



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 21, 2024 – 08:48 am BST

PDB ID : 1QMZ
Title : PHOSPHORYLATED CDK2-CYCLIN A-SUBSTRATE PEPTIDE COMPLEX
Authors : Brown, N.R.; Noble, M.E.M.; Endicott, J.A.; Johnson, L.N.
Deposited on : 1999-10-11
Resolution : 2.20 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

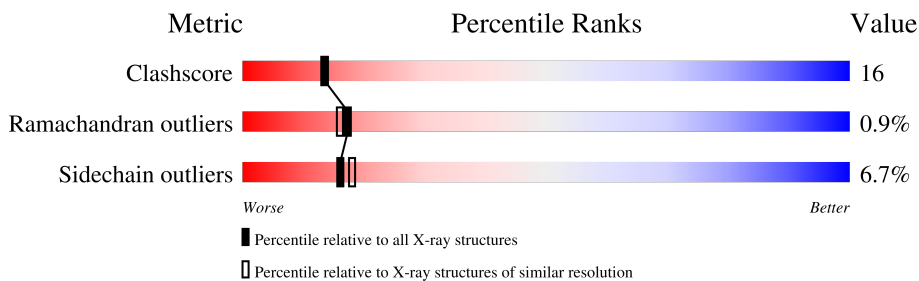
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	299	
1	C	299	
2	B	259	
2	D	259	
3	E	7	
3	F	7	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9889 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 CELL DIVISION PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	P				S
1	A	297	2388	1550	404	425	1	8	0	0	0
1	C	297	2388	1550	404	425	1	8	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	cloning artifact	UNP P24941
C	0	SER	-	cloning artifact	UNP P24941

- Molecule 2 is a protein called G2/MITOTIC-SPECIFIC CYCLIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	258	2083	1350	339	383	11	0	0	0
2	D	258	2083	1350	339	383	11	0	0	0

- Molecule 3 is a protein called SUBSTRATE PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	E	7	58	35	15	8	0	0	0
3	F	7	58	35	15	8	0	0	0

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	206	Total	O	0	0
			206	206		
6	B	166	Total	O	0	0
			166	166		
6	C	197	Total	O	0	0
			197	197		
6	D	185	Total	O	0	0
			185	185		
6	E	5	Total	O	0	0
			5	5		

Continued on next page...

Continued from previous page...

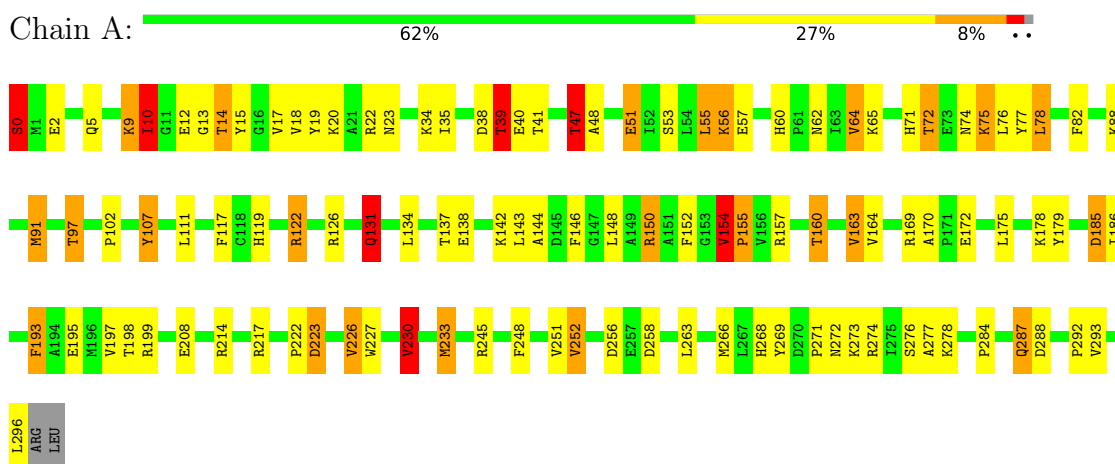
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	8	Total	O	0	0
			8	8		

3 Residue-property plots [i](#)

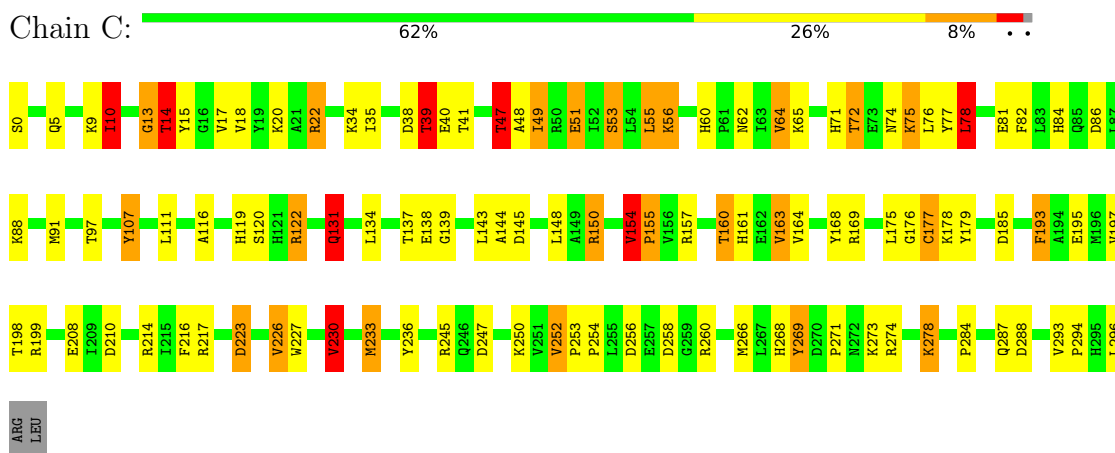
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

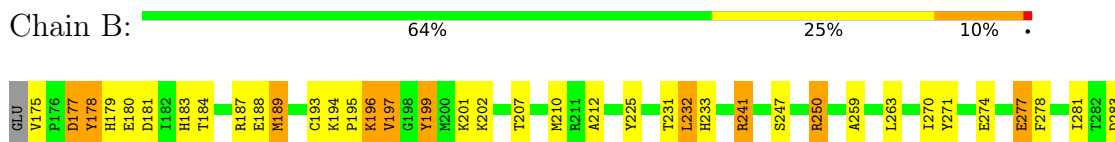
- Molecule 1: CELL DIVISION PROTEIN KINASE 2

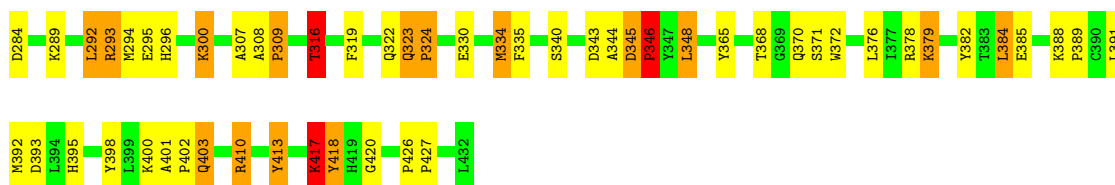


- Molecule 1: CELL DIVISION PROTEIN KINASE 2



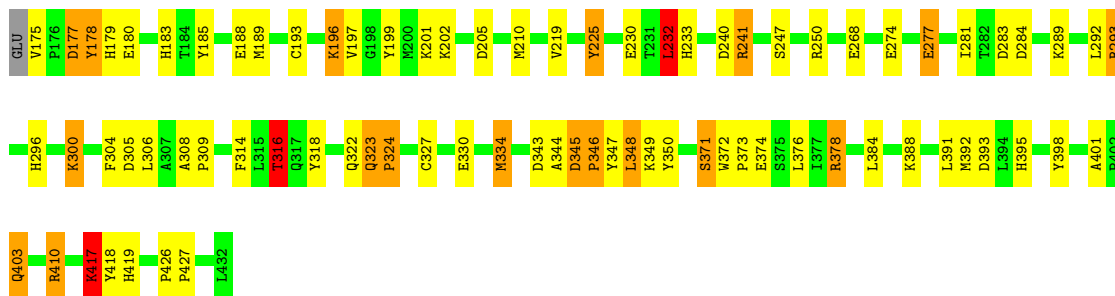
- Molecule 2: G2/MITOTIC-SPECIFIC CYCLIN A





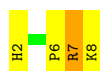
- Molecule 2: G2/MITOTIC-SPECIFIC CYCLIN A

Chain D: 69% 23% 7%



- Molecule 3: SUBSTRATE PEPTIDE

Chain E: 43% 43% 14%



- Molecule 3: SUBSTRATE PEPTIDE

Chain F: 57% 43%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	152.60Å 163.70Å 73.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20	Depositor
% Data completeness (in resolution range)	98.9 (20.00-2.20)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	0.10	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.220 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	9889	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.92	0/2438	1.98	60/3308 (1.8%)
1	C	0.95	1/2438 (0.0%)	2.03	69/3308 (2.1%)
2	B	0.95	1/2133 (0.0%)	1.89	61/2897 (2.1%)
2	D	0.96	1/2133 (0.0%)	1.96	57/2897 (2.0%)
3	E	0.95	0/60	3.08	5/79 (6.3%)
3	F	0.99	0/60	3.37	6/79 (7.6%)
All	All	0.94	3/9262 (0.0%)	1.99	258/12568 (2.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	C	0	3
2	B	0	5
2	D	0	5
All	All	0	17

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	340	SER	CB-OG	6.21	1.50	1.42
1	C	177	CYS	CB-SG	5.04	1.90	1.82
2	D	374	GLU	CD-OE1	5.01	1.31	1.25

All (258) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	245	ARG	NE-CZ-NH2	-28.38	106.11	120.30
1	C	245	ARG	NE-CZ-NH2	-23.75	108.43	120.30
2	D	241	ARG	NE-CZ-NH2	-19.92	110.34	120.30
1	C	22	ARG	NE-CZ-NH2	-18.85	110.88	120.30
3	E	7	ARG	CD-NE-CZ	18.43	149.40	123.60
3	F	7	ARG	CD-NE-CZ	16.05	146.07	123.60
2	D	241	ARG	NE-CZ-NH1	15.18	127.89	120.30
2	D	283	ASP	CB-CG-OD1	14.37	131.23	118.30
2	B	378	ARG	NE-CZ-NH1	-13.18	113.71	120.30
1	A	22	ARG	NE-CZ-NH2	-12.59	114.00	120.30
2	D	378	ARG	NE-CZ-NH2	12.58	126.59	120.30
2	D	293	ARG	NE-CZ-NH2	-12.46	114.07	120.30
1	A	47	THR	OG1-CB-CG2	-12.45	81.37	110.00
1	C	168	TYR	CB-CG-CD2	-12.10	113.74	121.00
2	B	393	ASP	CB-CG-OD2	11.92	129.03	118.30
1	C	51	GLU	OE1-CD-OE2	-11.65	109.32	123.30
1	A	245	ARG	NE-CZ-NH1	11.58	126.09	120.30
1	A	214	ARG	NE-CZ-NH2	-11.55	114.52	120.30
2	D	378	ARG	NE-CZ-NH1	-11.13	114.73	120.30
1	A	208	GLU	OE1-CD-OE2	-11.09	109.99	123.30
1	C	214	ARG	NE-CZ-NH2	-10.95	114.83	120.30
1	C	131	GLN	CG-CD-OE1	10.79	143.17	121.60
2	D	284	ASP	CB-CG-OD2	10.55	127.79	118.30
2	D	334	MET	CG-SD-CE	-10.42	83.53	100.20
1	A	185	ASP	CB-CG-OD1	10.35	127.61	118.30
2	B	283	ASP	CB-CG-OD1	10.30	127.57	118.30
3	F	7	ARG	NE-CZ-NH2	10.24	125.42	120.30
2	B	334	MET	CG-SD-CE	-10.21	83.86	100.20
2	B	324	PRO	CA-N-CD	-10.21	97.21	111.50
1	C	157	ARG	NE-CZ-NH1	-10.20	115.20	120.30
1	A	51	GLU	OE1-CD-OE2	-10.20	111.07	123.30
3	F	7	ARG	NE-CZ-NH1	10.19	125.39	120.30
2	D	324	PRO	CA-N-CD	-10.15	97.28	111.50
1	C	22	ARG	NE-CZ-NH1	10.09	125.34	120.30
2	D	205	ASP	CB-CG-OD2	10.00	127.30	118.30
2	D	277	GLU	OE1-CD-OE2	9.95	135.24	123.30
2	B	277	GLU	OE1-CD-OE2	9.94	135.22	123.30
2	D	345	ASP	CA-C-O	-9.91	99.29	120.10
2	D	240	ASP	CB-CG-OD2	9.84	127.16	118.30
1	C	77	TYR	CB-CG-CD1	9.80	126.88	121.00
1	A	131	GLN	CG-CD-OE1	9.57	140.73	121.60
1	A	230	VAL	CB-CA-C	-9.50	93.34	111.40
1	C	245	ARG	NE-CZ-NH1	9.43	125.01	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	217	ARG	NE-CZ-NH2	9.36	124.98	120.30
1	C	230	VAL	CB-CA-C	-9.33	93.67	111.40
1	C	214	ARG	NE-CZ-NH1	9.32	124.96	120.30
3	F	7	ARG	NH1-CZ-NH2	-9.29	109.18	119.40
2	D	316	THR	N-CA-CB	-9.29	92.66	110.30
2	D	230	GLU	OE1-CD-OE2	-9.19	112.28	123.30
2	B	323	GLN	CA-C-O	-9.08	101.04	120.10
2	B	293	ARG	NE-CZ-NH2	-9.01	115.79	120.30
1	C	77	TYR	CB-CG-CD2	-9.01	115.59	121.00
2	B	284	ASP	CB-CG-OD2	8.98	126.38	118.30
1	A	150	ARG	NE-CZ-NH1	8.89	124.75	120.30
2	B	379	LYS	CA-C-N	8.87	136.72	117.20
1	A	22	ARG	NE-CZ-NH1	8.83	124.72	120.30
2	D	374	GLU	OE1-CD-OE2	8.77	133.82	123.30
1	A	223	ASP	CB-CG-OD1	8.71	126.14	118.30
2	B	241	ARG	NE-CZ-NH1	8.53	124.57	120.30
1	C	150	ARG	NE-CZ-NH1	8.46	124.53	120.30
2	D	323	GLN	CA-C-O	-8.46	102.34	120.10
2	B	177	ASP	CB-CG-OD1	8.46	125.91	118.30
1	C	252	VAL	CG1-CB-CG2	-8.19	97.80	110.90
2	B	178	TYR	CA-CB-CG	-8.16	97.89	113.40
2	B	345	ASP	CA-C-O	-8.12	103.05	120.10
2	D	316	THR	CA-CB-CG2	8.10	123.74	112.40
1	A	131	GLN	OE1-CD-NE2	-7.99	103.53	121.90
1	A	214	ARG	NE-CZ-NH1	7.95	124.28	120.30
2	B	178	TYR	CG-CD2-CE2	-7.94	114.95	121.30
2	B	316	THR	N-CA-CB	-7.90	95.29	110.30
2	D	305	ASP	CB-CG-OD2	7.89	125.40	118.30
1	C	168	TYR	CG-CD1-CE1	-7.84	115.03	121.30
2	D	205	ASP	CB-CG-OD1	-7.83	111.25	118.30
1	C	223	ASP	CB-CG-OD1	7.75	125.27	118.30
1	C	269	TYR	CB-CG-CD1	-7.73	116.36	121.00
2	D	393	ASP	CB-CG-OD2	7.70	125.23	118.30
2	D	410	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	A	64	VAL	CA-CB-CG2	-7.67	99.40	110.90
2	B	410	ARG	NE-CZ-NH2	-7.65	116.47	120.30
1	A	155	PRO	CA-N-CD	-7.62	100.84	111.50
1	C	78	LEU	CA-CB-CG	7.61	132.80	115.30
1	A	245	ARG	NH1-CZ-NH2	7.60	127.76	119.40
2	D	403	GLN	CA-CB-CG	7.52	129.94	113.40
1	C	155	PRO	CA-N-CD	-7.51	100.98	111.50
2	D	178	TYR	CB-CG-CD2	-7.49	116.50	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	178	TYR	CB-CG-CD2	-7.46	116.52	121.00
1	A	163	VAL	N-CA-CB	-7.45	95.11	111.50
2	D	293	ARG	NH1-CZ-NH2	7.41	127.55	119.40
2	B	293	ARG	CG-CD-NE	-7.35	96.37	111.80
1	C	163	VAL	N-CA-CB	-7.33	95.37	111.50
2	D	232	LEU	CB-CG-CD2	7.29	123.40	111.00
1	C	64	VAL	CA-CB-CG2	-7.22	100.06	110.90
1	C	168	TYR	CB-CG-CD1	7.19	125.31	121.00
1	A	217	ARG	NE-CZ-NH2	7.18	123.89	120.30
1	A	122	ARG	NE-CZ-NH1	-7.16	116.72	120.30
2	D	300	LYS	CB-CA-C	-7.15	96.09	110.40
1	A	157	ARG	NE-CZ-NH1	-7.10	116.75	120.30
2	D	188	GLU	OE1-CD-OE2	7.10	131.81	123.30
1	A	258	ASP	CB-CG-OD2	7.04	124.64	118.30
1	C	258	ASP	CB-CG-OD2	7.01	124.61	118.30
2	B	232	LEU	CB-CG-CD2	7.00	122.90	111.00
1	C	163	VAL	CB-CA-C	6.99	124.69	111.40
2	D	240	ASP	CB-CG-OD1	-6.91	112.08	118.30
2	B	379	LYS	CA-C-O	-6.90	105.61	120.10
1	A	256	ASP	CB-CG-OD1	6.89	124.50	118.30
2	D	178	TYR	CA-CB-CG	-6.82	100.45	113.40
1	A	230	VAL	CA-CB-CG2	6.72	120.98	110.90
2	D	188	GLU	CG-CD-OE2	-6.70	104.91	118.30
1	A	78	LEU	CA-CB-CG	6.69	130.69	115.30
1	C	274	ARG	NE-CZ-NH1	6.67	123.63	120.30
2	B	403	GLN	CA-CB-CG	6.64	128.01	113.40
2	B	346	PRO	CA-N-CD	-6.62	102.22	111.50
1	C	157	ARG	NH1-CZ-NH2	6.62	126.69	119.40
3	E	7	ARG	N-CA-CB	-6.58	98.75	110.60
1	C	131	GLN	OE1-CD-NE2	-6.58	106.77	121.90
1	C	176	GLY	CA-C-O	-6.57	108.77	120.60
1	C	210	ASP	CB-CG-OD2	6.57	124.22	118.30
2	B	295	GLU	OE1-CD-OE2	-6.56	115.42	123.30
1	C	217	ARG	NE-CZ-NH1	-6.54	117.03	120.30
1	A	195	GLU	OE1-CD-OE2	-6.54	115.45	123.30
1	C	10	ILE	N-CA-CB	-6.53	95.79	110.80
3	F	7	ARG	N-CA-CB	-6.52	98.86	110.60
1	C	245	ARG	NH1-CZ-NH2	6.46	126.51	119.40
2	B	259	ALA	N-CA-CB	6.45	119.14	110.10
2	B	300	LYS	CB-CA-C	-6.45	97.50	110.40
2	D	293	ARG	CG-CD-NE	-6.45	98.27	111.80
1	A	157	ARG	CA-CB-CG	6.42	127.53	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	178	TYR	CG-CD2-CE2	-6.41	116.17	121.30
1	A	77	TYR	CB-CG-CD1	6.38	124.83	121.00
2	B	187	ARG	NE-CZ-NH1	6.34	123.47	120.30
2	B	294	MET	O-C-N	-6.31	112.61	122.70
1	C	236	TYR	CB-CG-CD1	6.31	124.78	121.00
1	A	274	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	A	163	VAL	CA-CB-CG1	6.24	120.26	110.90
1	A	39	THR	N-CA-CB	6.23	122.14	110.30
2	B	180	GLU	CG-CD-OE1	6.22	130.74	118.30
2	B	365	TYR	CB-CG-CD1	-6.22	117.27	121.00
1	A	252	VAL	CG1-CB-CG2	-6.21	100.96	110.90
2	B	197	VAL	CG1-CB-CG2	-6.19	100.99	110.90
1	C	208	GLU	OE1-CD-OE2	-6.17	115.89	123.30
1	A	150	ARG	NE-CZ-NH2	-6.17	117.22	120.30
2	B	278	PHE	CB-CG-CD2	6.14	125.10	120.80
1	C	258	ASP	OD1-CG-OD2	-6.14	111.64	123.30
1	A	154	VAL	CA-C-O	-6.07	107.36	120.10
1	C	233	MET	CG-SD-CE	6.06	109.90	100.20
2	B	324	PRO	N-CA-CB	6.05	110.56	103.30
1	C	230	VAL	CA-CB-CG2	6.05	119.97	110.90
1	C	258	ASP	CB-CG-OD1	6.02	123.72	118.30
1	C	216	PHE	CB-CG-CD2	-6.01	116.59	120.80
2	D	283	ASP	OD1-CG-OD2	-6.00	111.89	123.30
2	B	385	GLU	OE1-CD-OE2	-5.99	116.11	123.30
2	B	241	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	C	195	GLU	OE1-CD-OE2	-5.96	116.15	123.30
1	C	157	ARG	CB-CA-C	-5.93	98.53	110.40
1	A	107	TYR	CB-CG-CD1	5.92	124.55	121.00
2	D	241	ARG	CD-NE-CZ	5.88	131.84	123.60
2	B	188	GLU	OE1-CD-OE2	5.88	130.36	123.30
2	B	413	TYR	CB-CG-CD1	-5.86	117.48	121.00
2	D	180	GLU	CG-CD-OE2	-5.85	106.61	118.30
2	B	250	ARG	NE-CZ-NH1	5.84	123.22	120.30
2	B	384	LEU	CB-CA-C	5.83	121.27	110.20
2	D	284	ASP	OD1-CG-OD2	-5.82	112.24	123.30
2	B	177	ASP	N-CA-CB	-5.81	100.14	110.60
1	C	252	VAL	CA-CB-CG2	5.81	119.61	110.90
2	D	308	ALA	CB-CA-C	-5.77	101.44	110.10
2	B	418	TYR	CB-CG-CD1	-5.72	117.57	121.00
1	C	122	ARG	CD-NE-CZ	5.71	131.59	123.60
2	D	268	GLU	CA-CB-CG	5.70	125.93	113.40
2	B	382	TYR	CB-CG-CD1	5.69	124.42	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	MET	CA-CB-CG	-5.68	103.64	113.30
2	B	382	TYR	CB-CG-CD2	-5.68	117.59	121.00
1	C	138	GLU	OE1-CD-OE2	5.67	130.10	123.30
1	A	169	ARG	CD-NE-CZ	5.65	131.51	123.60
2	D	232	LEU	CB-CA-C	-5.65	99.46	110.20
1	A	23	ASN	O-C-N	-5.65	113.66	122.70
2	B	189	MET	CG-SD-CE	-5.65	91.17	100.20
2	B	417	LYS	CB-CG-CD	5.65	126.28	111.60
2	B	188	GLU	CG-CD-OE2	-5.63	107.03	118.30
1	A	77	TYR	CB-CG-CD2	-5.60	117.64	121.00
2	B	393	ASP	CB-CG-OD1	-5.60	113.26	118.30
1	C	154	VAL	CA-C-O	-5.59	108.36	120.10
1	A	146	PHE	CZ-CE2-CD2	5.58	126.80	120.10
2	B	184	THR	O-C-N	-5.55	113.82	122.70
1	C	120	SER	CA-CB-OG	-5.55	96.21	111.20
1	C	53	SER	N-CA-CB	5.55	118.83	110.50
1	C	39	THR	N-CA-CB	5.55	120.84	110.30
1	C	13	GLY	CA-C-O	5.54	130.57	120.60
1	C	226	VAL	CG1-CB-CG2	-5.54	102.04	110.90
2	D	300	LYS	N-CA-CB	5.52	120.54	110.60
1	A	12	GLU	N-CA-CB	5.52	120.54	110.60
2	B	212	ALA	CB-CA-C	-5.52	101.82	110.10
2	B	181	ASP	CB-CG-OD1	-5.49	113.36	118.30
1	A	13	GLY	C-N-CA	5.49	135.42	121.70
2	D	177	ASP	CB-CG-OD1	5.48	123.23	118.30
2	D	180	GLU	CG-CD-OE1	5.47	129.24	118.30
2	B	300	LYS	N-CA-CB	5.47	120.44	110.60
2	D	350	TYR	CB-CG-CD2	-5.47	117.72	121.00
2	D	417	LYS	CB-CG-CD	5.45	125.78	111.60
1	A	107	TYR	CB-CG-CD2	-5.45	117.73	121.00
1	C	247	ASP	CB-CG-OD1	-5.45	113.40	118.30
1	C	169	ARG	NE-CZ-NH2	5.44	123.02	120.30
1	A	10	ILE	N-CA-CB	-5.43	98.31	110.80
1	A	122	ARG	CA-CB-CG	5.41	125.31	113.40
2	D	346	PRO	CA-N-CD	-5.41	103.92	111.50
1	C	107	TYR	CB-CG-CD1	5.40	124.24	121.00
2	D	185	TYR	CB-CG-CD2	5.39	124.24	121.00
2	B	231	THR	CA-CB-OG1	-5.38	97.71	109.00
1	C	226	VAL	CA-CB-CG2	5.36	118.94	110.90
1	A	53	SER	N-CA-CB	5.36	118.53	110.50
2	B	187	ARG	CD-NE-CZ	-5.34	116.12	123.60
3	E	6	PRO	C-N-CA	5.32	135.00	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	86	ASP	CB-CG-OD2	5.30	123.07	118.30
2	D	324	PRO	N-CA-CB	5.29	109.65	103.30
2	B	420	GLY	O-C-N	-5.29	114.23	122.70
3	E	2	HIS	CA-CB-CG	5.29	122.58	113.60
1	C	157	ARG	CA-CB-CG	5.28	125.02	113.40
1	A	252	VAL	CA-CB-CG1	-5.28	102.98	110.90
2	D	189	MET	CG-SD-CE	-5.28	91.76	100.20
1	A	252	VAL	CA-CB-CG2	5.26	118.80	110.90
2	B	178	TYR	O-C-N	5.24	131.09	122.70
1	C	252	VAL	CA-CB-CG1	-5.24	103.05	110.90
1	A	117	PHE	CB-CG-CD1	-5.23	117.14	120.80
2	D	225	TYR	CB-CG-CD1	5.22	124.13	121.00
2	B	232	LEU	CA-CB-CG	5.21	127.29	115.30
1	C	116	ALA	N-CA-CB	5.21	117.40	110.10
2	B	178	TYR	CD1-CG-CD2	5.21	123.63	117.90
2	B	263	LEU	O-C-N	5.21	131.04	122.70
1	C	195	GLU	CG-CD-OE1	5.19	128.69	118.30
2	D	418	TYR	CB-CG-CD1	-5.18	117.89	121.00
2	D	314	PHE	CB-CG-CD1	-5.18	117.18	120.80
1	C	47	THR	OG1-CB-CG2	-5.17	98.12	110.00
1	A	91	MET	CA-CB-CG	5.16	122.08	113.30
1	C	177	CYS	N-CA-CB	5.16	119.89	110.60
2	D	349	LYS	CB-CG-CD	5.16	125.02	111.60
1	A	193	PHE	CB-CG-CD1	5.16	124.41	120.80
1	A	287	GLN	O-C-N	-5.15	114.45	122.70
1	C	193	PHE	CB-CG-CD1	5.15	124.41	120.80
2	D	343	ASP	CB-CG-OD1	5.12	122.91	118.30
1	C	84	HIS	CA-CB-CG	-5.12	104.90	113.60
1	A	142	LYS	N-CA-CB	-5.11	101.41	110.60
2	D	318	TYR	CB-CG-CD1	5.11	124.06	121.00
2	D	373	PRO	CA-C-O	5.10	132.45	120.20
1	C	256	ASP	CB-CG-OD1	5.10	122.89	118.30
2	D	371	SER	CB-CA-C	-5.10	100.41	110.10
1	C	81	GLU	OE1-CD-OE2	-5.10	117.19	123.30
1	A	19	TYR	CB-CA-C	-5.08	100.25	110.40
1	A	126	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	A	208	GLU	CG-CD-OE1	5.07	128.45	118.30
1	A	226	VAL	CG1-CB-CG2	-5.06	102.80	110.90
2	B	271	TYR	CZ-CE2-CD2	-5.06	115.24	119.80
3	F	6	PRO	O-C-N	-5.06	114.60	122.70
2	B	295	GLU	CG-CD-OE1	5.05	128.40	118.30
1	A	97	THR	CB-CA-C	-5.05	97.97	111.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	343	ASP	CB-CG-OD1	5.05	122.84	118.30
1	A	155	PRO	N-CD-CG	5.01	110.71	103.20
3	E	7	ARG	CA-C-N	5.01	128.22	117.20
1	C	214	ARG	CD-NE-CZ	5.01	130.61	123.60
1	C	233	MET	CA-CB-CG	-5.00	104.80	113.30

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	0	SER	Mainchain
1	A	152	PHE	Mainchain
1	A	154	VAL	Mainchain,Peptide
2	B	309	PRO	Mainchain
2	B	323	GLN	Mainchain,Peptide
2	B	345	ASP	Mainchain,Peptide
1	C	0	SER	Mainchain
1	C	154	VAL	Mainchain,Peptide
2	D	323	GLN	Mainchain,Peptide
2	D	345	ASP	Mainchain,Peptide
2	D	347	TYR	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2388	0	2430	102	0
1	C	2388	0	2430	101	0
2	B	2083	0	2107	58	1
2	D	2083	0	2107	48	1
3	E	58	0	56	3	0
3	F	58	0	56	1	0
4	A	31	0	12	2	0
4	C	31	0	12	2	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	206	0	0	18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	166	0	0	7	0
6	C	197	0	0	10	0
6	D	185	0	0	9	0
6	E	5	0	0	0	0
6	F	8	0	0	0	0
All	All	9889	0	9210	294	1

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 16.

All (294) 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:C:9:LYS:HZ2	1:C:17:VAL:HG11	1.32	0.94
1:C:266:MET:SD	6:C:2130:HOH:O	2.24	0.94
2:D:327:CYS:HB3	6:D:2125:HOH:O	1.73	0.88
1:C:9:LYS:NZ	1:C:17:VAL:HG11	1.89	0.87
1:A:266:MET:SD	6:A:2134:HOH:O	2.33	0.87
1:A:252:VAL:HB	6:A:2171:HOH:O	1.76	0.86
2:D:177:ASP:HB3	6:D:2033:HOH:O	1.75	0.85
1:A:60:HIS:HD2	1:A:62:ASN:H	1.27	0.82
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.59	0.81
1:C:252:VAL:HB	6:C:2168:HOH:O	1.80	0.81
1:C:88:LYS:HD2	1:C:131:GLN:HE21	1.47	0.80
1:C:60:HIS:HD2	1:C:62:ASN:H	1.30	0.79
1:A:9:LYS:HZ2	1:A:17:VAL:HG11	1.49	0.77
2:B:210:MET:CE	2:B:250:ARG:HB2	2.18	0.74
1:C:47:THR:HG22	6:C:2033:HOH:O	1.87	0.73
2:D:296:HIS:NE2	2:D:300:LYS:NZ	2.30	0.73
2:D:289:LYS:HE2	2:D:293:ARG:HE	1.53	0.73
1:C:88:LYS:HD2	1:C:131:GLN:NE2	2.04	0.72
1:A:60:HIS:CD2	1:A:62:ASN:H	2.07	0.72
1:C:65:LYS:HD2	6:C:2011:HOH:O	1.89	0.72
1:C:9:LYS:HZ2	1:C:17:VAL:HG21	1.55	0.72
2:B:316:THR:HG21	6:B:2012:HOH:O	1.89	0.71
1:A:14:THR:HB	1:A:15:TYR:CD1	2.25	0.71
2:B:296:HIS:NE2	2:B:300:LYS:NZ	2.30	0.70
1:C:60:HIS:CD2	1:C:62:ASN:H	2.09	0.70
1:A:64:VAL:HG21	1:A:134:LEU:HD12	1.72	0.70
1:A:131:GLN:HG3	6:A:2032:HOH:O	1.91	0.69
1:C:223:ASP:H	1:C:226:VAL:CG1	2.05	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:LYS:NZ	1:A:75:LYS:HG2	2.07	0.69
1:C:17:VAL:HG12	1:C:18:VAL:N	2.07	0.69
2:B:233:HIS:HD2	6:B:2102:HOH:O	1.76	0.68
2:B:289:LYS:HE2	2:B:293:ARG:HE	1.57	0.68
2:D:344:ALA:HB1	2:D:348:LEU:HD22	1.73	0.68
1:A:10:ILE:HG23	4:A:381:ATP:H1'	1.74	0.68
1:C:91:MET:HE3	6:C:2131:HOH:O	1.93	0.68
1:C:14:THR:HB	1:C:15:TYR:CD1	2.29	0.68
1:A:47:THR:HG22	6:A:2010:HOH:O	1.94	0.67
2:D:210:MET:HE3	2:D:250:ARG:HB2	1.75	0.67
1:C:119:HIS:HD2	6:D:2034:HOH:O	1.77	0.67
1:A:20:LYS:HE3	1:A:82:PHE:CZ	2.29	0.67
2:D:210:MET:CE	2:D:250:ARG:HB2	2.24	0.67
1:C:34:LYS:NZ	1:C:75:LYS:HG2	2.09	0.67
1:A:17:VAL:HG12	1:A:18:VAL:N	2.10	0.67
2:D:330:GLU:O	2:D:334:MET:HG3	1.94	0.66
1:A:197:VAL:HG11	1:A:252:VAL:CG1	2.25	0.66
1:C:64:VAL:HG21	1:C:144:ALA:HB2	1.77	0.66
1:A:71:HIS:CD2	1:A:76:LEU:HD13	2.31	0.66
2:B:289:LYS:HE2	2:B:293:ARG:NE	2.11	0.66
1:A:193:PHE:HD2	1:A:266:MET:HE1	1.62	0.65
1:C:39:THR:HG21	2:D:289:LYS:NZ	2.12	0.65
1:C:71:HIS:CD2	1:C:76:LEU:HD13	2.31	0.65
2:D:196:LYS:O	2:D:196:LYS:HG3	1.96	0.65
1:C:131:GLN:CD	1:C:131:GLN:H	1.99	0.64
1:A:88:LYS:HB2	1:A:131:GLN:NE2	2.13	0.64
1:A:223:ASP:H	1:A:226:VAL:CG1	2.10	0.64
1:C:17:VAL:CG1	1:C:18:VAL:N	2.61	0.63
1:A:119:HIS:HD2	6:B:2024:HOH:O	1.80	0.63
1:A:88:LYS:HB2	1:A:131:GLN:HE21	1.64	0.63
1:A:227:TRP:O	1:A:230:VAL:HG22	1.98	0.63
2:B:210:MET:HE1	2:B:250:ARG:HB2	1.81	0.62
1:C:227:TRP:O	1:C:230:VAL:HG22	1.99	0.62
1:C:230:VAL:HG12	1:C:233:MET:CE	2.30	0.62
1:C:230:VAL:CG1	1:C:233:MET:HE1	2.30	0.62
2:D:289:LYS:HE2	2:D:293:ARG:NE	2.15	0.62
1:A:119:HIS:HE1	1:A:185:ASP:OD2	1.82	0.62
1:C:64:VAL:HG21	1:C:134:LEU:HD12	1.82	0.61
6:A:2047:HOH:O	2:B:178:TYR:HB2	2.00	0.61
1:C:193:PHE:HD2	1:C:266:MET:CE	2.13	0.61
1:A:175:LEU:CD1	1:A:233:MET:HE3	2.30	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:TPO:O3P	3:E:8:LYS:NZ	2.34	0.61
1:C:53:SER:HB3	2:D:304:PHE:O	2.01	0.60
1:C:137:THR:HG22	1:C:296:LEU:HD12	1.82	0.60
1:C:230:VAL:HG13	1:C:233:MET:HE1	1.83	0.60
2:B:289:LYS:HD2	2:B:289:LYS:O	2.01	0.60
2:B:330:GLU:O	2:B:334:MET:HG3	2.02	0.60
1:C:71:HIS:CE1	2:D:296:HIS:ND1	2.70	0.60
1:C:14:THR:HB	1:C:15:TYR:HD1	1.67	0.60
2:B:210:MET:HE3	2:B:250:ARG:HB2	1.84	0.60
1:A:91:MET:HE3	6:A:2137:HOH:O	2.01	0.60
1:A:131:GLN:CD	1:A:131:GLN:H	2.05	0.60
1:A:154:VAL:O	2:B:316:THR:HG23	2.02	0.60
1:A:230:VAL:HG13	1:A:233:MET:HE1	1.82	0.60
2:D:233:HIS:HD2	6:D:2114:HOH:O	1.85	0.59
1:C:20:LYS:HE3	1:C:82:PHE:CZ	2.37	0.59
1:A:0:SER:O	6:A:2001:HOH:O	2.17	0.59
2:B:196:LYS:O	2:B:196:LYS:HG3	2.02	0.59
2:B:201:LYS:HD3	2:B:202:LYS:HD2	1.85	0.59
1:C:230:VAL:HG12	1:C:233:MET:HE2	1.86	0.58
1:C:9:LYS:HZ2	1:C:17:VAL:CG1	2.13	0.58
1:C:88:LYS:HB2	1:C:131:GLN:NE2	2.19	0.57
1:A:88:LYS:HD2	1:A:131:GLN:NE2	2.19	0.57
1:C:160:TPO:O3P	3:F:8:LYS:NZ	2.37	0.57
2:D:183:HIS:HD2	6:D:2036:HOH:O	1.87	0.57
1:A:39:THR:HG21	2:B:289:LYS:NZ	2.19	0.57
2:B:388:LYS:O	2:B:392:MET:HG2	2.05	0.57
2:D:201:LYS:HD3	2:D:202:LYS:HD2	1.87	0.57
1:A:223:ASP:OD1	1:A:226:VAL:HG12	2.05	0.56
1:A:230:VAL:HG12	1:A:233:MET:HE2	1.87	0.56
1:A:278:LYS:HD2	6:A:2191:HOH:O	2.05	0.56
1:A:193:PHE:HD2	1:A:266:MET:CE	2.18	0.56
1:A:272:ASN:ND2	6:A:2187:HOH:O	2.38	0.56
2:D:193:CYS:O	2:D:241:ARG:HD2	2.03	0.56
2:B:400:LYS:HE2	6:B:2143:HOH:O	2.05	0.56
1:A:175:LEU:HD12	1:A:233:MET:HE3	1.87	0.56
1:A:193:PHE:CD2	1:A:266:MET:HE1	2.40	0.55
1:A:230:VAL:HG12	1:A:233:MET:CE	2.36	0.55
2:B:189:MET:HE2	6:B:2099:HOH:O	2.07	0.55
1:C:64:VAL:HG23	1:C:143:LEU:O	2.07	0.55
1:C:197:VAL:HG11	1:C:252:VAL:CG1	2.36	0.55
2:D:197:VAL:HG22	2:D:348:LEU:O	2.04	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:LYS:HZ3	1:C:75:LYS:HG2	1.71	0.54
1:A:230:VAL:CG1	1:A:233:MET:HE1	2.37	0.54
1:C:119:HIS:HE1	1:C:185:ASP:OD2	1.89	0.54
1:A:64:VAL:HG21	1:A:144:ALA:HB2	1.88	0.54
2:D:316:THR:HG21	6:D:2020:HOH:O	2.07	0.54
1:A:2:GLU:OE2	2:D:293:ARG:HD3	2.08	0.54
1:C:10:ILE:HG23	4:C:381:ATP:H1'	1.90	0.54
2:D:296:HIS:CD2	2:D:300:LYS:HE2	2.43	0.54
6:A:2049:HOH:O	2:B:175:VAL:HG21	2.08	0.53
1:C:278:LYS:HE2	2:D:178:TYR:CE1	2.44	0.53
1:C:137:THR:HA	1:C:296:LEU:HD11	1.91	0.53
2:D:388:LYS:O	2:D:392:MET:HG2	2.09	0.53
1:A:131:GLN:NE2	1:A:131:GLN:N	2.55	0.53
1:C:137:THR:HG22	1:C:296:LEU:CD1	2.39	0.53
1:C:223:ASP:OD1	1:C:226:VAL:HG12	2.08	0.53
1:C:284:PRO:O	1:C:287:GLN:HG2	2.08	0.53
1:A:14:THR:HB	1:A:15:TYR:HD1	1.74	0.52
1:A:131:GLN:NE2	1:A:131:GLN:H	2.08	0.52
2:B:183:HIS:HD2	6:B:2030:HOH:O	1.93	0.52
2:B:193:CYS:O	2:B:241:ARG:HD2	2.10	0.52
1:A:10:ILE:HG23	4:A:381:ATP:C1'	2.39	0.52
1:C:72:THR:HG22	1:C:75:LYS:H	1.74	0.52
1:C:175:LEU:CD1	1:C:233:MET:HE3	2.39	0.52
2:D:289:LYS:HD2	2:D:289:LYS:O	2.09	0.52
1:A:51:GLU:O	1:A:55:LEU:HB2	2.10	0.52
2:B:207:THR:OG1	2:B:210:MET:HG3	2.09	0.52
1:C:35:ILE:HD13	1:C:48:ALA:HB2	1.91	0.51
2:D:274:GLU:HG2	2:D:277:GLU:HG3	1.91	0.51
1:A:88:LYS:HD2	1:A:131:GLN:HE21	1.74	0.51
6:A:2191:HOH:O	2:B:177:ASP:HB3	2.11	0.51
2:B:196:LYS:HG3	2:B:199:TYR:HB3	1.92	0.51
1:A:9:LYS:HZ2	1:A:17:VAL:CG1	2.21	0.51
2:D:395:HIS:HE1	2:D:427:PRO:O	1.93	0.51
1:A:137:THR:HA	1:A:296:LEU:HD11	1.93	0.51
1:C:197:VAL:HG11	1:C:252:VAL:HG12	1.92	0.51
1:A:197:VAL:HG11	1:A:252:VAL:HG12	1.91	0.51
2:D:371:SER:O	2:D:372:TRP:C	2.49	0.50
1:A:9:LYS:HD3	1:A:17:VAL:HG13	1.93	0.50
1:A:197:VAL:CG1	1:A:252:VAL:CG1	2.89	0.50
2:D:322:GLN:NE2	2:D:330:GLU:OE2	2.44	0.50
1:A:65:LYS:HD2	6:A:2013:HOH:O	2.10	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:ILE:HG22	1:C:18:VAL:HB	1.92	0.50
2:B:319:PHE:O	2:B:322:GLN:HG3	2.12	0.50
1:A:276:SER:HB3	2:B:177:ASP:OD2	2.11	0.50
2:D:219:VAL:HG22	2:D:232:LEU:HD11	1.94	0.50
1:A:91:MET:HG2	6:A:2136:HOH:O	2.11	0.50
1:A:230:VAL:CG1	1:A:233:MET:CE	2.89	0.50
1:A:17:VAL:CG1	1:A:18:VAL:N	2.74	0.50
1:A:0:SER:C	1:A:2:GLU:H	2.15	0.49
1:A:10:ILE:HG22	1:A:18:VAL:HB	1.95	0.49
1:A:34:LYS:HZ3	1:A:75:LYS:HG2	1.75	0.49
2:D:289:LYS:CE	2:D:293:ARG:HE	2.24	0.49
1:C:175:LEU:HD13	1:C:233:MET:CE	2.43	0.49
2:B:296:HIS:CD2	2:B:300:LYS:HE2	2.48	0.49
1:A:71:HIS:CE1	2:B:296:HIS:ND1	2.81	0.49
1:C:9:LYS:NZ	1:C:17:VAL:HG21	2.26	0.49
2:B:270:ILE:O	3:E:8:LYS:HE3	2.13	0.48
1:C:193:PHE:HD2	1:C:266:MET:HE1	1.78	0.48
1:A:284:PRO:O	1:A:287:GLN:HG2	2.13	0.48
1:A:64:VAL:HG23	1:A:143:LEU:O	2.13	0.48
1:A:175:LEU:HD13	1:A:233:MET:HE3	1.96	0.47
1:A:292:PRO:HB3	6:A:2081:HOH:O	2.13	0.47
2:B:289:LYS:CE	2:B:293:ARG:HE	2.25	0.47
1:A:198:THR:O	1:A:199:ARG:HB2	2.14	0.47
2:B:197:VAL:HG22	2:B:348:LEU:O	2.14	0.47
1:C:230:VAL:CG1	1:C:233:MET:CE	2.89	0.47
1:A:35:ILE:HD13	1:A:48:ALA:HB2	1.95	0.47
1:A:57:GLU:OE2	2:B:307:ALA:HB3	2.14	0.47
2:D:309:PRO:HD2	6:D:2113:HOH:O	2.13	0.47
1:A:72:THR:HG22	1:A:75:LYS:H	1.79	0.47
2:B:292:LEU:HD12	2:B:292:LEU:HA	1.76	0.47
2:D:384:LEU:HD12	2:D:384:LEU:HA	1.79	0.47
1:C:198:THR:HG23	1:C:252:VAL:HG13	1.97	0.47
2:B:225:TYR:HE2	2:B:281:ILE:HG21	1.80	0.46
2:B:379:LYS:O	2:B:379:LYS:HG2	2.15	0.46
1:C:250:LYS:HE3	6:C:2166:HOH:O	2.14	0.46
1:A:175:LEU:HD13	1:A:233:MET:CE	2.45	0.46
1:C:197:VAL:CG1	1:C:252:VAL:CG1	2.93	0.46
2:B:384:LEU:HB2	6:B:2136:HOH:O	2.16	0.46
1:C:56:LYS:HB3	1:C:56:LYS:HE2	1.57	0.46
1:C:175:LEU:HD13	1:C:233:MET:HE3	1.98	0.46
2:D:274:GLU:CG	2:D:277:GLU:HG3	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:LYS:HD3	1:C:179:TYR:CE2	2.50	0.46
1:C:39:THR:HG21	2:D:289:LYS:HD3	1.97	0.46
2:D:225:TYR:HE2	2:D:281:ILE:HG21	1.81	0.46
2:D:417:LYS:HE3	6:D:2180:HOH:O	2.16	0.46
1:A:178:LYS:HD3	1:A:179:TYR:CE2	2.50	0.46
1:C:137:THR:O	1:C:293:VAL:HG13	2.15	0.46
1:A:154:VAL:O	2:B:316:THR:CG2	2.64	0.46
1:A:154:VAL:HG22	6:A:2101:HOH:O	2.15	0.46
2:D:378:ARG:NH1	6:D:2148:HOH:O	2.48	0.46
2:B:274:GLU:CG	2:B:277:GLU:HG3	2.46	0.46
2:B:308:ALA:HA	2:B:309:PRO:HD3	1.72	0.46
2:B:395:HIS:HE1	2:B:427:PRO:O	1.99	0.45
1:C:22:ARG:HD2	6:C:2005:HOH:O	2.16	0.45
2:B:196:LYS:CB	2:B:196:LYS:NZ	2.79	0.45
1:A:137:THR:O	1:A:293:VAL:HG13	2.16	0.45
1:A:197:VAL:HG11	1:A:252:VAL:HG11	1.98	0.45
2:D:401:ALA:HB1	2:D:410:ARG:HD2	1.97	0.45
2:D:196:LYS:HG3	2:D:199:TYR:HB3	1.98	0.45
1:A:88:LYS:CB	1:A:131:GLN:HE21	2.28	0.45
1:A:102:PRO:HB2	1:A:292:PRO:HG3	1.98	0.45
1:A:263:LEU:HA	1:A:266:MET:HE3	1.98	0.45
1:A:268:HIS:CD2	1:A:273:LYS:HB2	2.51	0.45
1:C:227:TRP:CE3	1:C:230:VAL:HG13	2.52	0.45
1:A:56:LYS:HB3	1:A:56:LYS:HE2	1.59	0.45
1:A:148:LEU:HD12	1:A:148:LEU:HA	1.87	0.45
2:B:289:LYS:HD2	2:B:293:ARG:HG3	1.99	0.45
1:C:39:THR:HG22	1:C:40:GLU:H	1.82	0.45
6:A:2049:HOH:O	2:B:175:VAL:HG11	2.17	0.45
2:B:368:THR:CB	2:B:370:GLN:HE21	2.30	0.44
1:C:15:TYR:CD1	1:C:15:TYR:N	2.86	0.44
1:C:107:TYR:O	1:C:111:LEU:HG	2.17	0.44
1:A:199:ARG:HG2	6:A:2074:HOH:O	2.18	0.44
2:B:398:TYR:CD2	2:B:426:PRO:HB3	2.53	0.44
1:A:39:THR:HG22	1:A:40:GLU:H	1.82	0.44
1:A:137:THR:HG22	1:A:296:LEU:HD12	1.98	0.44
1:C:34:LYS:NZ	1:C:75:LYS:NZ	2.66	0.44
1:C:253:PRO:HB2	1:C:254:PRO:HD3	1.99	0.44
1:C:198:THR:O	1:C:199:ARG:HB2	2.18	0.44
1:C:51:GLU:O	1:C:55:LEU:HB2	2.17	0.44
1:C:148:LEU:HD12	1:C:148:LEU:HA	1.80	0.44
1:C:60:HIS:HE1	6:C:2080:HOH:O	2.01	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:GLN:NE2	1:C:131:GLN:N	2.65	0.44
1:C:223:ASP:H	1:C:226:VAL:HG12	1.82	0.44
1:C:178:LYS:HD3	1:C:179:TYR:CZ	2.53	0.44
1:C:193:PHE:HD2	1:C:266:MET:HE2	1.80	0.43
3:E:7:ARG:O	3:E:7:ARG:HG2	2.17	0.43
1:C:34:LYS:HZ1	1:C:75:LYS:HE2	1.82	0.43
1:C:193:PHE:CD2	1:C:266:MET:CE	2.98	0.43
1:A:88:LYS:HD3	6:A:2026:HOH:O	2.18	0.43
1:A:170:ALA:HB1	1:A:172:GLU:OE1	2.18	0.43
1:C:268:HIS:CD2	1:C:273:LYS:HB2	2.53	0.43
1:C:154:VAL:O	2:D:316:THR:HG23	2.18	0.43
1:C:9:LYS:HZ2	1:C:17:VAL:CG2	2.27	0.43
1:A:2:GLU:OE2	2:D:293:ARG:NH1	2.52	0.43
1:C:177:CYS:SG	1:C:178:LYS:N	2.91	0.43
1:A:88:LYS:HA	1:A:91:MET:HE2	2.01	0.42
1:A:269:TYR:O	1:A:271:PRO:HD3	2.19	0.42
1:A:186:ILE:HD11	1:A:277:ALA:HB2	2.01	0.42
2:B:401:ALA:N	2:B:402:PRO:CD	2.82	0.42
1:A:107:TYR:O	1:A:111:LEU:HG	2.19	0.42
2:B:417:LYS:HE2	2:B:418:TYR:CE2	2.54	0.42
1:C:193:PHE:CD2	1:C:266:MET:HE1	2.54	0.42
2:D:289:LYS:HD2	2:D:293:ARG:HG3	2.01	0.42
2:B:388:LYS:HB3	2:B:389:PRO:HD3	1.99	0.42
1:A:9:LYS:CD	1:A:17:VAL:HG13	2.50	0.42
1:A:39:THR:HG21	2:B:289:LYS:HZ1	1.83	0.42
1:C:269:TYR:O	1:C:271:PRO:HD3	2.19	0.42
2:D:196:LYS:CB	2:D:196:LYS:NZ	2.83	0.42
1:A:10:ILE:HG21	1:A:18:VAL:HG12	2.02	0.42
1:A:248:PHE:HA	1:A:251:VAL:HB	2.02	0.42
2:B:417:LYS:NZ	2:B:417:LYS:CB	2.83	0.42
2:B:401:ALA:HB1	2:B:410:ARG:HD2	2.00	0.42
1:A:34:LYS:HZ1	1:A:75:LYS:HE2	1.84	0.42
2:B:376:LEU:HD23	2:B:376:LEU:HA	1.87	0.42
2:B:322:GLN:NE2	2:B:330:GLU:OE2	2.52	0.42
1:C:10:ILE:HD13	1:C:10:ILE:HG21	1.65	0.42
1:C:260:ARG:HH11	1:C:260:ARG:HD3	1.63	0.41
1:C:131:GLN:NE2	1:C:131:GLN:H	2.18	0.41
2:D:376:LEU:HD23	2:D:376:LEU:HA	1.88	0.41
2:B:335:PHE:HB2	2:B:413:TYR:CD2	2.56	0.41
2:D:175:VAL:HG12	2:D:175:VAL:O	2.20	0.41
1:A:193:PHE:CD2	1:A:266:MET:CE	3.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:274:GLU:HG2	2:B:277:GLU:HG3	2.03	0.41
2:D:327:CYS:HB2	2:D:419:HIS:CE1	2.56	0.41
1:A:227:TRP:CE3	1:A:230:VAL:HG13	2.56	0.41
1:C:49:ILE:HG23	2:D:306:LEU:HD12	2.02	0.41
1:C:227:TRP:CE3	1:C:269:TYR:HB3	2.55	0.41
1:C:131:GLN:CD	1:C:131:GLN:N	2.72	0.41
1:C:226:VAL:HG12	1:C:226:VAL:H	1.62	0.41
1:A:222:PRO:HA	1:A:226:VAL:HG11	2.02	0.41
1:A:226:VAL:HG12	1:A:226:VAL:H	1.61	0.41
2:B:194:LYS:HA	2:B:195:PRO:HD3	1.84	0.41
1:C:35:ILE:HD12	1:C:78:LEU:HD21	2.02	0.41
1:C:13:GLY:HA3	4:C:381:ATP:O1B	2.21	0.41
1:C:10:ILE:HD11	1:C:82:PHE:HE1	1.87	0.40
1:C:137:THR:HA	1:C:296:LEU:CD1	2.51	0.40
1:C:161:HIS:HE1	6:C:2145:HOH:O	2.04	0.40
2:D:398:TYR:CD2	2:D:426:PRO:HB3	2.57	0.40
2:B:371:SER:O	2:B:372:TRP:C	2.59	0.40
1:C:139:GLY:HA2	1:C:294:PRO:HD3	2.04	0.40
1:C:250:LYS:HD2	6:C:2166:HOH:O	2.21	0.40
1:A:178:LYS:HD3	1:A:179:TYR:CZ	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:379:LYS:O	2:D:378:ARG:NH2[2_665]	1.70	0.50

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	294/299 (98%)	277 (94%)	15 (5%)	2 (1%)	22 22

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	294/299 (98%)	279 (95%)	11 (4%)	4 (1%)	11	8
2	B	256/259 (99%)	251 (98%)	3 (1%)	2 (1%)	19	19
2	D	256/259 (99%)	251 (98%)	3 (1%)	2 (1%)	19	19
3	E	5/7 (71%)	5 (100%)	0	0	100	100
3	F	5/7 (71%)	5 (100%)	0	0	100	100
All	All	1110/1130 (98%)	1068 (96%)	32 (3%)	10 (1%)	17	16

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	ASP
1	C	38	ASP
1	A	164	VAL
1	C	164	VAL
2	B	346	PRO
1	C	14	THR
2	D	324	PRO
2	B	324	PRO
1	C	145	ASP
2	D	346	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	261/263 (99%)	238 (91%)	23 (9%)	10	10
1	C	261/263 (99%)	239 (92%)	22 (8%)	11	11
2	B	232/233 (100%)	220 (95%)	12 (5%)	23	28
2	D	232/233 (100%)	222 (96%)	10 (4%)	29	36
3	E	6/6 (100%)	6 (100%)	0	100	100
3	F	6/6 (100%)	6 (100%)	0	100	100
All	All	998/1004 (99%)	931 (93%)	67 (7%)	16	18

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	SER
1	A	5	GLN
1	A	9	LYS
1	A	10	ILE
1	A	14	THR
1	A	39	THR
1	A	41	THR
1	A	47	THR
1	A	55	LEU
1	A	56	LYS
1	A	72	THR
1	A	74	ASN
1	A	75	LYS
1	A	78	LEU
1	A	97	THR
1	A	122	ARG
1	A	131	GLN
1	A	138	GLU
1	A	150	ARG
1	A	155	PRO
1	A	163	VAL
1	A	230	VAL
1	A	288	ASP
2	B	179	HIS
2	B	196	LYS
2	B	199	TYR
2	B	232	LEU
2	B	247	SER
2	B	292	LEU
2	B	316	THR
2	B	346	PRO
2	B	348	LEU
2	B	391	LEU
2	B	403	GLN
2	B	417	LYS
1	C	5	GLN
1	C	10	ILE
1	C	14	THR
1	C	39	THR
1	C	41	THR
1	C	47	THR
1	C	49	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	55	LEU
1	C	56	LYS
1	C	72	THR
1	C	74	ASN
1	C	75	LYS
1	C	78	LEU
1	C	97	THR
1	C	122	ARG
1	C	131	GLN
1	C	150	ARG
1	C	155	PRO
1	C	163	VAL
1	C	230	VAL
1	C	278	LYS
1	C	288	ASP
2	D	179	HIS
2	D	196	LYS
2	D	232	LEU
2	D	247	SER
2	D	292	LEU
2	D	316	THR
2	D	348	LEU
2	D	391	LEU
2	D	403	GLN
2	D	417	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	71	HIS
1	A	84	HIS
1	A	119	HIS
1	A	131	GLN
1	A	268	HIS
2	B	183	HIS
2	B	233	HIS
2	B	254	GLN
2	B	317	GLN
2	B	370	GLN
2	B	395	HIS
1	C	60	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	71	HIS
1	C	119	HIS
1	C	131	GLN
1	C	161	HIS
2	D	183	HIS
2	D	233	HIS
2	D	254	GLN
2	D	317	GLN
2	D	370	GLN
2	D	395	HIS
2	D	396	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	TPO	C	160	1	8,10,11	2.18	2 (25%)	10,14,16	2.07	3 (30%)
1	TPO	A	160	1	8,10,11	2.04	1 (12%)	10,14,16	1.86	2 (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
1	TPO	C	160	1	-	1/9/11/13	-
1	TPO	A	160	1	-	1/9/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	160	TPO	P-OG1	-5.50	1.48	1.59
1	A	160	TPO	P-OG1	-4.62	1.50	1.59
1	C	160	TPO	P-O3P	-2.15	1.46	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	TPO	P-OG1-CB	4.31	136.24	123.21
1	C	160	TPO	O-C-CA	-3.71	115.05	124.78
1	C	160	TPO	P-OG1-CB	3.50	133.79	123.21
1	C	160	TPO	CG2-CB-CA	3.39	119.85	113.16
1	A	160	TPO	CG2-CB-CA	2.76	118.61	113.16

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	160	TPO	O-C-CA-CB
1	C	160	TPO	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	160	TPO	1	0
1	A	160	TPO	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	ATP	A	381	5	26,33,33	1.56	4 (15%)	31,52,52	1.78	7 (22%)
4	ATP	C	381	5	26,33,33	1.67	5 (19%)	31,52,52	1.71	6 (19%)

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	ATP	A	381	5	-	3/18/38/38	0/3/3/3
4	ATP	C	381	5	-	4/18/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	381	ATP	C8-N7	-4.17	1.27	1.34
4	A	381	ATP	C8-N7	-4.03	1.27	1.34
4	A	381	ATP	C2-N1	2.96	1.39	1.33
4	C	381	ATP	PB-O2B	-2.93	1.41	1.55
4	C	381	ATP	C2-N1	2.88	1.39	1.33
4	C	381	ATP	O4'-C1'	-2.82	1.37	1.41
4	A	381	ATP	PB-O2B	-2.65	1.42	1.55
4	A	381	ATP	O4'-C1'	-2.47	1.37	1.41
4	C	381	ATP	C5-C4	-2.38	1.34	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	381	ATP	PB-O3B-PG	-4.00	119.11	132.83
4	C	381	ATP	C4-C5-N7	3.71	113.27	109.40
4	C	381	ATP	O2G-PG-O3B	3.32	115.76	104.64
4	A	381	ATP	C4-C5-N7	3.19	112.72	109.40
4	C	381	ATP	C5-C6-N6	2.98	124.88	120.35
4	A	381	ATP	C5-C6-N1	-2.92	113.73	120.35
4	C	381	ATP	PB-O3B-PG	-2.90	122.89	132.83
4	C	381	ATP	C5-C6-N1	-2.84	113.92	120.35
4	C	381	ATP	C1'-N9-C4	2.81	131.59	126.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	381	ATP	C5-C6-N6	2.78	124.58	120.35
4	A	381	ATP	O2G-PG-O3B	2.71	113.71	104.64
4	A	381	ATP	PA-O5'-C5'	2.56	136.70	121.68
4	A	381	ATP	O3G-PG-O1G	-2.52	100.80	110.68

There are no chirality outliers.

All (7) torsion outliers are listed below:

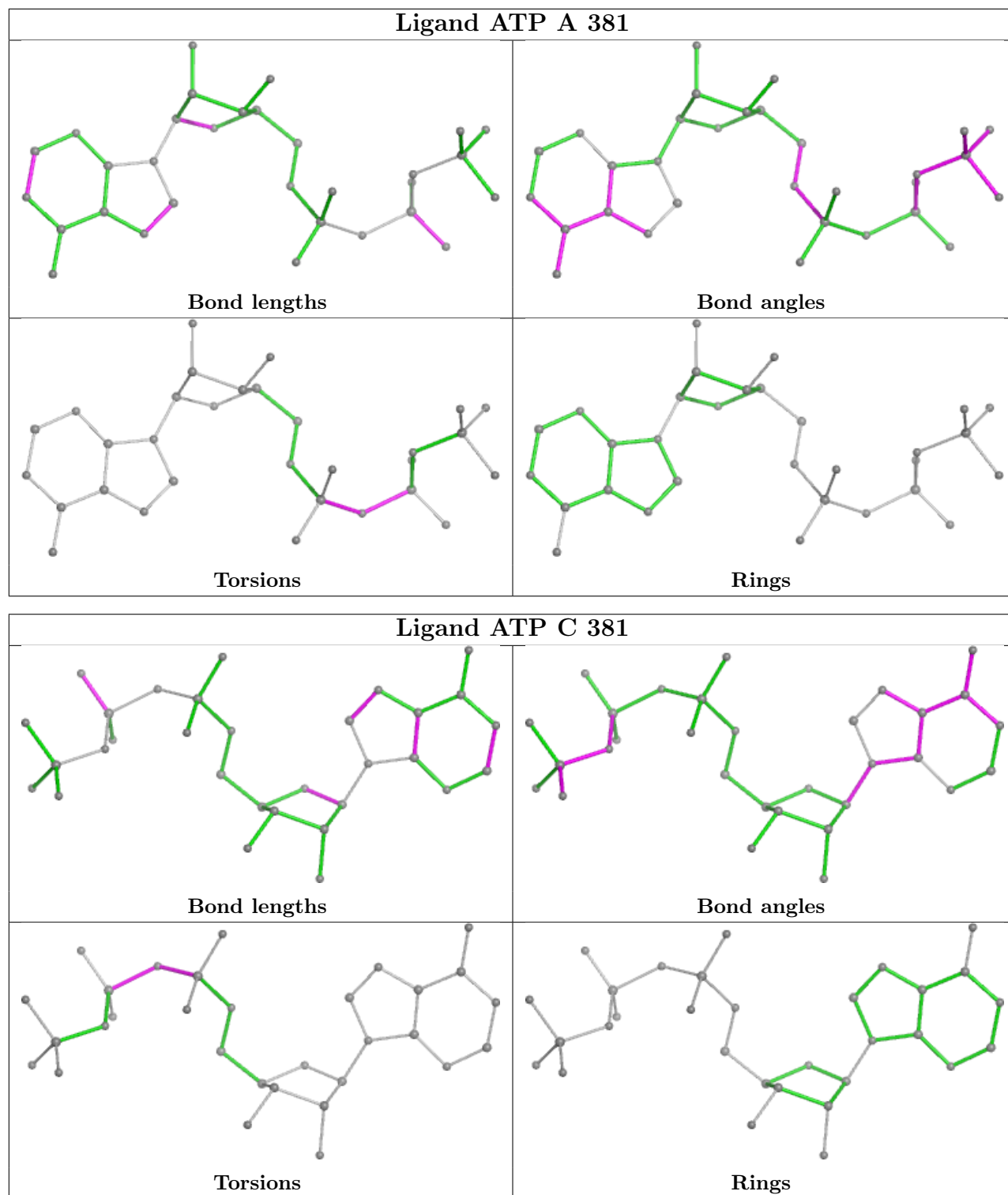
Mol	Chain	Res	Type	Atoms
4	C	381	ATP	PB-O3A-PA-O1A
4	A	381	ATP	PB-O3A-PA-O1A
4	C	381	ATP	PA-O3A-PB-O3B
4	C	381	ATP	PB-O3A-PA-O2A
4	A	381	ATP	PA-O3A-PB-O3B
4	A	381	ATP	PA-O3A-PB-O2B
4	C	381	ATP	PA-O3A-PB-O2B

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	381	ATP	2	0
4	C	381	ATP	2	0

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



5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.