



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 02:19 pm BST

PDB ID : 1SVM
Title : Co-crystal structure of SV40 large T antigen helicase domain and ATP
Authors : Gai, D.; Zhao, R.; Finkielstein, C.V.; Chen, X.S.
Deposited on : 2004-03-29
Resolution : 1.94 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

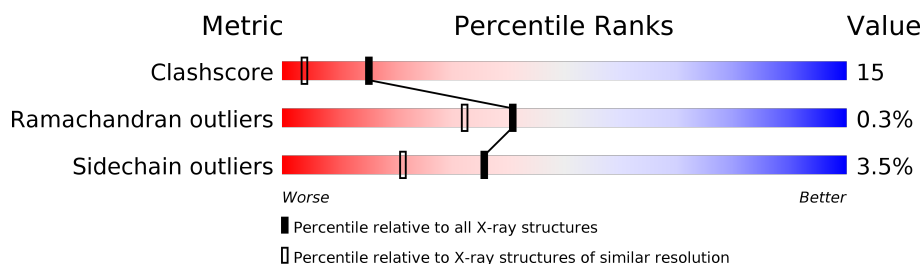
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	377	
1	B	377	
1	C	377	
1	D	377	
1	E	377	
1	F	377	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18609 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 large T antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2933	1888	493	531	21			
1	B	362	Total	C	N	O	S	0	0	0
			2929	1885	492	531	21			
1	C	363	Total	C	N	O	S	0	0	0
			2940	1892	494	533	21			
1	D	362	Total	C	N	O	S	0	0	0
			2933	1888	493	531	21			
1	E	362	Total	C	N	O	S	0	0	0
			2929	1885	492	531	21			
1	F	363	Total	C	N	O	S	0	0	0
			2940	1892	494	533	21			

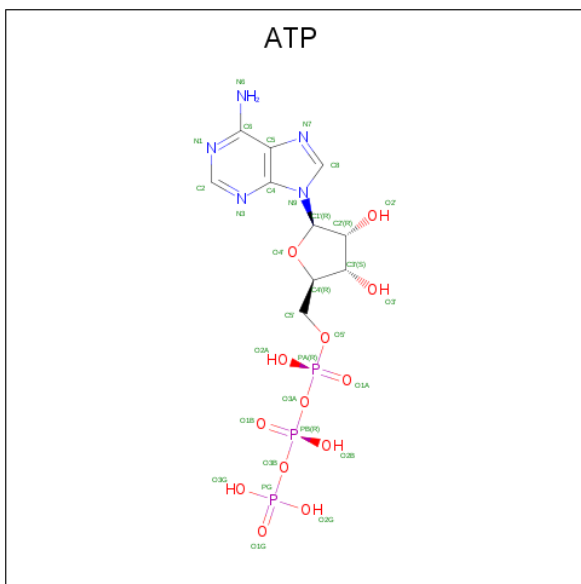
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$).



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

Continued on next page...

Continued from previous page...

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

- Molecule 5 is water.

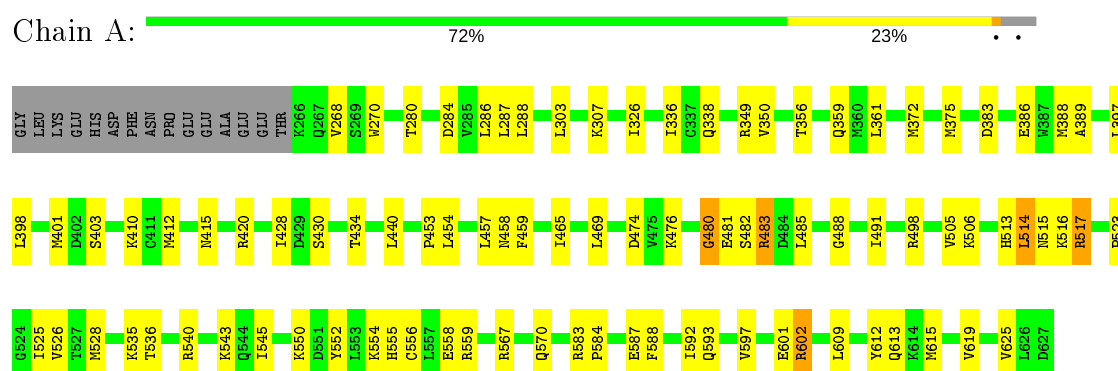
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	136	Total	O	0	0
			136	136		
5	B	140	Total	O	0	0
			140	140		
5	C	127	Total	O	0	0
			127	127		
5	D	123	Total	O	0	0
			123	123		
5	E	159	Total	O	0	0
			159	159		
5	F	122	Total	O	0	0
			122	122		

3 Residue-property plots

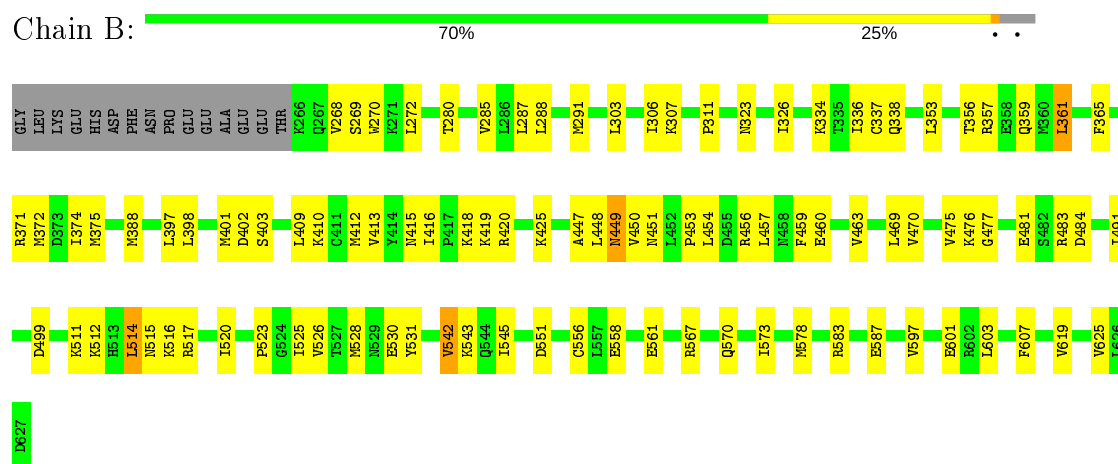
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

Note EDS was not executed.

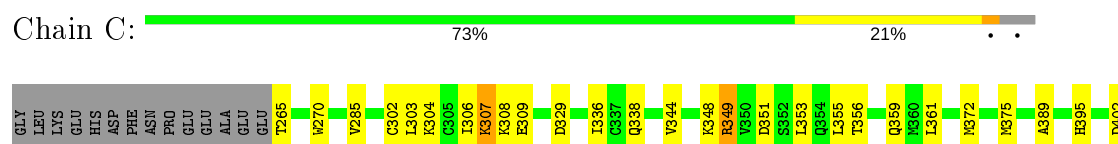
- Molecule 1: large T antigen

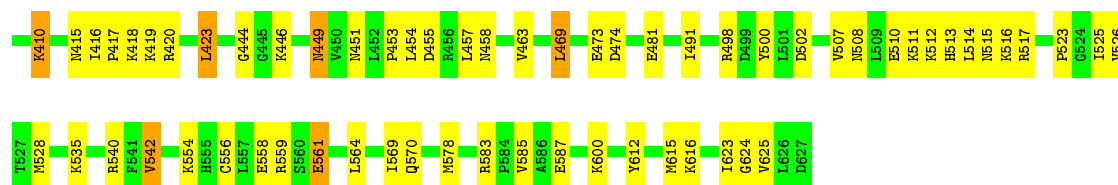


- Molecule 1: large T antigen

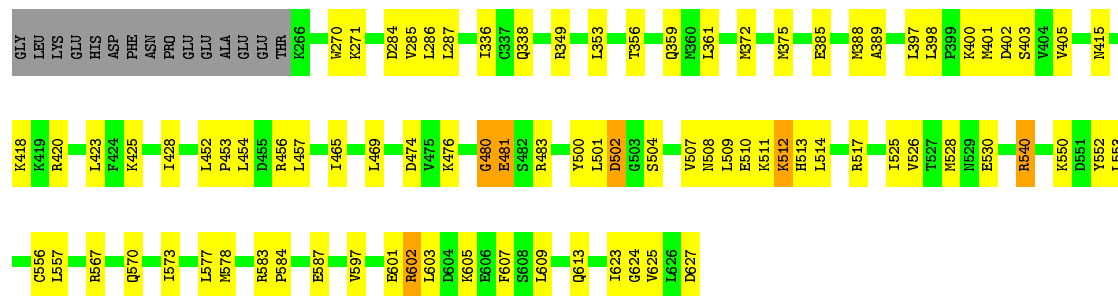


- Molecule 1: large T antigen

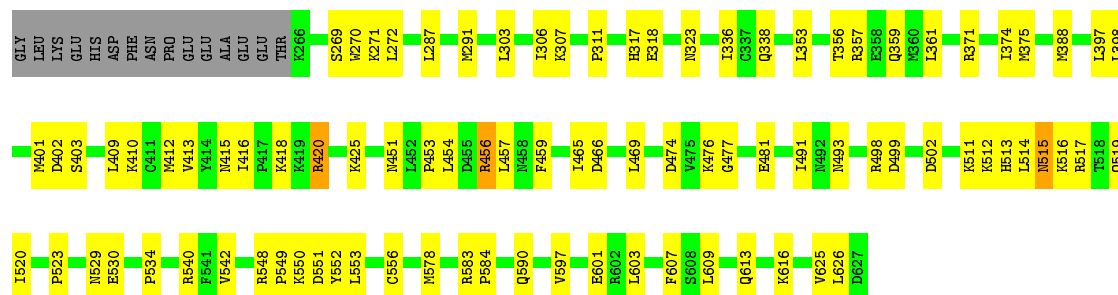




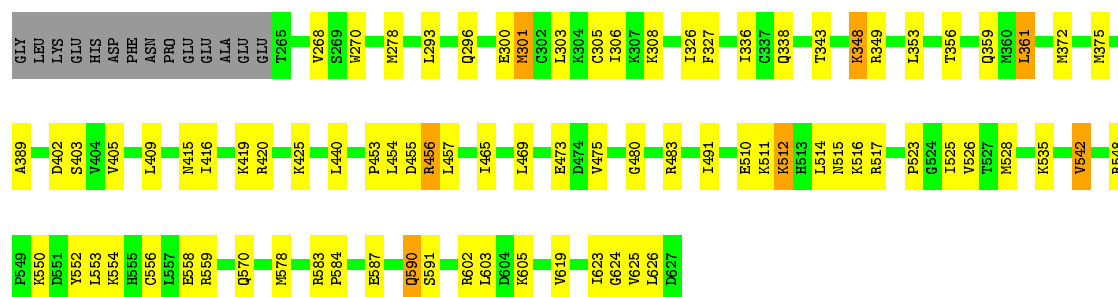
- Molecule 1: large T antigen



- Molecule 1: large T antigen



- Molecule 1: large T antigen



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	125.02Å 89.38Å 148.51Å 90.00° 91.31° 90.00°	Depositor
Resolution (Å)	30.00 – 1.94	Depositor
% Data completeness (in resolution range)	92.3 (30.00-1.94)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.241	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18609	wwPDB-VP
Average B, all atoms (Å ²)	34.0	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: MG, ZN, ATP

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	0.33	0/2992	0.54	0/4030
1	B	0.34	0/2988	0.56	0/4026
1	C	0.32	0/2999	0.54	0/4040
1	D	0.32	0/2992	0.54	0/4030
1	E	0.34	0/2988	0.55	0/4026
1	F	0.33	0/2999	0.54	0/4040
All	All	0.33	0/17958	0.55	0/24192

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	2933	0	2981	94	0
1	B	2929	0	2970	116	0
1	C	2940	0	2988	91	0
1	D	2933	0	2981	89	0
1	E	2929	0	2970	92	0
1	F	2940	0	2988	89	0
2	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	31	0	12	1	0
4	B	31	0	12	0	0
4	C	31	0	12	1	0
4	D	31	0	12	1	0
4	E	31	0	12	3	0
4	F	31	0	12	3	0
5	A	136	0	0	2	0
5	B	140	0	0	2	0
5	C	127	0	0	0	0
5	D	123	0	0	1	0
5	E	159	0	0	3	0
5	F	122	0	0	1	0
All	All	18609	0	17950	531	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (531) 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:E:491:ILE:HD11	1:E:534:PRO:HD3	1.28	1.10
1:E:269:SER:H	1:E:323:ASN:HD21	1.03	1.00
1:B:450:VAL:HG23	1:B:457:LEU:HD11	1.44	0.99
1:E:425:LYS:HE2	1:E:530:GLU:HA	1.45	0.99
1:F:415:ASN:HD21	1:F:420:ARG:HH11	1.11	0.92
1:B:269:SER:H	1:B:323:ASN:HD21	1.13	0.91
1:B:475:VAL:HG12	1:B:491:ILE:HD12	1.50	0.91
1:F:454:LEU:HA	1:F:457:LEU:HB2	1.52	0.89
1:F:602:ARG:HA	1:F:605:LYS:HE2	1.55	0.87
1:B:415:ASN:HD21	1:B:420:ARG:HH11	1.23	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:LEU:HA	1:B:512:LYS:HG3	1.56	0.86
1:C:415:ASN:HD21	1:C:420:ARG:HH11	1.20	0.86
1:B:412:MET:HE3	1:B:523:PRO:HG2	1.57	0.86
1:A:412:MET:HE1	1:A:523:PRO:HG2	1.57	0.85
1:C:454:LEU:H	1:C:454:LEU:HD12	1.43	0.83
1:D:415:ASN:HD21	1:D:420:ARG:HH11	1.23	0.83
1:C:410:LYS:HA	1:C:410:LYS:HE3	1.58	0.83
1:E:477:GLY:HA2	1:E:491:ILE:HG22	1.60	0.83
1:B:285:VAL:HG21	1:B:338:GLN:NE2	1.95	0.82
1:D:500:TYR:CZ	1:D:507:VAL:HG11	2.15	0.82
1:C:498:ARG:NH2	1:D:476:LYS:HD3	1.95	0.81
1:B:425:LYS:HE2	1:B:530:GLU:HA	1.63	0.80
1:E:491:ILE:HD11	1:E:534:PRO:CD	2.10	0.80
1:B:412:MET:CE	1:B:523:PRO:HG2	2.11	0.80
1:A:415:ASN:HD21	1:A:420:ARG:HH11	1.28	0.79
1:C:307:LYS:HA	1:C:307:LYS:HE2	1.64	0.79
1:E:415:ASN:HD21	1:E:420:ARG:HH11	1.30	0.79
1:F:349:ARG:NH1	1:F:517:ARG:HD3	1.97	0.79
1:E:454:LEU:HD12	1:E:457:LEU:HD22	1.65	0.79
1:E:466:ASP:H	1:E:519:GLN:HE22	1.31	0.78
1:A:303:LEU:HD11	1:A:307:LYS:HE3	1.66	0.78
1:B:454:LEU:HD12	1:B:454:LEU:H	1.48	0.78
1:A:535:LYS:HE3	1:B:484:ASP:HB2	1.64	0.78
1:A:434:THR:HG23	1:A:570:GLN:HG3	1.66	0.77
1:D:425:LYS:HE2	1:D:530:GLU:HA	1.65	0.77
1:B:291:MET:HA	1:B:291:MET:HE2	1.66	0.77
1:F:419:LYS:HA	1:F:542:VAL:HG13	1.67	0.77
1:F:356:THR:OG1	1:F:359:GLN:HG3	1.87	0.75
1:A:505:VAL:HG11	1:B:447:ALA:HB2	1.67	0.75
1:B:397:LEU:HG	1:B:398:LEU:HD12	1.67	0.75
1:D:480:GLY:HA2	1:D:483:ARG:HH21	1.52	0.75
1:C:535:LYS:HE2	1:D:428:ILE:HD12	1.67	0.74
1:E:303:LEU:HA	1:E:306:ILE:HG12	1.67	0.74
1:C:402:ASP:HA	1:C:578:MET:HE3	1.70	0.74
1:B:454:LEU:HA	1:B:457:LEU:HB2	1.70	0.74
1:F:590:GLN:NE2	1:F:590:GLN:H	1.86	0.73
1:C:454:LEU:HA	1:C:457:LEU:HG	1.69	0.73
1:E:454:LEU:HD11	1:E:493:ASN:ND2	2.03	0.73
1:B:517:ARG:HH11	1:B:517:ARG:HG2	1.54	0.73
1:B:556:CYS:SG	1:B:625:VAL:HG13	2.29	0.73
1:E:409:LEU:O	1:E:413:VAL:HG12	1.89	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:THR:OG1	1:A:359:GLN:HG3	1.89	0.72
1:F:349:ARG:HD3	1:F:517:ARG:NH1	2.02	0.72
1:D:514:LEU:HB2	1:E:514:LEU:HD11	1.71	0.72
1:F:514:LEU:HB3	1:F:516:LYS:NZ	2.05	0.72
1:F:349:ARG:CZ	1:F:517:ARG:HD3	2.20	0.72
1:F:491:ILE:HD11	1:F:528:MET:HE2	1.72	0.72
1:B:397:LEU:HG	1:B:398:LEU:CD1	2.20	0.71
1:D:502:ASP:OD2	1:D:540:ARG:HD2	1.90	0.71
1:E:477:GLY:HA2	1:E:491:ILE:CG2	2.20	0.71
1:C:402:ASP:HA	1:C:578:MET:CE	2.20	0.71
1:A:453:PRO:HG2	1:F:454:LEU:HB2	1.71	0.71
1:A:612:TYR:HA	1:A:615:MET:HE3	1.72	0.70
1:B:460:GLU:O	1:B:463:VAL:HG22	1.91	0.70
1:A:454:LEU:H	1:A:454:LEU:HD12	1.56	0.70
1:F:349:ARG:CZ	1:F:353:LEU:HD21	2.22	0.70
1:C:517:ARG:HH22	1:D:286:LEU:HD12	1.56	0.69
1:F:583:ARG:HD2	1:F:587:GLU:OE1	1.92	0.69
1:B:412:MET:HE2	1:B:469:LEU:HB3	1.72	0.69
1:B:454:LEU:HB2	1:C:453:PRO:HG2	1.75	0.69
1:B:449:ASN:HD22	1:B:449:ASN:C	1.96	0.68
1:C:449:ASN:ND2	1:C:451:ASN:H	1.91	0.68
1:E:303:LEU:HD22	1:E:306:ILE:HD11	1.73	0.68
1:C:285:VAL:HG21	1:C:338:GLN:NE2	2.08	0.68
1:E:454:LEU:HB2	1:F:453:PRO:HG2	1.76	0.68
1:A:514:LEU:HD11	1:B:514:LEU:HD11	1.76	0.68
1:C:454:LEU:HB2	1:D:453:PRO:HG2	1.75	0.68
1:F:348:LYS:NZ	1:F:348:LYS:HB2	2.09	0.68
1:F:454:LEU:H	1:F:454:LEU:HD12	1.59	0.67
1:D:415:ASN:HD21	1:D:420:ARG:NH1	1.92	0.67
1:C:303:LEU:H	1:C:303:LEU:HD23	1.60	0.67
1:A:410:LYS:HA	1:A:410:LYS:HE2	1.76	0.67
1:E:416:ILE:O	1:E:420:ARG:HG2	1.95	0.67
1:A:505:VAL:HG11	1:B:447:ALA:CB	2.24	0.66
1:B:449:ASN:ND2	1:B:451:ASN:H	1.92	0.66
1:F:415:ASN:HD21	1:F:420:ARG:NH1	1.89	0.66
1:E:402:ASP:HA	1:E:578:MET:CE	2.25	0.66
1:D:454:LEU:H	1:D:454:LEU:HD12	1.61	0.65
1:F:510:GLU:HA	1:F:515:ASN:HA	1.78	0.65
1:B:291:MET:HA	1:B:291:MET:CE	2.26	0.65
1:E:353:LEU:HD21	1:E:517:ARG:HH22	1.62	0.65
1:E:397:LEU:HG	1:E:398:LEU:CD1	2.27	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:451:ASN:HD21	1:E:476:LYS:H	1.45	0.65
1:C:395:HIS:HD2	1:C:616:LYS:NZ	1.93	0.65
1:D:402:ASP:HA	1:D:578:MET:CE	2.27	0.65
1:B:402:ASP:HA	1:B:578:MET:CE	2.27	0.65
1:F:514:LEU:HB3	1:F:516:LYS:HZ2	1.60	0.64
1:C:449:ASN:HD22	1:C:451:ASN:H	1.43	0.64
1:D:556:CYS:SG	1:D:625:VAL:HG13	2.37	0.64
1:C:514:LEU:HD13	1:D:512:LYS:HA	1.79	0.64
1:C:449:ASN:HD22	1:C:449:ASN:C	2.01	0.63
1:E:454:LEU:H	1:E:454:LEU:HD22	1.64	0.63
1:B:409:LEU:O	1:B:413:VAL:HG12	1.98	0.63
1:D:602:ARG:HH11	1:D:602:ARG:HG3	1.64	0.63
1:B:412:MET:HE2	1:B:469:LEU:CB	2.29	0.63
1:D:454:LEU:HB2	1:E:453:PRO:HG2	1.79	0.63
1:E:454:LEU:HA	1:E:457:LEU:HB2	1.81	0.62
1:F:454:LEU:HD12	1:F:454:LEU:N	2.14	0.62
1:C:416:ILE:O	1:C:420:ARG:HG2	1.99	0.62
1:E:491:ILE:CD1	1:E:534:PRO:HD3	2.19	0.62
1:A:454:LEU:HA	1:A:457:LEU:HB2	1.81	0.62
1:E:454:LEU:N	1:E:454:LEU:HD22	2.14	0.62
1:A:454:LEU:HB2	1:B:453:PRO:HG2	1.81	0.62
1:A:412:MET:HE2	1:A:469:LEU:HB2	1.80	0.62
1:D:584:PRO:HG2	1:D:587:GLU:HG3	1.81	0.62
1:E:269:SER:H	1:E:323:ASN:ND2	1.87	0.62
1:E:498:ARG:HD3	1:E:540:ARG:NH2	2.15	0.61
1:E:556:CYS:SG	1:E:625:VAL:HG13	2.40	0.61
1:D:480:GLY:HA2	1:D:483:ARG:NH2	2.16	0.61
1:C:511:LYS:HE2	1:C:516:LYS:HG3	1.82	0.61
1:C:612:TYR:HA	1:C:615:MET:HE3	1.81	0.61
1:A:428:ILE:HD12	1:F:535:LYS:HE2	1.83	0.61
1:B:499:ASP:HB3	1:C:473:GLU:HG2	1.82	0.61
1:A:584:PRO:HG2	1:A:587:GLU:HG3	1.81	0.61
1:D:356:THR:OG1	1:D:359:GLN:HG3	2.01	0.61
1:D:397:LEU:HG	1:D:398:LEU:CD1	2.31	0.61
1:F:415:ASN:ND2	1:F:420:ARG:HH11	1.91	0.61
1:D:454:LEU:HA	1:D:457:LEU:HB2	1.82	0.61
1:A:412:MET:CE	1:A:523:PRO:HG2	2.29	0.60
1:D:285:VAL:HG21	1:D:338:GLN:NE2	2.16	0.60
1:B:397:LEU:C	1:B:398:LEU:HD12	2.22	0.60
1:D:500:TYR:CE2	1:D:507:VAL:HG11	2.35	0.60
1:E:412:MET:CE	1:E:523:PRO:HG2	2.31	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:415:ASN:ND2	1:D:420:ARG:HH11	1.97	0.60
1:F:415:ASN:ND2	1:F:420:ARG:HD2	2.17	0.60
1:B:448:LEU:HG	1:B:470:VAL:HG13	1.82	0.60
1:F:416:ILE:O	1:F:420:ARG:HG2	2.02	0.59
1:C:623:ILE:HG22	1:C:624:GLY:N	2.17	0.59
1:F:419:LYS:HB3	1:F:542:VAL:HG11	1.82	0.59
1:F:554:LYS:O	1:F:558:GLU:HG3	2.02	0.59
1:E:597:VAL:O	1:E:601:GLU:HG3	2.02	0.59
1:D:372:MET:HA	1:D:375:MET:HG2	1.84	0.59
1:A:454:LEU:N	1:A:454:LEU:HD12	2.18	0.59
1:D:550:LYS:HD3	1:D:552:TYR:OH	2.03	0.59
1:A:554:LYS:O	1:A:558:GLU:HG3	2.02	0.59
1:B:545:ILE:N	1:B:545:ILE:HD12	2.18	0.59
1:E:465:ILE:HD12	1:E:511:LYS:HG3	1.85	0.58
1:E:388:MET:HG3	1:E:607:PHE:CE1	2.37	0.58
1:E:456:ARG:HD2	1:E:456:ARG:N	2.19	0.58
1:F:483:ARG:HG3	1:F:483:ARG:HH11	1.68	0.58
1:A:588:PHE:HB3	1:A:592:ILE:CD1	2.34	0.58
1:E:287:LEU:HG	1:E:291:MET:CE	2.34	0.58
1:B:269:SER:OG	1:B:272:LEU:HD13	2.03	0.58
1:B:597:VAL:O	1:B:601:GLU:HG3	2.04	0.58
1:F:623:ILE:HG22	1:F:624:GLY:N	2.18	0.58
1:A:280:THR:O	1:A:280:THR:HG22	2.03	0.58
1:E:425:LYS:CE	1:E:530:GLU:HA	2.28	0.58
1:B:402:ASP:HA	1:B:578:MET:HE1	1.85	0.57
1:A:588:PHE:HB3	1:A:592:ILE:HD11	1.85	0.57
1:D:454:LEU:HD12	1:D:454:LEU:N	2.19	0.57
1:C:415:ASN:ND2	1:C:420:ARG:HD2	2.20	0.57
1:E:454:LEU:CB	1:F:453:PRO:HG2	2.34	0.57
1:D:481:GLU:H	1:D:481:GLU:CD	2.07	0.57
1:D:397:LEU:O	1:D:398:LEU:HD12	2.05	0.57
1:E:397:LEU:C	1:E:398:LEU:HD12	2.25	0.57
1:F:349:ARG:O	1:F:353:LEU:HD23	2.05	0.57
1:A:415:ASN:HD22	1:A:420:ARG:HG2	1.70	0.57
1:E:418:LYS:NZ	4:F:800:ATP:O2G	2.29	0.57
1:E:311:PRO:HG2	1:E:374:ILE:HD13	1.87	0.57
1:F:268:VAL:HG11	1:F:327:PHE:HA	1.87	0.57
1:A:513:HIS:O	1:A:514:LEU:HB2	2.04	0.56
1:D:398:LEU:HD13	1:D:401:MET:HE1	1.86	0.56
1:B:583:ARG:HD2	1:B:587:GLU:OE1	2.05	0.56
1:C:500:TYR:CZ	1:C:507:VAL:HG11	2.41	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:ASN:HD21	1:A:420:ARG:NH1	2.02	0.56
1:B:449:ASN:HD22	1:B:451:ASN:H	1.51	0.56
1:C:500:TYR:CE2	1:C:507:VAL:HG11	2.41	0.56
1:E:412:MET:HE1	1:E:523:PRO:HG2	1.87	0.56
1:C:454:LEU:N	1:C:454:LEU:HD12	2.17	0.56
1:D:397:LEU:HG	1:D:398:LEU:HD12	1.86	0.56
1:C:612:TYR:HA	1:C:615:MET:CE	2.35	0.56
1:B:483:ARG:HE	1:B:483:ARG:HA	1.69	0.56
1:B:416:ILE:O	1:B:420:ARG:HG2	2.06	0.56
1:A:535:LYS:HG3	1:A:536:THR:N	2.20	0.56
1:B:280:THR:O	1:B:280:THR:HG22	2.05	0.56
1:F:372:MET:HA	1:F:375:MET:HG2	1.88	0.56
1:A:412:MET:HE2	1:A:469:LEU:CB	2.36	0.56
1:D:507:VAL:HG13	5:E:846:HOH:O	2.06	0.56
1:E:357:ARG:NH2	5:E:816:HOH:O	2.38	0.56
1:A:458:ASN:HD22	1:B:456:ARG:HD3	1.71	0.55
1:A:350:VAL:CG2	1:B:291:MET:HE3	2.36	0.55
1:B:476:LYS:C	1:B:491:ILE:HD13	2.26	0.55
1:E:397:LEU:HG	1:E:398:LEU:HD12	1.88	0.55
1:A:481:GLU:HA	1:A:485:LEU:O	2.06	0.55
1:B:412:MET:CE	1:B:469:LEU:HB3	2.35	0.55
1:E:412:MET:HE2	1:E:469:LEU:CB	2.37	0.55
1:E:402:ASP:HA	1:E:578:MET:HE1	1.88	0.55
1:B:520:ILE:HG22	5:B:826:HOH:O	2.07	0.55
1:C:356:THR:OG1	1:C:359:GLN:HG3	2.06	0.55
1:A:397:LEU:HG	1:A:398:LEU:HD13	1.89	0.54
1:B:398:LEU:HD13	1:B:401:MET:CE	2.37	0.54
1:C:372:MET:HA	1:C:375:MET:HG2	1.88	0.54
1:F:425:LYS:HD3	1:F:528:MET:HG3	1.89	0.54
1:F:349:ARG:NH1	1:F:353:LEU:HD21	2.22	0.54
1:B:543:LYS:HG2	1:B:545:ILE:CD1	2.37	0.54
1:A:480:GLY:HA2	1:A:483:ARG:NH2	2.22	0.54
1:C:454:LEU:CD1	1:C:454:LEU:H	2.17	0.54
1:C:449:ASN:HD21	1:C:451:ASN:HB2	1.72	0.54
1:F:348:LYS:HZ3	1:F:348:LYS:HB2	1.71	0.54
1:F:301:MET:HE3	1:F:301:MET:H	1.72	0.54
1:B:306:ILE:HD12	1:B:307:LYS:N	2.23	0.54
1:B:450:VAL:HG22	1:B:450:VAL:O	2.08	0.54
1:C:623:ILE:HG22	1:C:624:GLY:H	1.72	0.53
1:B:356:THR:OG1	1:B:359:GLN:HG3	2.07	0.53
1:E:356:THR:OG1	1:E:359:GLN:HG3	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:ARG:O	1:B:375:MET:HG3	2.08	0.53
1:A:482:SER:OG	1:A:483:ARG:HD3	2.08	0.53
1:D:402:ASP:HA	1:D:578:MET:HE3	1.90	0.53
1:D:402:ASP:HA	1:D:578:MET:HE1	1.91	0.53
1:F:419:LYS:HA	1:F:542:VAL:CG1	2.36	0.53
1:F:454:LEU:HG	1:F:457:LEU:HD22	1.89	0.53
1:A:397:LEU:O	1:A:398:LEU:HD12	2.08	0.53
1:D:514:LEU:CB	1:E:514:LEU:HD11	2.38	0.53
1:E:397:LEU:O	1:E:398:LEU:HD12	2.09	0.53
1:B:517:ARG:HG2	1:B:517:ARG:NH1	2.23	0.53
1:C:583:ARG:HB3	1:C:587:GLU:OE1	2.09	0.53
1:F:268:VAL:HG13	1:F:326:ILE:HG22	1.91	0.53
1:F:420:ARG:HB3	1:F:523:PRO:HB3	1.90	0.53
1:B:415:ASN:ND2	1:B:420:ARG:HD2	2.24	0.53
1:C:349:ARG:NH1	1:C:353:LEU:HD11	2.24	0.53
1:C:508:ASN:HB3	1:C:515:ASN:HD21	1.74	0.52
1:E:303:LEU:CD2	1:E:306:ILE:HD11	2.40	0.52
1:A:268:VAL:HG22	1:A:326:ILE:HG22	1.91	0.52
1:B:454:LEU:HD12	1:B:454:LEU:N	2.22	0.52
1:C:444:GLY:O	1:C:469:LEU:HD22	2.10	0.52
1:C:415:ASN:HD21	1:C:420:ARG:NH1	1.99	0.52
1:D:500:TYR:CZ	1:D:507:VAL:CG1	2.90	0.52
1:D:507:VAL:HG12	1:D:508:ASN:N	2.23	0.52
1:E:454:LEU:CD1	1:E:457:LEU:HD22	2.36	0.52
1:F:475:VAL:HG22	1:F:528:MET:HB3	1.90	0.52
1:C:554:LYS:O	1:C:558:GLU:HG3	2.10	0.52
1:F:300:GLU:HB2	1:F:301:MET:HE2	1.92	0.52
1:A:480:GLY:HA2	1:A:483:ARG:CZ	2.40	0.52
1:D:418:LYS:HZ1	4:E:800:ATP:PG	2.32	0.52
1:D:454:LEU:CB	1:E:453:PRO:HG2	2.40	0.52
1:E:306:ILE:HG13	1:E:307:LYS:N	2.25	0.52
1:A:609:LEU:HB3	1:A:613:GLN:HE21	1.74	0.52
1:B:285:VAL:HG13	1:B:337:CYS:SG	2.49	0.52
1:C:270:TRP:CE2	1:C:336:ILE:HG12	2.45	0.52
1:A:543:LYS:NZ	1:A:545:ILE:HG12	2.25	0.51
1:C:303:LEU:HA	1:C:306:ILE:HG22	1.91	0.51
1:B:403:SER:HA	1:B:583:ARG:NH2	2.26	0.51
1:D:583:ARG:HD2	1:D:587:GLU:OE1	2.10	0.51
1:D:583:ARG:CD	1:D:587:GLU:OE1	2.58	0.51
1:D:602:ARG:HG3	1:D:602:ARG:NH1	2.25	0.51
1:F:300:GLU:HB2	1:F:301:MET:CE	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:LEU:HD22	1:A:516:LYS:HG3	1.93	0.51
1:A:609:LEU:HB3	1:A:613:GLN:NE2	2.25	0.51
1:C:308:LYS:O	1:C:309:GLU:HB2	2.10	0.51
1:D:507:VAL:CG1	1:D:508:ASN:N	2.73	0.51
1:B:415:ASN:ND2	1:B:420:ARG:HH11	2.02	0.51
1:E:609:LEU:O	1:E:613:GLN:HG3	2.11	0.51
1:F:454:LEU:H	1:F:454:LEU:CD1	2.24	0.51
1:A:453:PRO:HG2	1:F:454:LEU:CB	2.40	0.51
1:C:559:ARG:HH11	1:C:559:ARG:HG3	1.76	0.51
1:E:415:ASN:HD21	1:E:420:ARG:NH1	2.05	0.51
1:E:469:LEU:HD12	1:E:469:LEU:C	2.31	0.51
1:A:498:ARG:HB3	1:A:540:ARG:NH2	2.26	0.51
1:C:395:HIS:HD2	1:C:616:LYS:HZ1	1.57	0.51
1:E:311:PRO:CG	1:E:374:ILE:HD13	2.41	0.51
1:F:303:LEU:HA	1:F:306:ILE:HG22	1.93	0.51
1:D:388:MET:HE2	1:D:577:LEU:HD13	1.93	0.50
1:A:583:ARG:HD2	1:A:587:GLU:OE1	2.11	0.50
1:D:397:LEU:C	1:D:398:LEU:HD12	2.31	0.50
1:D:609:LEU:O	1:D:613:GLN:HG3	2.11	0.50
1:D:389:ALA:HB1	1:D:625:VAL:HG21	1.92	0.50
1:F:268:VAL:CG1	1:F:326:ILE:HG22	2.41	0.50
1:A:383:ASP:HB3	1:A:386:GLU:HG3	1.93	0.50
1:B:303:LEU:HA	1:B:306:ILE:HG13	1.93	0.50
1:E:403:SER:OG	1:E:583:ARG:NH2	2.44	0.50
1:E:418:LYS:HZ1	4:F:800:ATP:PG	2.34	0.50
1:A:270:TRP:CE2	1:A:336:ILE:HG12	2.47	0.50
1:B:288:LEU:HD23	1:B:337:CYS:HB2	1.93	0.50
1:B:415:ASN:HD21	1:B:420:ARG:NH1	2.01	0.50
1:B:561:GLU:CD	1:B:561:GLU:H	2.15	0.50
1:B:412:MET:CE	1:B:469:LEU:CB	2.89	0.50
1:B:483:ARG:NE	1:B:483:ARG:HA	2.27	0.50
1:E:520:ILE:HG22	5:E:817:HOH:O	2.11	0.50
1:B:454:LEU:CD1	1:B:454:LEU:H	2.22	0.50
1:A:593:GLN:O	1:A:597:VAL:HG23	2.11	0.50
1:D:353:LEU:HD21	1:D:517:ARG:HH22	1.77	0.50
1:E:402:ASP:HA	1:E:578:MET:HE3	1.92	0.50
1:C:418:LYS:HE3	1:C:540:ARG:NH1	2.26	0.49
1:F:511:LYS:O	1:F:512:LYS:HB3	2.12	0.49
1:D:623:ILE:HG13	1:D:623:ILE:O	2.12	0.49
1:F:389:ALA:HB1	1:F:625:VAL:HG21	1.94	0.49
1:A:454:LEU:H	1:A:454:LEU:CD1	2.23	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:ARG:N	1:A:483:ARG:HD3	2.27	0.49
1:B:543:LYS:HG2	1:B:545:ILE:HD11	1.92	0.49
1:D:270:TRP:CE2	1:D:336:ILE:HG12	2.46	0.49
1:E:412:MET:HE2	1:E:469:LEU:HB2	1.92	0.49
1:F:469:LEU:HD12	1:F:469:LEU:C	2.33	0.49
1:F:483:ARG:NH1	1:F:483:ARG:HG3	2.28	0.49
1:F:623:ILE:HG22	1:F:624:GLY:H	1.76	0.49
1:D:415:ASN:HD22	1:D:420:ARG:HG2	1.76	0.49
1:A:412:MET:CE	1:A:469:LEU:CB	2.91	0.49
1:D:469:LEU:C	1:D:469:LEU:HD12	2.32	0.49
1:C:389:ALA:HB1	1:C:625:VAL:HG11	1.94	0.49
1:C:507:VAL:CG1	1:C:508:ASN:N	2.76	0.49
1:E:511:LYS:O	1:E:512:LYS:HB2	2.12	0.49
1:A:389:ALA:HB1	1:A:625:VAL:HG21	1.94	0.48
1:C:420:ARG:HB3	1:C:523:PRO:HB3	1.95	0.48
1:A:412:MET:CE	1:A:469:LEU:HB3	2.43	0.48
1:A:583:ARG:CD	1:A:587:GLU:OE1	2.61	0.48
1:B:397:LEU:O	1:B:398:LEU:HD12	2.13	0.48
1:C:491:ILE:HD11	1:C:528:MET:HE1	1.95	0.48
1:F:456:ARG:HH11	1:F:456:ARG:HG3	1.79	0.48
1:C:351:ASP:HB3	1:C:355:LEU:HD12	1.95	0.48
1:E:511:LYS:HD3	1:E:515:ASN:HB3	1.95	0.48
1:E:502:ASP:OD1	1:E:540:ARG:HD2	2.13	0.48
1:A:372:MET:HA	1:A:375:MET:HG2	1.95	0.48
1:F:556:CYS:SG	1:F:625:VAL:HG13	2.54	0.48
1:B:403:SER:OG	1:B:583:ARG:NH2	2.46	0.48
1:D:597:VAL:O	1:D:601:GLU:HG3	2.13	0.48
1:D:385:GLU:HA	1:D:607:PHE:CZ	2.48	0.48
1:B:398:LEU:HD13	1:B:401:MET:HE1	1.94	0.48
1:C:418:LYS:NZ	4:D:800:ATP:O2G	2.37	0.48
1:E:287:LEU:HG	1:E:291:MET:HE2	1.96	0.48
1:A:567:ARG:NH1	1:A:567:ARG:HG3	2.29	0.47
1:A:350:VAL:HG21	1:B:291:MET:HE3	1.95	0.47
1:C:419:LYS:HA	1:C:542:VAL:HG22	1.95	0.47
1:A:415:ASN:ND2	1:A:420:ARG:HG2	2.29	0.47
1:E:410:LYS:HA	1:E:413:VAL:CG1	2.44	0.47
1:A:525:ILE:HG22	1:A:526:VAL:N	2.29	0.47
1:E:454:LEU:CD2	1:E:454:LEU:H	2.26	0.47
1:D:423:LEU:HD11	1:D:528:MET:HE3	1.97	0.47
1:D:418:LYS:NZ	4:E:800:ATP:PG	2.88	0.47
1:F:550:LYS:HD2	1:F:553:LEU:HD11	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:ILE:C	1:B:306:ILE:HD12	2.35	0.47
1:D:418:LYS:NZ	4:E:800:ATP:O2G	2.30	0.47
1:F:480:GLY:HA2	1:F:483:ARG:NH2	2.29	0.47
1:F:525:ILE:HG22	1:F:526:VAL:N	2.29	0.47
1:B:419:LYS:HA	1:B:542:VAL:HG13	1.97	0.47
1:C:349:ARG:HD2	1:C:517:ARG:CZ	2.44	0.47
1:C:458:ASN:HB2	1:D:456:ARG:HE	1.80	0.47
1:E:412:MET:CE	1:E:469:LEU:CB	2.93	0.47
1:F:402:ASP:HA	1:F:578:MET:CE	2.45	0.47
1:E:418:LYS:NZ	4:F:800:ATP:PG	2.88	0.47
1:B:269:SER:H	1:B:323:ASN:ND2	1.96	0.47
1:E:512:LYS:C	1:E:514:LEU:H	2.17	0.47
1:D:415:ASN:ND2	1:D:420:ARG:HG2	2.30	0.47
1:A:550:LYS:HD3	1:A:552:TYR:OH	2.15	0.47
1:B:357:ARG:NH2	5:B:802:HOH:O	2.47	0.47
1:B:412:MET:HE1	1:B:523:PRO:HG2	1.93	0.47
1:C:511:LYS:CE	1:C:516:LYS:HG3	2.45	0.47
1:B:469:LEU:HD12	1:B:469:LEU:C	2.36	0.47
1:B:583:ARG:CD	1:B:587:GLU:OE1	2.63	0.47
1:D:501:LEU:HB2	1:D:540:ARG:HG2	1.97	0.47
1:D:425:LYS:CE	1:D:530:GLU:HA	2.41	0.47
1:F:465:ILE:HG23	1:F:517:ARG:HD2	1.97	0.47
1:A:398:LEU:HB2	1:A:401:MET:HE2	1.96	0.46
1:F:491:ILE:CD1	1:F:528:MET:HE2	2.45	0.46
1:A:415:ASN:ND2	1:A:420:ARG:HH11	2.04	0.46
1:B:311:PRO:HG2	1:B:374:ILE:HD13	1.97	0.46
1:F:293:LEU:O	1:F:296:GLN:HG2	2.15	0.46
1:F:419:LYS:CB	1:F:542:VAL:HG11	2.45	0.46
1:D:454:LEU:H	1:D:454:LEU:CD1	2.26	0.46
1:C:513:HIS:HB3	1:D:513:HIS:HD2	1.81	0.46
1:F:270:TRP:CE2	1:F:336:ILE:HG12	2.50	0.46
1:F:619:VAL:HG22	1:F:625:VAL:HG12	1.97	0.46
1:D:405:VAL:HG21	1:D:578:MET:HE2	1.96	0.46
1:D:514:LEU:HD12	1:D:514:LEU:O	2.15	0.46
1:B:459:PHE:CD2	1:B:459:PHE:N	2.84	0.46
1:D:550:LYS:HD3	1:D:552:TYR:CZ	2.51	0.46
1:F:361:LEU:HD11	1:F:409:LEU:HD22	1.97	0.46
1:F:514:LEU:HB3	1:F:516:LYS:HZ1	1.81	0.46
1:B:410:LYS:HA	1:B:413:VAL:CG1	2.46	0.45
1:B:448:LEU:HD22	1:B:463:VAL:CG2	2.47	0.45
1:C:349:ARG:CZ	1:C:517:ARG:HD2	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:465:ILE:HG23	1:E:517:ARG:HD3	1.99	0.45
1:E:481:GLU:H	1:E:481:GLU:CD	2.20	0.45
1:B:353:LEU:HD21	1:B:517:ARG:HH21	1.80	0.45
1:B:514:LEU:N	1:B:514:LEU:HD23	2.31	0.45
1:C:415:ASN:ND2	1:C:420:ARG:HH11	2.00	0.45
1:D:400:LYS:HB3	1:D:400:LYS:NZ	2.31	0.45
1:D:525:ILE:HG22	1:D:526:VAL:N	2.29	0.45
1:C:444:GLY:O	1:C:469:LEU:CD2	2.65	0.45
1:A:476:LYS:HG2	1:A:488:GLY:HA3	1.98	0.45
1:B:334:LYS:HA	1:B:337:CYS:SG	2.57	0.45
1:E:269:SER:OG	1:E:272:LEU:HD13	2.15	0.45
1:F:548:ARG:HH11	1:F:548:ARG:HG2	1.82	0.45
1:F:590:GLN:HG2	1:F:591:SER:N	2.32	0.45
1:D:605:LYS:O	1:D:605:LYS:HG2	2.16	0.45
1:E:529:ASN:O	1:E:530:GLU:HB3	2.17	0.45
1:E:412:MET:HE2	1:E:469:LEU:HD22	1.99	0.45
1:C:349:ARG:CD	1:C:517:ARG:CZ	2.95	0.44
1:A:602:ARG:HH11	1:A:602:ARG:HG3	1.82	0.44
1:A:430:SER:N	4:A:800:ATP:O1B	2.50	0.44
1:B:525:ILE:HG22	1:B:526:VAL:N	2.32	0.44
1:B:270:TRP:CE2	1:B:336:ILE:HG12	2.51	0.44
1:C:516:LYS:O	1:C:517:ARG:HD3	2.17	0.44
1:F:550:LYS:HD3	1:F:552:TYR:CZ	2.52	0.44
1:A:555:HIS:O	1:A:559:ARG:HG3	2.18	0.44
1:C:302:CYS:SG	1:C:304:LYS:HB2	2.57	0.44
1:C:559:ARG:HG3	1:C:559:ARG:NH1	2.32	0.44
1:D:465:ILE:HG23	1:D:517:ARG:HD3	1.99	0.44
1:D:511:LYS:O	1:D:512:LYS:HB2	2.17	0.44
1:D:517:ARG:HG3	1:D:517:ARG:HH11	1.83	0.44
1:C:561:GLU:N	1:C:561:GLU:CD	2.71	0.44
1:D:271:LYS:HB3	1:D:271:LYS:NZ	2.32	0.44
1:C:417:PRO:HG2	1:D:570:GLN:NE2	2.33	0.44
1:E:412:MET:CE	1:E:469:LEU:HB3	2.48	0.44
1:F:625:VAL:HG23	1:F:626:LEU:HG	1.99	0.44
1:C:265:THR:HG22	1:C:265:THR:O	2.17	0.44
1:A:514:LEU:HD23	1:A:515:ASN:N	2.33	0.44
1:A:597:VAL:O	1:A:601:GLU:HG3	2.17	0.44
1:C:512:LYS:O	1:C:512:LYS:HG2	2.18	0.44
1:F:559:ARG:HG3	1:F:559:ARG:HH11	1.83	0.44
1:A:388:MET:HB3	1:A:615:MET:HE1	1.99	0.43
1:F:456:ARG:NH1	1:F:456:ARG:HG3	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:CYS:SG	1:A:625:VAL:HG13	2.57	0.43
1:F:405:VAL:HG21	1:F:578:MET:CE	2.48	0.43
1:B:372:MET:HG3	1:B:573:ILE:HD12	2.00	0.43
1:F:550:LYS:HD3	1:F:552:TYR:OH	2.18	0.43
1:A:567:ARG:HH11	1:A:567:ARG:HG3	1.83	0.43
1:C:525:ILE:HG22	1:C:526:VAL:N	2.34	0.43
1:D:510:GLU:O	1:D:510:GLU:HG3	2.19	0.43
1:C:511:LYS:HE2	1:C:516:LYS:CB	2.48	0.43
1:E:371:ARG:O	1:E:375:MET:HG3	2.18	0.43
1:F:583:ARG:HA	1:F:584:PRO:HD3	1.84	0.43
1:B:410:LYS:HA	1:B:413:VAL:HG12	2.00	0.43
1:B:477:GLY:N	1:B:491:ILE:HD13	2.34	0.43
1:B:556:CYS:SG	1:B:625:VAL:CG1	3.04	0.43
5:A:801:HOH:O	1:B:567:ARG:HD3	2.19	0.43
1:C:458:ASN:CG	1:D:456:ARG:HD3	2.39	0.43
1:E:451:ASN:ND2	1:E:476:LYS:H	2.12	0.43
1:B:419:LYS:HB3	1:B:542:VAL:HG11	2.01	0.43
1:C:303:LEU:HD23	1:C:303:LEU:N	2.31	0.43
1:C:481:GLU:H	1:C:481:GLU:CD	2.21	0.43
1:A:491:ILE:CD1	1:A:528:MET:HE1	2.49	0.43
1:A:505:VAL:HG12	1:A:506:LYS:N	2.34	0.43
1:B:449:ASN:ND2	1:B:449:ASN:C	2.69	0.43
1:B:511:LYS:O	1:B:512:LYS:HB2	2.19	0.43
1:B:280:THR:O	1:B:280:THR:CG2	2.67	0.42
1:C:517:ARG:HH22	1:D:286:LEU:CD1	2.27	0.42
1:E:412:MET:CE	1:E:469:LEU:HB2	2.48	0.42
1:E:548:ARG:HA	1:E:549:PRO:HD3	1.94	0.42
1:F:278:MET:CE	1:F:343:THR:HG22	2.49	0.42
1:F:278:MET:HE1	5:F:855:HOH:O	2.18	0.42
1:B:361:LEU:HD22	1:B:365:PHE:CE1	2.54	0.42
1:B:567:ARG:HG3	1:B:567:ARG:NH1	2.34	0.42
1:E:499:ASP:HB3	1:F:473:GLU:HG2	2.00	0.42
1:A:415:ASN:O	1:B:567:ARG:NH2	2.53	0.42
1:C:416:ILE:O	1:C:420:ARG:CG	2.67	0.42
1:E:270:TRP:CE2	1:E:336:ILE:HG12	2.54	0.42
1:F:556:CYS:SG	1:F:625:VAL:CG1	3.08	0.42
1:F:405:VAL:HG21	1:F:578:MET:HE2	2.00	0.42
1:A:458:ASN:HB2	1:B:456:ARG:HE	1.85	0.42
1:B:481:GLU:H	1:B:481:GLU:CD	2.23	0.42
1:C:511:LYS:HE2	1:C:516:LYS:CG	2.49	0.42
1:F:348:LYS:NZ	1:F:348:LYS:CB	2.81	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:ALA:C	1:B:448:LEU:HD23	2.40	0.42
1:A:415:ASN:HB3	1:B:567:ARG:NH2	2.34	0.42
1:D:372:MET:HG3	1:D:573:ILE:HD12	2.02	0.42
1:E:556:CYS:SG	1:E:625:VAL:CG1	3.07	0.42
1:A:514:LEU:HB3	1:A:516:LYS:NZ	2.35	0.42
1:E:398:LEU:HD13	1:E:401:MET:HE1	2.01	0.42
1:B:268:VAL:HG22	1:B:326:ILE:HG22	2.02	0.42
1:D:512:LYS:O	1:D:514:LEU:HG	2.20	0.42
1:F:403:SER:HA	1:F:583:ARG:NH2	2.35	0.42
1:C:454:LEU:HB2	1:D:453:PRO:CG	2.47	0.42
1:E:583:ARG:HA	1:E:584:PRO:HD3	1.82	0.42
1:F:305:CYS:O	1:F:308:LYS:HD3	2.18	0.42
1:A:516:LYS:HB2	5:A:876:HOH:O	2.19	0.42
1:B:448:LEU:HG	1:B:470:VAL:CG1	2.49	0.42
1:C:455:ASP:HA	1:D:456:ARG:HH12	1.85	0.42
1:C:510:GLU:HA	1:C:515:ASN:HA	2.01	0.42
1:C:585:VAL:HG13	1:C:600:LYS:HE3	2.01	0.42
1:D:385:GLU:HA	1:D:607:PHE:CE2	2.55	0.42
1:E:550:LYS:HB2	1:E:553:LEU:HD12	2.02	0.42
1:C:564:LEU:HD21	1:C:569:ILE:HD11	2.02	0.41
1:E:287:LEU:HG	1:E:291:MET:HE1	2.02	0.41
1:C:402:ASP:HA	1:C:578:MET:HE1	1.99	0.41
1:C:498:ARG:HD3	1:C:540:ARG:NH2	2.35	0.41
1:E:459:PHE:CE2	1:E:512:LYS:HD3	2.56	0.41
1:E:625:VAL:HG23	1:E:626:LEU:HG	2.01	0.41
1:F:625:VAL:HG23	1:F:626:LEU:N	2.34	0.41
1:A:514:LEU:HD22	1:A:516:LYS:CG	2.51	0.41
1:A:465:ILE:CG2	1:A:517:ARG:HG3	2.50	0.41
1:A:612:TYR:HA	1:A:615:MET:CE	2.47	0.41
1:A:403:SER:OG	1:A:583:ARG:NH2	2.53	0.41
1:B:388:MET:HG3	1:B:607:PHE:CE1	2.54	0.41
1:A:454:LEU:CB	1:B:453:PRO:HG2	2.46	0.41
1:C:446:LYS:HG3	1:C:463:VAL:HG12	2.02	0.41
1:B:420:ARG:HB3	1:B:523:PRO:HB3	2.01	0.41
1:C:458:ASN:HD21	1:D:452:LEU:HD13	1.85	0.41
1:A:284:ASP:HB3	1:A:287:LEU:HB3	2.03	0.41
1:C:423:LEU:HD21	1:C:528:MET:HE3	2.02	0.41
1:F:583:ARG:CD	1:F:587:GLU:OE1	2.62	0.41
1:A:476:LYS:HG2	1:A:488:GLY:N	2.36	0.41
1:B:558:GLU:O	1:B:561:GLU:OE1	2.39	0.41
1:A:280:THR:CG2	1:A:280:THR:O	2.69	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:475:VAL:O	1:F:475:VAL:HG23	2.20	0.41
1:A:286:LEU:HB2	1:F:517:ARG:HH22	1.84	0.41
1:E:515:ASN:HD22	1:E:516:LYS:N	2.19	0.41
1:B:418:LYS:HZ1	4:C:800:ATP:PG	2.43	0.41
1:B:528:MET:HE3	1:B:531:TYR:HB2	2.03	0.41
1:B:619:VAL:HG22	1:B:625:VAL:HG12	2.03	0.41
1:E:271:LYS:NZ	1:E:271:LYS:HB3	2.36	0.41
1:F:535:LYS:HE3	1:F:535:LYS:HB2	1.83	0.41
1:A:615:MET:O	1:A:619:VAL:HG23	2.20	0.41
1:B:398:LEU:HD13	1:B:401:MET:HE2	2.02	0.41
1:C:502:ASP:OD1	1:C:540:ARG:HD2	2.21	0.41
1:D:403:SER:OG	1:D:583:ARG:NH2	2.54	0.41
1:E:550:LYS:HD3	1:E:552:TYR:OH	2.21	0.41
1:B:543:LYS:HG2	1:B:545:ILE:HD12	2.03	0.40
1:E:616:LYS:HE3	1:E:616:LYS:HB3	1.89	0.40
1:D:284:ASP:HB3	1:D:287:LEU:HB3	2.03	0.40
1:A:398:LEU:HB2	1:A:401:MET:CE	2.50	0.40
1:B:475:VAL:CG1	1:B:491:ILE:HD12	2.36	0.40
1:C:556:CYS:SG	1:C:625:VAL:HG22	2.60	0.40
1:A:525:ILE:CG2	1:A:526:VAL:N	2.84	0.40
1:A:592:ILE:HD12	1:A:592:ILE:C	2.42	0.40
1:D:550:LYS:HB2	1:D:553:LEU:HD12	2.03	0.40
1:A:480:GLY:C	1:A:482:SER:H	2.25	0.40
1:A:415:ASN:HB3	1:B:567:ARG:HH21	1.86	0.40
1:C:344:VAL:O	1:C:348:LYS:HG2	2.21	0.40
1:C:449:ASN:C	1:C:449:ASN:ND2	2.73	0.40
1:C:491:ILE:CD1	1:C:528:MET:HE1	2.52	0.40
1:D:567:ARG:HA	5:D:820:HOH:O	2.21	0.40
1:D:567:ARG:NH1	1:D:567:ARG:HG3	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	360/377 (96%)	348 (97%)	10 (3%)	2 (1%)	25	13
1	B	360/377 (96%)	347 (96%)	12 (3%)	1 (0%)	41	32
1	C	361/377 (96%)	349 (97%)	12 (3%)	0	100	100
1	D	360/377 (96%)	349 (97%)	8 (2%)	3 (1%)	19	9
1	E	360/377 (96%)	350 (97%)	10 (3%)	0	100	100
1	F	361/377 (96%)	351 (97%)	9 (2%)	1 (0%)	41	32
All	All	2162/2262 (96%)	2094 (97%)	61 (3%)	7 (0%)	41	32

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	512	LYS
1	D	624	GLY
1	A	514	LEU
1	B	514	LEU
1	A	480	GLY
1	F	512	LYS
1	D	480	GLY

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	323/336 (96%)	313 (97%)	10 (3%)	40	26
1	B	322/336 (96%)	313 (97%)	9 (3%)	43	29
1	C	324/336 (96%)	312 (96%)	12 (4%)	34	19
1	D	323/336 (96%)	311 (96%)	12 (4%)	34	19
1	E	322/336 (96%)	309 (96%)	13 (4%)	31	16
1	F	324/336 (96%)	313 (97%)	11 (3%)	37	22
All	All	1938/2016 (96%)	1871 (96%)	67 (4%)	36	21

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

Mol	Chain	Res	Type
1	A	288	LEU
1	A	338	GLN
1	A	349	ARG
1	A	361	LEU
1	A	440	LEU
1	A	459	PHE
1	A	474	ASP
1	A	483	ARG
1	A	517	ARG
1	A	602	ARG
1	B	287	LEU
1	B	361	LEU
1	B	449	ASN
1	B	515	ASN
1	B	516	LYS
1	B	542	VAL
1	B	551	ASP
1	B	570	GLN
1	B	603	LEU
1	C	307	LYS
1	C	329	ASP
1	C	349	ARG
1	C	361	LEU
1	C	410	LYS
1	C	423	LEU
1	C	449	ASN
1	C	469	LEU
1	C	474	ASP
1	C	542	VAL
1	C	561	GLU
1	C	570	GLN
1	D	349	ARG
1	D	361	LEU
1	D	474	ASP
1	D	481	GLU
1	D	502	ASP
1	D	504	SER
1	D	509	LEU
1	D	540	ARG
1	D	557	LEU
1	D	602	ARG
1	D	603	LEU
1	D	627	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	317	HIS
1	E	318	GLU
1	E	338	GLN
1	E	361	LEU
1	E	420	ARG
1	E	456	ARG
1	E	474	ASP
1	E	513	HIS
1	E	515	ASN
1	E	542	VAL
1	E	551	ASP
1	E	590	GLN
1	E	603	LEU
1	F	301	MET
1	F	338	GLN
1	F	348	LYS
1	F	361	LEU
1	F	440	LEU
1	F	455	ASP
1	F	456	ARG
1	F	542	VAL
1	F	570	GLN
1	F	590	GLN
1	F	603	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	267	GLN
1	A	296	GLN
1	A	333	GLN
1	A	415	ASN
1	A	458	ASN
1	A	467	GLN
1	A	508	ASN
1	A	544	GLN
1	A	613	GLN
1	B	323	ASN
1	B	333	GLN
1	B	338	GLN
1	B	415	ASN
1	B	449	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	493	ASN
1	B	515	ASN
1	B	590	GLN
1	B	613	GLN
1	C	267	GLN
1	C	310	GLN
1	C	333	GLN
1	C	338	GLN
1	C	395	HIS
1	C	415	ASN
1	C	449	ASN
1	C	458	ASN
1	C	515	ASN
1	C	544	GLN
1	C	613	GLN
1	D	333	GLN
1	D	338	GLN
1	D	415	ASN
1	D	467	GLN
1	D	508	ASN
1	D	544	GLN
1	D	570	GLN
1	E	296	GLN
1	E	317	HIS
1	E	323	ASN
1	E	333	GLN
1	E	354	GLN
1	E	415	ASN
1	E	451	ASN
1	E	489	GLN
1	E	492	ASN
1	E	493	ASN
1	E	513	HIS
1	E	519	GLN
1	F	310	GLN
1	F	333	GLN
1	F	338	GLN
1	F	395	HIS
1	F	415	ASN
1	F	544	GLN
1	F	590	GLN
1	F	613	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ATP	C	800	3	26,33,33	1.37	4 (15%)	31,52,52	1.79	5 (16%)
4	ATP	B	800	3	26,33,33	1.44	3 (11%)	31,52,52	2.38	9 (29%)
4	ATP	F	800	3	26,33,33	1.39	5 (19%)	31,52,52	1.80	6 (19%)
4	ATP	D	800	3	26,33,33	1.36	4 (15%)	31,52,52	1.84	6 (19%)
4	ATP	A	800	3	26,33,33	1.37	3 (11%)	31,52,52	2.38	8 (25%)
4	ATP	E	800	3	26,33,33	1.39	4 (15%)	31,52,52	1.78	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	C	800	3	-	2/18/38/38	0/3/3/3
4	ATP	B	800	3	-	5/18/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	F	800	3	-	3/18/38/38	0/3/3/3
4	ATP	D	800	3	-	4/18/38/38	0/3/3/3
4	ATP	A	800	3	-	4/18/38/38	0/3/3/3
4	ATP	E	800	3	-	3/18/38/38	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	800	ATP	C2-N3	4.21	1.38	1.32
4	E	800	ATP	C2-N3	4.09	1.38	1.32
4	A	800	ATP	C2-N3	4.06	1.38	1.32
4	D	800	ATP	C2-N3	3.98	1.38	1.32
4	F	800	ATP	C2-N3	3.97	1.38	1.32
4	C	800	ATP	C2-N3	3.83	1.38	1.32
4	D	800	ATP	O4'-C1'	3.22	1.45	1.41
4	B	800	ATP	O4'-C1'	3.22	1.45	1.41
4	C	800	ATP	O4'-C1'	3.11	1.45	1.41
4	E	800	ATP	O4'-C1'	2.97	1.45	1.41
4	F	800	ATP	O4'-C1'	2.80	1.45	1.41
4	A	800	ATP	O4'-C1'	2.79	1.45	1.41
4	F	800	ATP	C2-N1	2.50	1.38	1.33
4	A	800	ATP	C2-N1	2.42	1.38	1.33
4	C	800	ATP	C2-N1	2.38	1.38	1.33
4	B	800	ATP	C2-N1	2.36	1.38	1.33
4	F	800	ATP	C4-N3	2.29	1.38	1.35
4	D	800	ATP	C2-N1	2.23	1.38	1.33
4	E	800	ATP	C2-N1	2.17	1.37	1.33
4	F	800	ATP	C2'-C1'	-2.14	1.50	1.53
4	C	800	ATP	C2'-C1'	-2.06	1.50	1.53
4	E	800	ATP	C2'-C1'	-2.04	1.50	1.53
4	D	800	ATP	C2'-C1'	-2.01	1.50	1.53

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	800	ATP	O5'-PA-O1A	-6.75	82.70	109.07
4	B	800	ATP	O5'-PA-O1A	-6.63	83.15	109.07
4	F	800	ATP	N3-C2-N1	-5.63	119.88	128.68
4	C	800	ATP	N3-C2-N1	-5.53	120.03	128.68
4	A	800	ATP	N3-C2-N1	-5.46	120.14	128.68
4	B	800	ATP	N3-C2-N1	-5.42	120.21	128.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	800	ATP	N3-C2-N1	-5.39	120.25	128.68
4	E	800	ATP	N3-C2-N1	-5.36	120.31	128.68
4	A	800	ATP	O2A-PA-O5'	-4.50	86.87	107.75
4	B	800	ATP	O2A-PA-O5'	-4.45	87.10	107.75
4	D	800	ATP	C4-C5-N7	-4.12	105.11	109.40
4	D	800	ATP	C5-C6-N6	4.04	126.48	120.35
4	E	800	ATP	C4-C5-N7	-4.01	105.22	109.40
4	C	800	ATP	C4-C5-N7	-3.91	105.33	109.40
4	E	800	ATP	C5-C6-N6	3.89	126.27	120.35
4	F	800	ATP	C4-C5-N7	-3.84	105.39	109.40
4	A	800	ATP	C4-C5-N7	-3.79	105.45	109.40
4	B	800	ATP	C4-C5-N7	-3.75	105.49	109.40
4	C	800	ATP	C5-C6-N6	3.72	126.00	120.35
4	F	800	ATP	C5-C6-N6	3.69	125.96	120.35
4	A	800	ATP	C5-C6-N6	3.58	125.79	120.35
4	B	800	ATP	C5-C6-N6	3.56	125.76	120.35
4	B	800	ATP	O2A-PA-O1A	3.22	128.18	112.24
4	A	800	ATP	O2A-PA-O1A	3.16	127.84	112.24
4	D	800	ATP	O2B-PB-O1B	2.79	126.01	112.24
4	C	800	ATP	O2B-PB-O1B	2.66	125.42	112.24
4	A	800	ATP	O2B-PB-O1B	2.58	124.97	112.24
4	B	800	ATP	O2B-PB-O1B	2.57	124.96	112.24
4	E	800	ATP	O2B-PB-O1B	2.56	124.88	112.24
4	C	800	ATP	O2G-PG-O3B	2.56	113.20	104.64
4	D	800	ATP	O2G-PG-O3B	2.46	112.89	104.64
4	E	800	ATP	O2G-PG-O3B	2.46	112.87	104.64
4	F	800	ATP	O2G-PG-O3B	2.42	112.74	104.64
4	F	800	ATP	O2B-PB-O1B	2.41	124.14	112.24
4	B	800	ATP	O2G-PG-O3B	2.34	112.47	104.64
4	A	800	ATP	O2G-PG-O3B	2.32	112.42	104.64
4	D	800	ATP	N6-C6-N1	-2.08	114.25	118.57
4	F	800	ATP	PB-O3B-PG	-2.08	125.70	132.83
4	E	800	ATP	PB-O3B-PG	-2.05	125.80	132.83
4	B	800	ATP	C5'-C4'-C3'	-2.02	107.61	115.18

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	800	ATP	C5'-O5'-PA-O2A
4	B	800	ATP	C3'-C4'-C5'-O5'
4	B	800	ATP	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

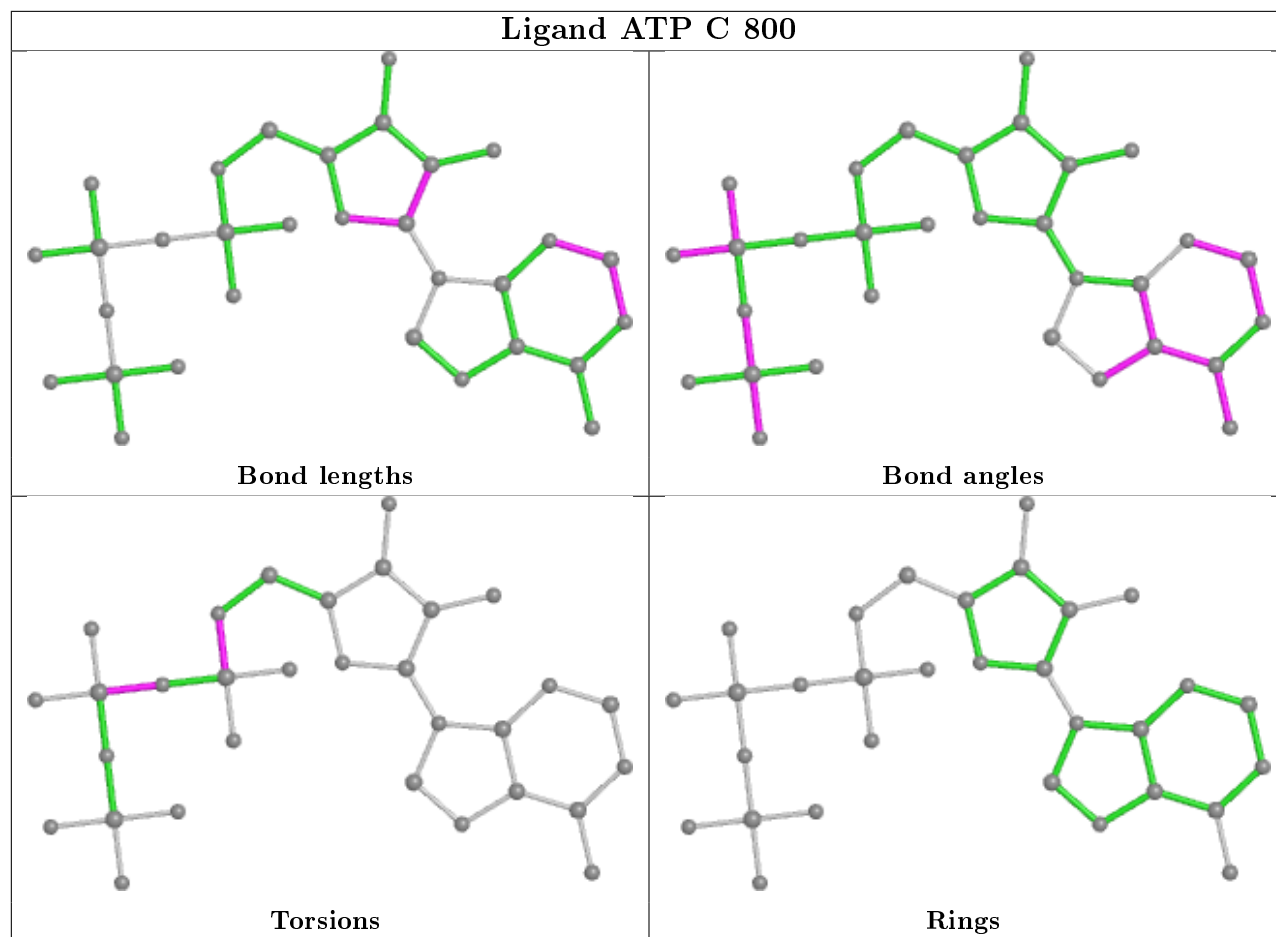
Mol	Chain	Res	Type	Atoms
4	F	800	ATP	C5'-O5'-PA-O3A
4	D	800	ATP	C5'-O5'-PA-O3A
4	E	800	ATP	C5'-O5'-PA-O3A
4	A	800	ATP	C3'-C4'-C5'-O5'
4	D	800	ATP	C5'-O5'-PA-O1A
4	A	800	ATP	O4'-C4'-C5'-O5'
4	F	800	ATP	PA-O3A-PB-O2B
4	C	800	ATP	PA-O3A-PB-O2B
4	D	800	ATP	PA-O3A-PB-O2B
4	B	800	ATP	PA-O3A-PB-O2B
4	A	800	ATP	PA-O3A-PB-O2B
4	E	800	ATP	PA-O3A-PB-O2B
4	C	800	ATP	C5'-O5'-PA-O3A
4	B	800	ATP	PB-O3A-PA-O1A
4	F	800	ATP	C5'-O5'-PA-O1A
4	B	800	ATP	C5'-O5'-PA-O1A
4	A	800	ATP	C5'-O5'-PA-O1A
4	E	800	ATP	C5'-O5'-PA-O1A

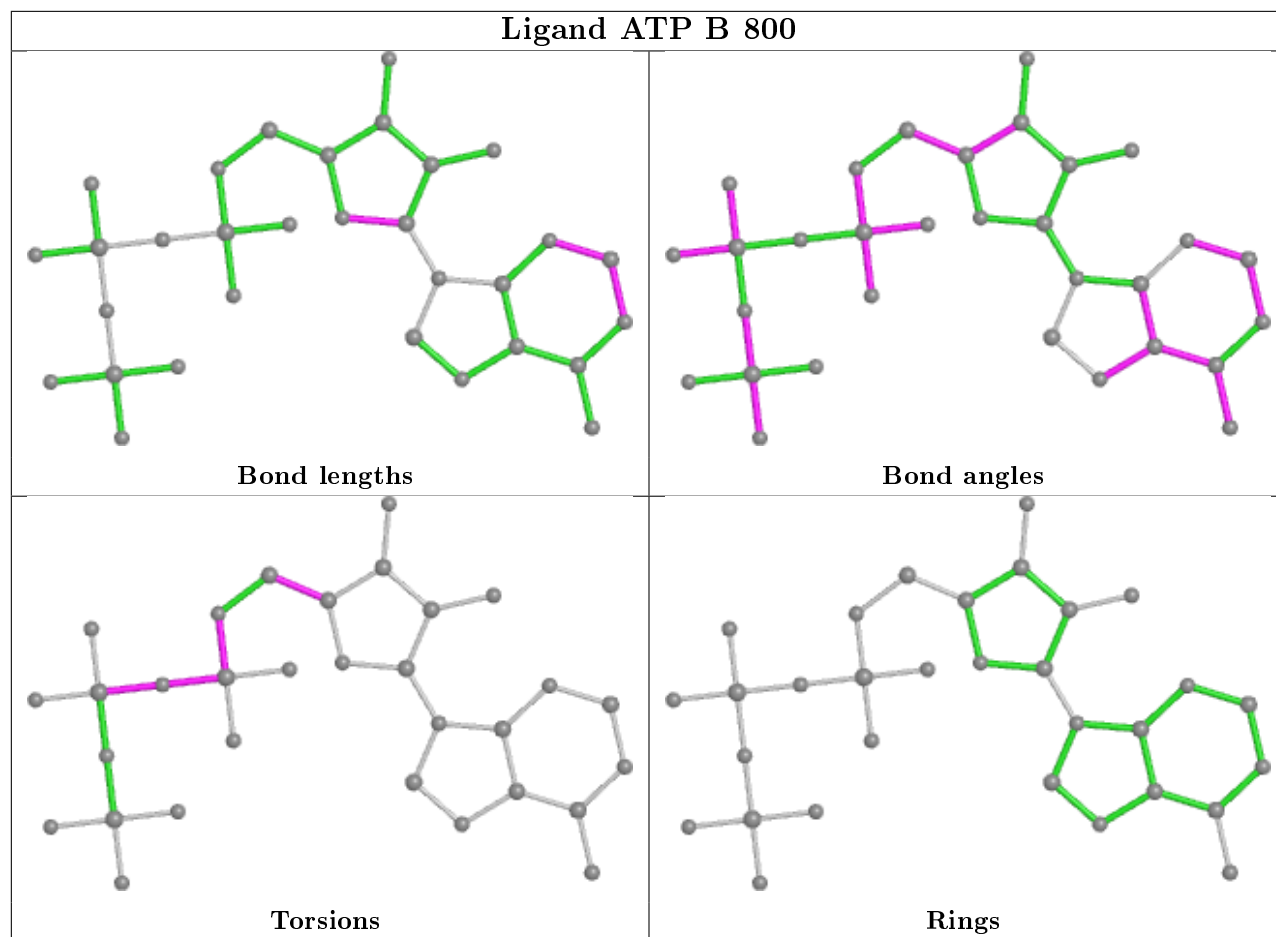
There are no ring outliers.

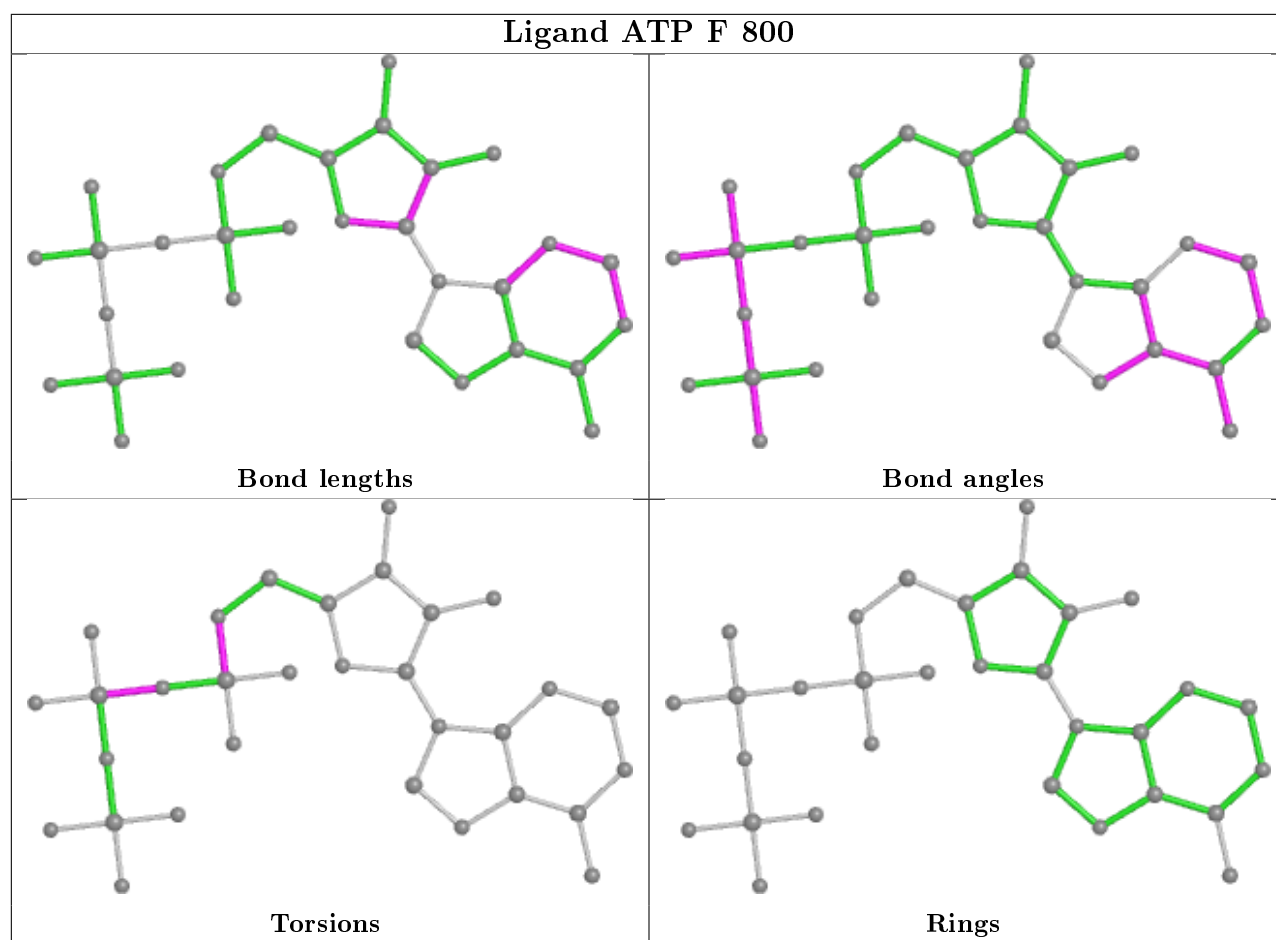
5 monomers are involved in 9 short contacts:

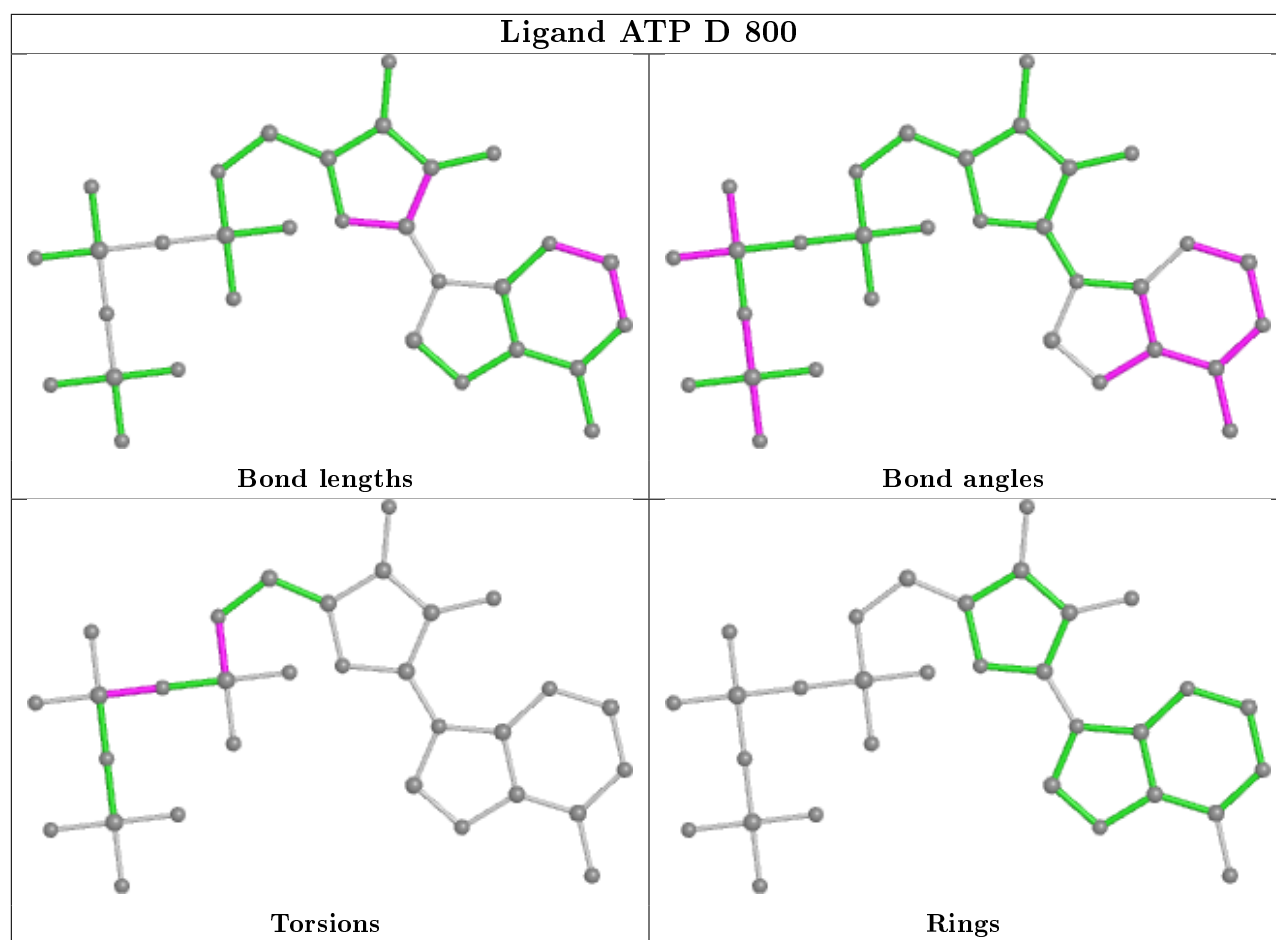
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	800	ATP	1	0
4	F	800	ATP	3	0
4	D	800	ATP	1	0
4	A	800	ATP	1	0
4	E	800	ATP	3	0

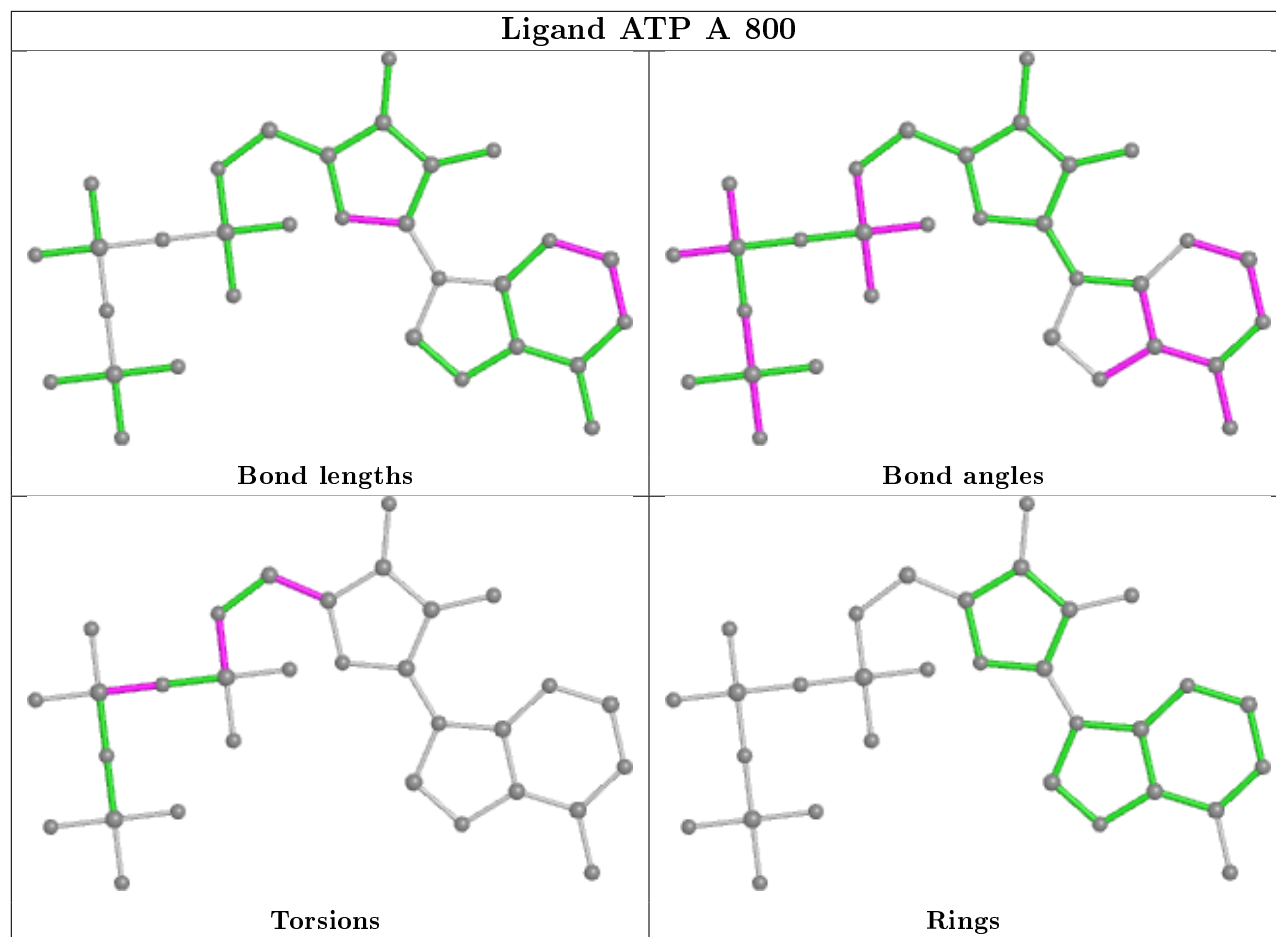
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

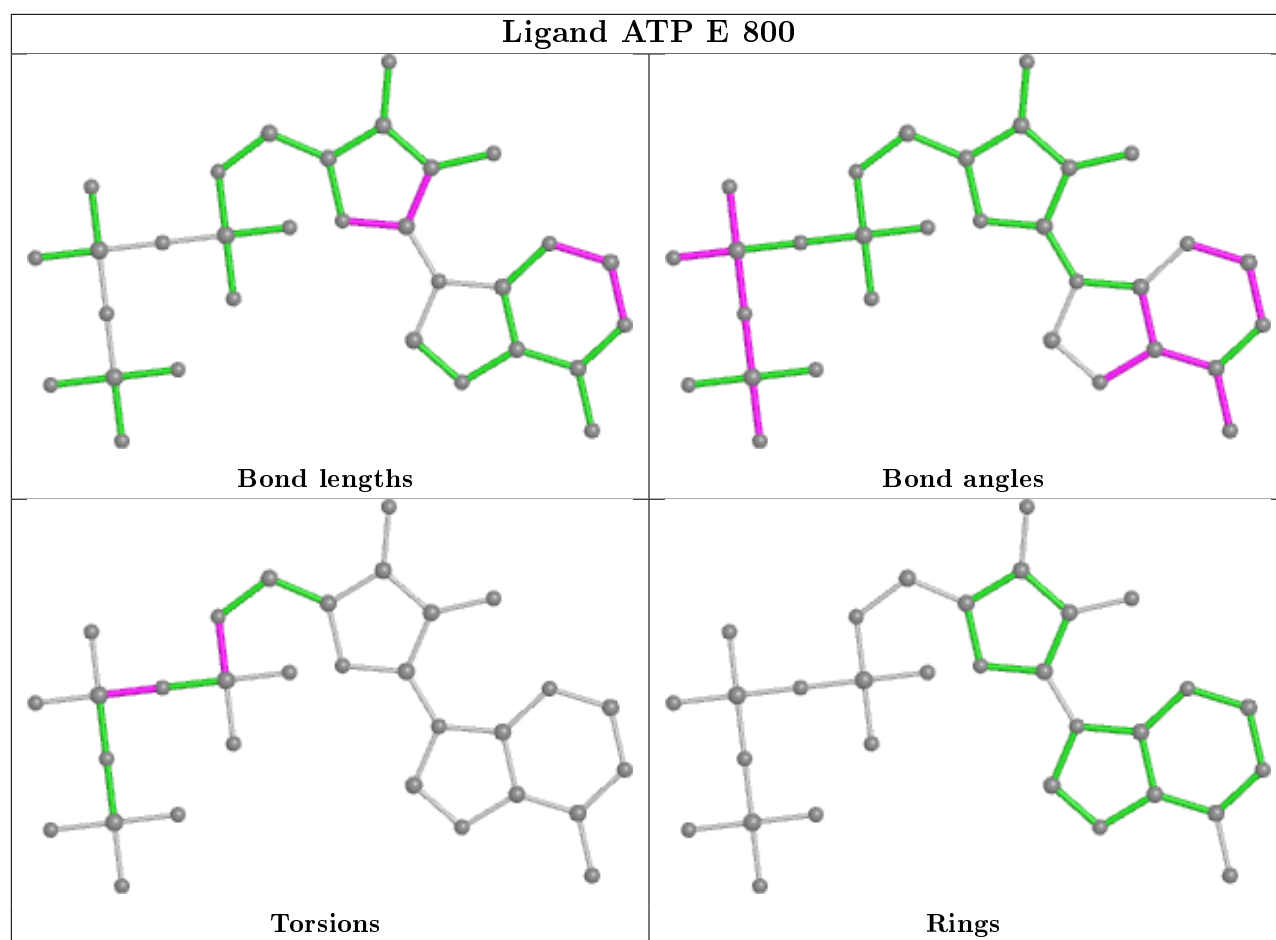












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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.