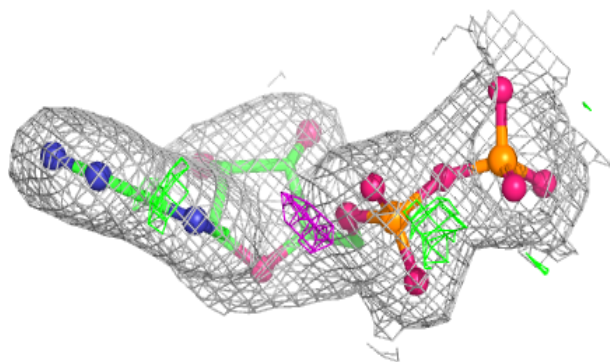
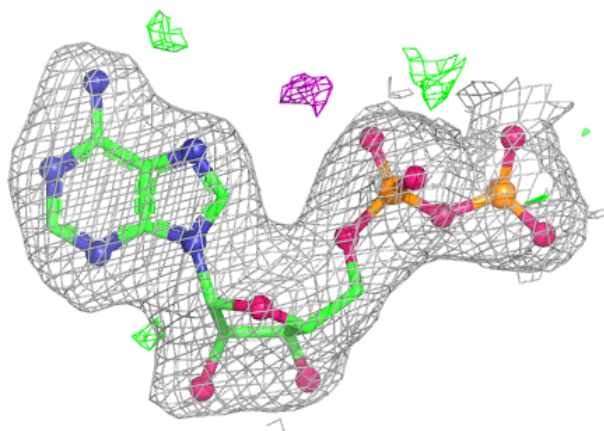
Electron density around ADP C 2:

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

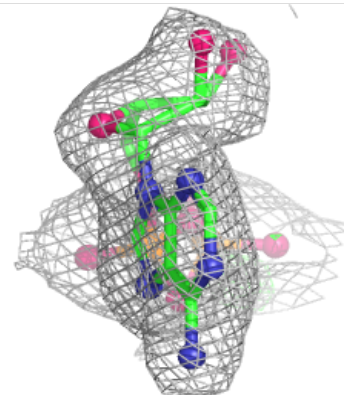
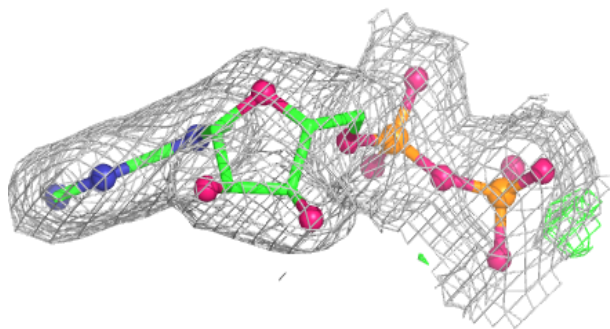
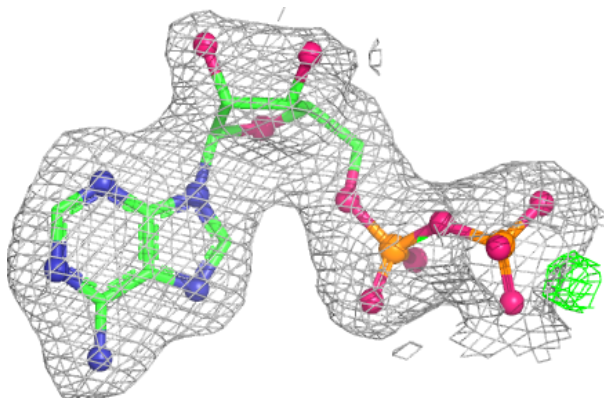


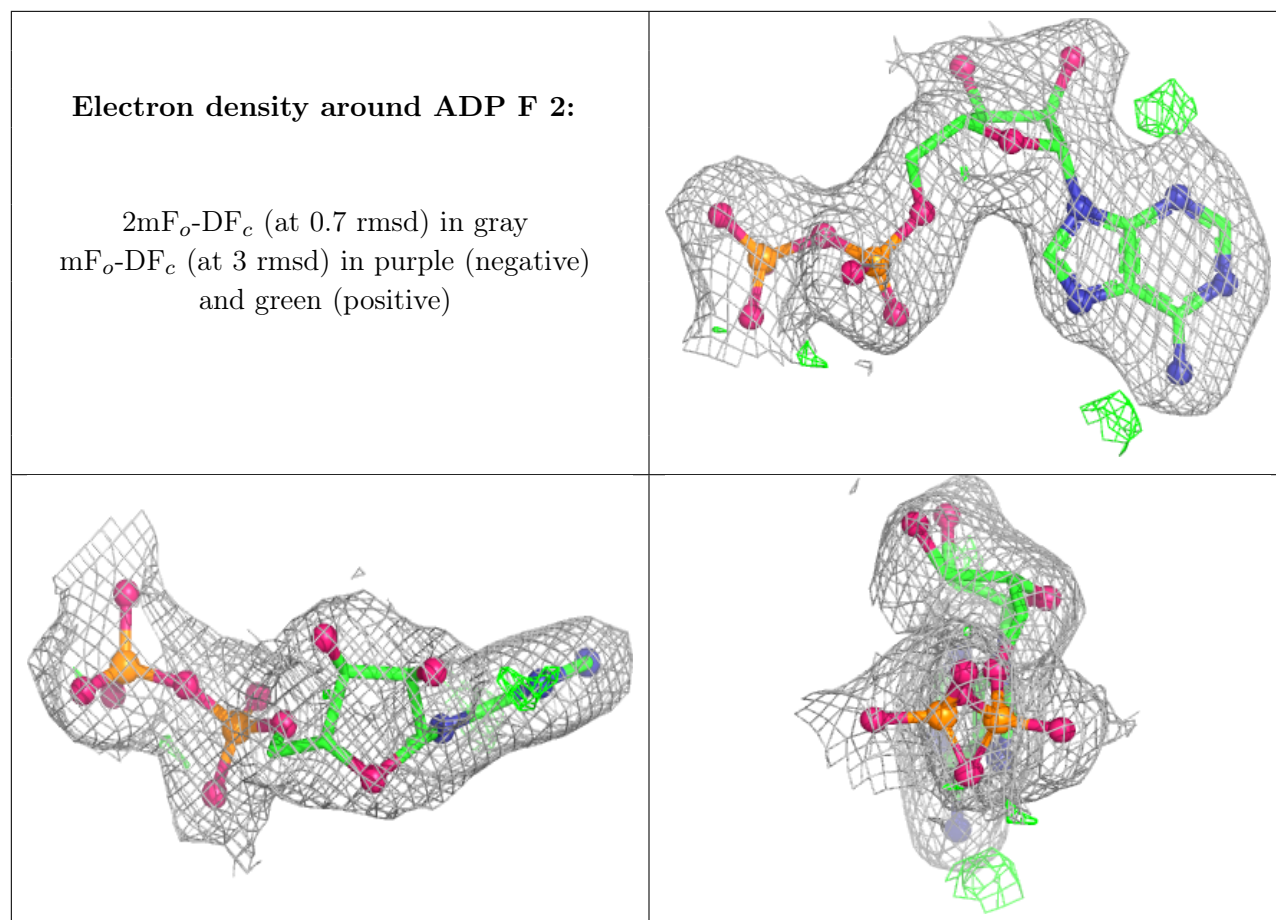
Electron density around ADP D 2:

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

**Electron density around ADP E 2:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.