



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:49 AM UTC

PDB ID : 1SVM / pdb_00001svm
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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

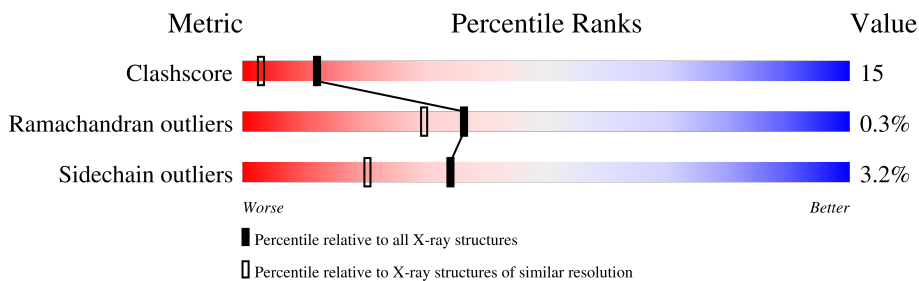
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (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 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	377	71% 23% . .
1	B	377	68% 26% . .
1	C	377	70% 23% . .
1	D	377	72% 21% . .
1	E	377	71% 22% . .
1	F	377	73% 20% . .

2 Entry composition [i](#)

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			

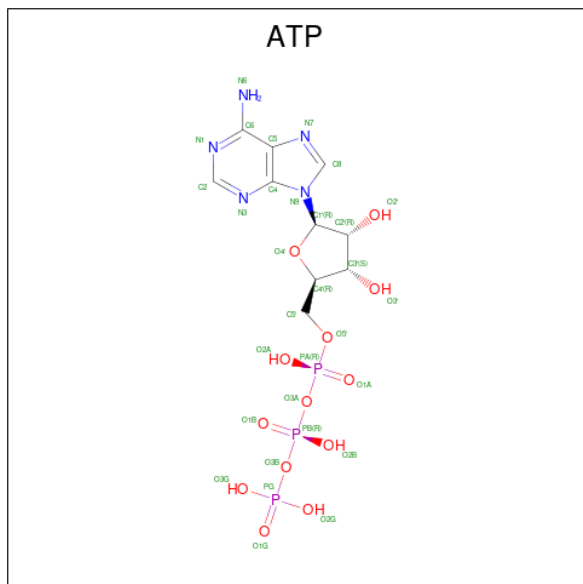
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 5 is water.

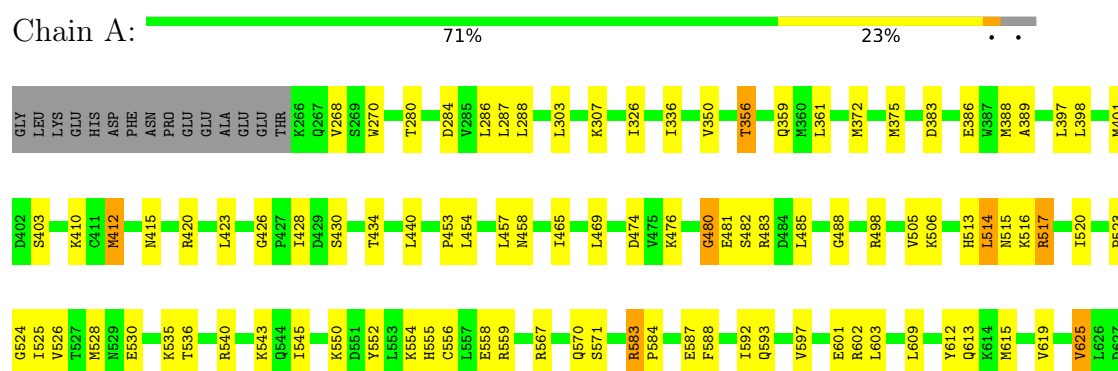
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	136	Total 136	O 136	0	0
5	B	140	Total 140	O 140	0	0
5	C	127	Total 127	O 127	0	0
5	D	123	Total 123	O 123	0	0
5	E	159	Total 159	O 159	0	0
5	F	122	Total 122	O 122	0	0

3 Residue-property plots

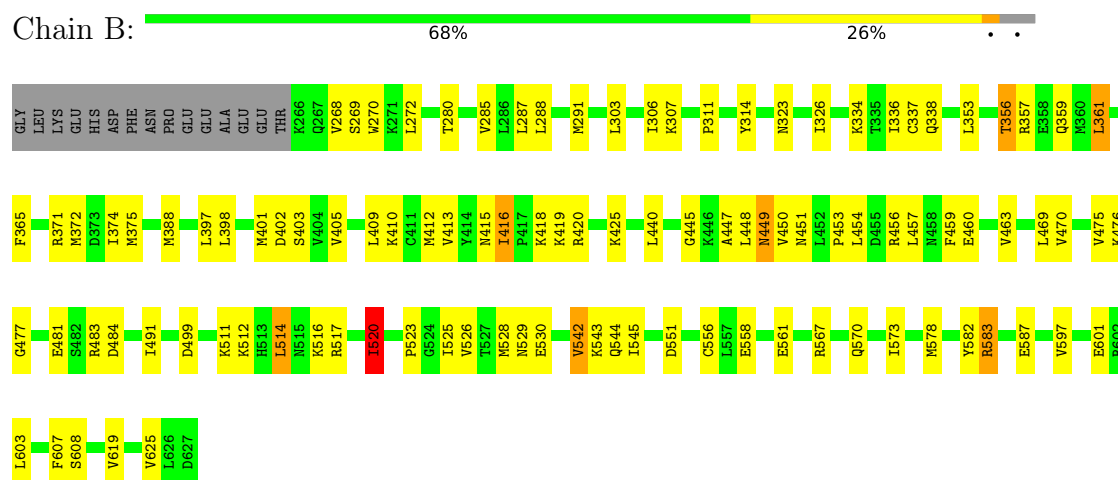
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

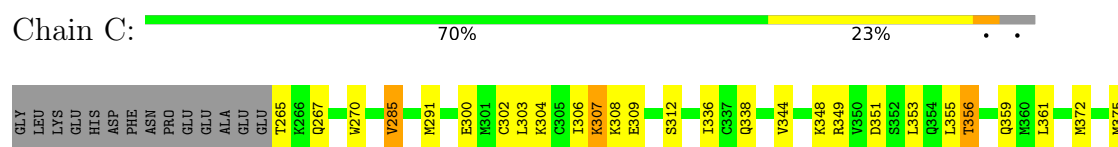
- Molecule 1: large T antigen

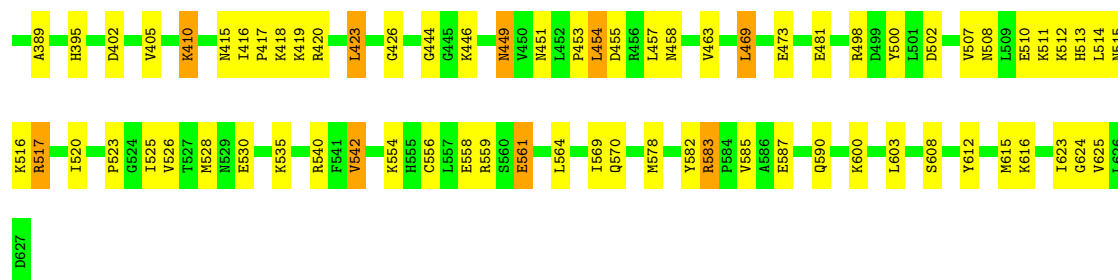


- Molecule 1: large T antigen



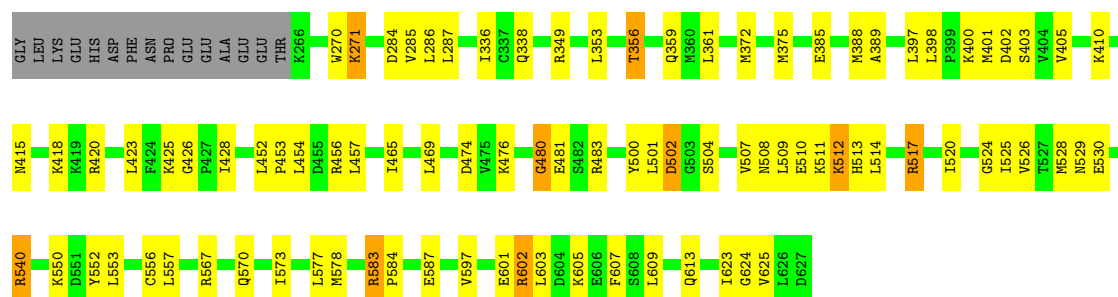
- Molecule 1: large T antigen





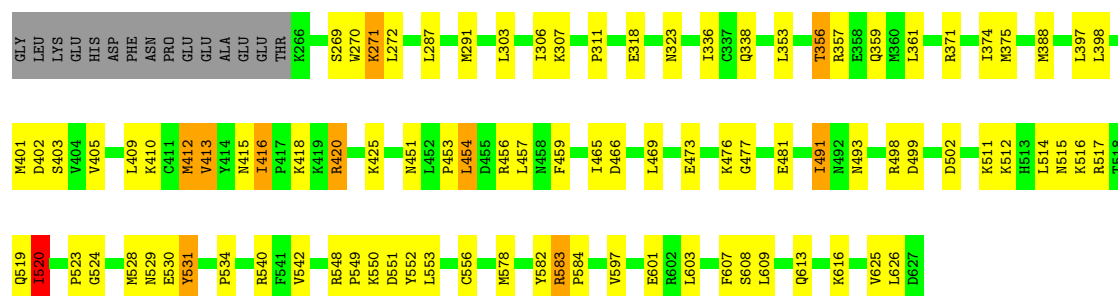
- Molecule 1: large T antigen

Chain D: 72% 21% . .



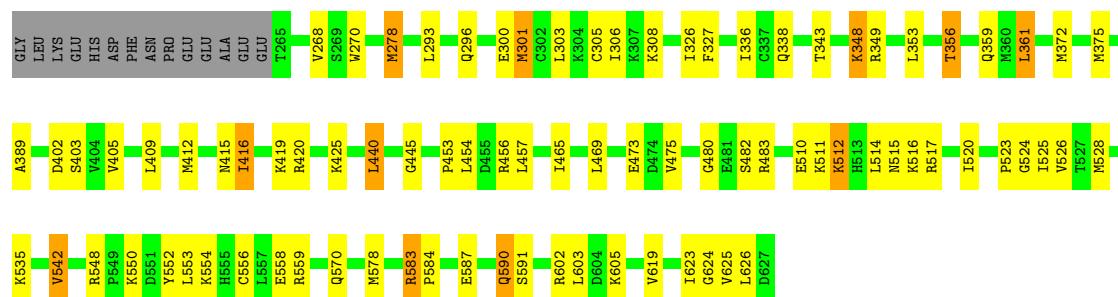
- Molecule 1: large T antigen

Chain E: 71% 22% . .



- Molecule 1: large T antigen

Chain F: 73% 20% . .



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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, 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	0.38	1/2992 (0.0%)	0.86	9/4030 (0.2%)
1	B	0.39	0/2988	0.87	9/4026 (0.2%)
1	C	0.35	0/2999	0.85	10/4040 (0.2%)
1	D	0.36	0/2992	0.85	8/4030 (0.2%)
1	E	0.39	1/2988 (0.0%)	0.84	9/4026 (0.2%)
1	F	0.36	0/2999	0.84	5/4040 (0.1%)
All	All	0.37	2/17958 (0.0%)	0.85	50/24192 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	412	MET	SD-CE	-6.93	1.62	1.79
1	E	412	MET	SD-CE	-5.92	1.64	1.79

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	583	ARG	N-CA-C	8.10	119.98	109.93
1	E	583	ARG	N-CA-C	7.60	119.35	109.93
1	A	524	GLY	N-CA-C	7.28	120.41	110.58
1	F	416	ILE	N-CA-C	7.11	114.74	108.63
1	A	583	ARG	N-CA-C	7.08	118.71	109.93
1	B	583	ARG	N-CA-C	6.98	118.58	109.93
1	B	356	THR	N-CA-C	-6.97	101.14	110.55
1	D	583	ARG	N-CA-C	6.91	118.77	110.07
1	B	529	ASN	N-CA-C	6.86	121.69	111.81
1	D	356	THR	N-CA-C	-6.55	101.70	110.55
1	C	582	TYR	N-CA-C	6.44	121.40	112.45
1	D	517	ARG	N-CA-C	6.41	118.83	108.32
1	C	426	GLY	CA-C-N	6.29	126.25	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	426	GLY	C-N-CA	6.29	126.25	120.21
1	A	356	THR	N-CA-C	-6.27	102.26	110.53
1	C	583	ARG	N-CA-C	6.13	118.75	110.29
1	F	356	THR	N-CA-C	-6.10	102.32	110.55
1	C	356	THR	N-CA-C	-6.09	102.33	110.55
1	C	517	ARG	N-CA-C	6.00	118.16	108.32
1	E	524	GLY	N-CA-C	6.00	120.48	111.42
1	C	520	ILE	N-CA-C	-5.88	101.94	109.30
1	A	625	VAL	N-CA-C	5.88	117.32	110.62
1	E	356	THR	N-CA-C	-5.88	102.62	110.55
1	B	582	TYR	N-CA-C	5.78	120.48	112.45
1	E	531	TYR	N-CA-C	-5.72	101.49	110.36
1	D	524	GLY	N-CA-C	5.65	119.95	111.42
1	F	524	GLY	N-CA-C	5.63	118.19	110.58
1	D	520	ILE	N-CA-C	-5.61	102.28	109.30
1	B	314	TYR	N-CA-C	5.55	118.10	111.71
1	D	529	ASN	N-CA-C	5.48	119.70	111.81
1	F	520	ILE	N-CA-C	-5.46	102.47	109.30
1	B	608	SER	N-CA-C	-5.46	103.18	110.55
1	E	416	ILE	N-CA-C	5.38	113.25	108.63
1	D	426	GLY	CA-C-N	5.33	125.33	120.21
1	D	426	GLY	C-N-CA	5.33	125.33	120.21
1	E	582	TYR	N-CA-C	5.32	119.85	112.45
1	B	416	ILE	N-CA-C	5.28	114.13	108.95
1	A	426	GLY	CA-C-N	5.28	125.28	120.21
1	A	426	GLY	C-N-CA	5.28	125.28	120.21
1	E	608	SER	N-CA-C	-5.27	103.73	110.53
1	A	571	SER	N-CA-C	5.25	118.78	109.96
1	E	473	GLU	N-CA-C	5.24	118.47	110.20
1	C	530	GLU	N-CA-C	5.20	117.66	109.39
1	A	520	ILE	N-CA-C	-5.17	102.83	109.30
1	C	608	SER	N-CA-C	-5.12	102.95	110.52
1	B	520	ILE	N-CA-C	-5.07	102.96	109.30
1	A	530	GLU	N-CA-C	5.05	118.53	110.70
1	E	520	ILE	N-CA-C	-5.04	102.99	109.30
1	B	529	ASN	CB-CA-C	-5.01	105.03	111.50
1	C	285	VAL	N-CA-C	5.01	115.63	110.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2933	0	2981	103	0
1	B	2929	0	2970	123	0
1	C	2940	0	2988	93	0
1	D	2933	0	2981	90	0
1	E	2929	0	2970	94	0
1	F	2940	0	2988	92	0
2	A	1	0	0	0	0
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	553	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 (553) 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:C:402:ASP:HA	1:C:578:MET:HE3	1.40	1.03
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:287:LEU:HG	1:E:291:MET:HE2	1.41	0.99
1:E:425:LYS:HE2	1:E:530:GLU:HA	1.45	0.99
1:B:291:MET:HE2	1:B:291:MET:HA	1.45	0.98
1:D:402:ASP:HA	1:D:578:MET:HE3	1.47	0.93
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:E:402:ASP:HA	1:E:578:MET:HE3	1.54	0.89
1:F:454:LEU:HA	1:F:457:LEU:HB2	1.52	0.89
1:B:402:ASP:HA	1:B:578:MET:HE3	1.56	0.88
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
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:C:454:LEU:HD12	1:C:454:LEU:H	1.43	0.83
1:D:415:ASN:HD21	1:D:420:ARG:HH11	1.23	0.83
1:C:410:LYS:HE3	1:C:410:LYS:HA	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:F:300:GLU:HB2	1:F:301:MET:HE2	1.60	0.81
1:B:412:MET:CE	1:B:523:PRO:HG2	2.11	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: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:F:402:ASP:HA	1:F:578:MET:HE3	1.67	0.77
1:D:425:LYS:HE2	1:D:530:GLU:HA	1.65	0.77
1:F:419:LYS:HA	1:F:542:VAL:HG13	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:612:TYR:HA	1:C:615:MET:HE3	1.68	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:B:449:ASN:C	1:B:449:ASN:HD22	1.96	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:HG2	1:B:517:ARG:HH11	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
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: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:A:453:PRO:HG2	1:F:454:LEU:HB2	1.71	0.71
1:B:412:MET:HE2	1:B:469:LEU:HB3	1.71	0.71
1:B:460:GLU:O	1:B:463:VAL:HG22	1.91	0.70
1:A:454:LEU:HD12	1:A:454:LEU:H	1.56	0.70
1:C:423:LEU:HD21	1:C:528:MET:HE3	1.74	0.70
1:F:349:ARG:CZ	1:F:353:LEU:HD21	2.22	0.70
1:B:412:MET:HE2	1:B:469:LEU:CB	2.21	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:454:LEU:HB2	1:C:453:PRO:HG2	1.75	0.69
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:449:ASN:HD22	1:C:449:ASN:C	2.01	0.68
1:B:412:MET:HE3	1:B:523:PRO:HG2	1.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:348:LYS:HB2	1:F:348:LYS:NZ	2.09	0.68
1:F:454:LEU:HD12	1:F:454:LEU:H	1.59	0.67
1:D:415:ASN:HD21	1:D:420:ARG:NH1	1.92	0.67
1:D:388:MET:HE1	1:D:577:LEU:HB3	1.75	0.67
1:C:303:LEU:H	1:C:303:LEU:HD23	1.60	0.67
1:C:402:ASP:HA	1:C:578:MET:CE	2.20	0.67
1:A:410:LYS:HE2	1:A:410:LYS:HA	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:B:412:MET:HE1	1:B:523:PRO:HG2	1.77	0.66
1:B:398:LEU:HD13	1:B:401:MET:HE1	1.78	0.65
1:D:454:LEU:HD12	1:D:454:LEU:H	1.61	0.65
1:F:510:GLU:HA	1:F:515:ASN:HA	1.78	0.65
1:B:397:LEU:C	1:B:398:LEU:HD12	2.22	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
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: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:B:402:ASP:HA	1:B:578:MET:CE	2.27	0.64
1:C:514:LEU:HD13	1:D:512:LYS:HA	1.79	0.64
1:E:402:ASP:HA	1:E:578:MET:CE	2.25	0.64
1:E:454:LEU:HD22	1:E:454:LEU:H	1.64	0.63
1:B:409:LEU:O	1:B:413:VAL:HG12	1.98	0.63
1:A:412:MET:HE3	1:A:523:PRO:HG2	1.79	0.63
1:D:602:ARG:HG3	1:D:602:ARG:HH11	1.64	0.63
1:D:454:LEU:HB2	1:E:453:PRO:HG2	1.79	0.63
1:A:412:MET:CE	1:A:523:PRO:HG2	2.29	0.62
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:HD22	1:E:454:LEU:N	2.14	0.62
1:A:454:LEU:HB2	1:B:453:PRO:HG2	1.81	0.62
1:D:481:GLU:H	1:D:481:GLU:CD	2.07	0.62
1:D:584:PRO:HG2	1:D:587:GLU:HG3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:269:SER:H	1:E:323:ASN:ND2	1.87	0.62
1:B:405:VAL:HG21	1:B:578:MET:HE1	1.80	0.61
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: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:E:397:LEU:C	1:E:398:LEU:HD12	2.25	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:D:285:VAL:HG21	1:D:338:GLN:NE2	2.16	0.60
1:D:388:MET:HE2	1:D:577:LEU:HD13	1.84	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
1:D:415:ASN:ND2	1:D:420:ARG:HH11	1.97	0.60
1:E:405:VAL:HG21	1:E:578:MET:HE1	1.82	0.60
1:F:415:ASN:ND2	1:F:420:ARG:HD2	2.17	0.60
1:A:412:MET:HE2	1:A:469:LEU:CB	2.32	0.60
1:B:448:LEU:HG	1:B:470:VAL:HG13	1.82	0.60
1:B:476:LYS:C	1:B:491:ILE:HD13	2.26	0.60
1:E:412:MET:HE3	1:E:523:PRO:HG2	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:D:402:ASP:HA	1:D:578:MET:CE	2.27	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:HD12	1:A:454:LEU:N	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:HD12	1:B:545:ILE:N	2.18	0.59
1:E:405:VAL:CG2	1:E:578:MET:HE1	2.33	0.59
1:F:405:VAL:HG21	1:F:578:MET:HE1	1.84	0.58
1:E:465:ILE:HD12	1:E:511:LYS:HG3	1.85	0.58
1:A:423:LEU:HD11	1:A:528:MET:HE3	1.85	0.58
1:E:388:MET:HG3	1:E:607:PHE:CE1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:456:ARG:N	1:E:456:ARG:HD2	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: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:HG22	1:A:280:THR:O	2.03	0.58
1:E:425:LYS:CE	1:E:530:GLU:HA	2.28	0.58
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:B:405:VAL:CG2	1:B:578:MET:HE1	2.35	0.57
1:D:418:LYS:NZ	4:E:800:ATP:O2G	2.30	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:397:LEU:O	1:D:398:LEU:HD12	2.05	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:A:423:LEU:CD1	1:A:528:MET:HE3	2.34	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:350:VAL:CG2	1:B:291:MET:HE3	2.35	0.56
1:A:415:ASN:HD21	1:A:420:ARG:NH1	2.02	0.56
1:A:513:HIS:O	1:A:514:LEU:HB2	2.04	0.56
1:B:449:ASN:HD22	1:B:451:ASN:H	1.51	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
1:C:500:TYR:CE2	1:C:507:VAL:HG11	2.41	0.56
1:C:454:LEU:HD12	1:C:454:LEU:N	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:412:MET:CE	1:B:469:LEU:HB3	2.35	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:HG22	1:B:280:THR:O	2.05	0.56
1:F:372:MET:HA	1:F:375:MET:HG2	1.88	0.56
1:B:291:MET:HA	1:B:291:MET:CE	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:469:LEU:C	1:E:469:LEU:HD12	2.31	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:D:397:LEU:C	1:D:398:LEU:HD12	2.31	0.55
1:D:405:VAL:HG21	1:D:578:MET:HE1	1.89	0.55
1:B:561:GLU:CD	1:B:561:GLU:H	2.15	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:398:LEU:HB2	1:A:401:MET:HE2	1.87	0.55
1:A:397:LEU:HG	1:A:398:LEU:HD13	1.89	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:H	1:C:454:LEU:CD1	2.17	0.54
1:C:449:ASN:HD21	1:C:451:ASN:HB2	1.72	0.54
1:F:348:LYS:HB2	1:F:348:LYS:HZ3	1.71	0.54
1:F:469:LEU:HD12	1:F:469:LEU:C	2.33	0.54
1:B:306:ILE:HD12	1:B:307:LYS:N	2.23	0.54
1:B:450:VAL:O	1:B:450:VAL:HG22	2.08	0.54
1:D:469:LEU:C	1:D:469:LEU:HD12	2.32	0.53
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
1:B:371:ARG:O	1:B:375:MET:HG3	2.08	0.53
1:B:398:LEU:HD13	1:B:401:MET:CE	2.37	0.53
1:A:482:SER:OG	1:A:483:ARG:HD3	2.08	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:E:412:MET:HE2	1:E:469:LEU:CB	2.39	0.53
1:C:508:ASN:HB3	1:C:515:ASN:HD21	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:398:LEU:HD13	1:D:401:MET:HE1	1.91	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:A:480:GLY:HA2	1:A:483:ARG:CZ	2.40	0.52
1:B:306:ILE:HD12	1:B:306:ILE:C	2.35	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:E:512:LYS:C	1:E:514:LEU:H	2.17	0.51
1:B:469:LEU:C	1:B:469:LEU:HD12	2.36	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: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:HG3	1:C:559:ARG:HH11	1.76	0.51
1:E:415:ASN:HD21	1:E:420:ARG:NH1	2.05	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:A:583:ARG:HD2	1:A:587:GLU:OE1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:389:ALA:HB1	1:D:625:VAL:HG21	1.92	0.50
1:D:609:LEU:O	1:D:613:GLN:HG3	2.11	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:A:412:MET:HE2	1:A:469:LEU:HD22	1.92	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:E:481:GLU:CD	1:E:481:GLU:H	2.20	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:412:MET:CE	1:B:469:LEU:CB	2.89	0.50
1:B:483:ARG:HA	1:B:483:ARG:NE	2.27	0.50
1:E:520:ILE:HG22	5:E:817:HOH:O	2.11	0.50
1:B:454:LEU:H	1:B:454:LEU:CD1	2.22	0.50
1:F:405:VAL:CG2	1:F:578:MET:HE1	2.41	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: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
1:A:483:ARG:HD3	1:A:483:ARG:N	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:A:388:MET:HB3	1:A:615:MET:HE1	1.95	0.49
1:F:483:ARG:HG3	1:F:483:ARG:NH1	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: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:C:561:GLU:N	1:C:561:GLU:CD	2.71	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:412:MET:HE2	1:A:469:LEU:CD2	2.44	0.48
1:A:583:ARG:CD	1:A:587:GLU:OE1	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:LEU:O	1:B:398:LEU:HD12	2.13	0.48
1:F:456:ARG:HG3	1:F:456:ARG:HH11	1.79	0.48
1:C:351:ASP:HB3	1:C:355:LEU:HD12	1.95	0.48
1:D:418:LYS:HZ1	4:E:800:ATP:PG	2.36	0.48
1:E:502:ASP:OD1	1:E:540:ARG:HD2	2.13	0.48
1:E:511:LYS:HD3	1:E:515:ASN:HB3	1.95	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:385:GLU:HA	1:D:607:PHE:CZ	2.48	0.48
1:D:597:VAL:O	1:D:601:GLU:HG3	2.13	0.48
1:C:418:LYS:NZ	4:D:800:ATP:O2G	2.37	0.48
1:A:567:ARG:HG3	1:A:567:ARG:NH1	2.29	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:C:481:GLU:CD	1:C:481:GLU:H	2.21	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:A:412:MET:HE1	1:A:523:PRO:C	2.39	0.47
1:D:423:LEU:HD11	1:D:528:MET:HE3	1.97	0.47
1:E:454:LEU:H	1:E:454:LEU:CD2	2.26	0.47
1:B:481:GLU:H	1:B:481:GLU:CD	2.23	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
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:269:SER:H	1:B:323:ASN:ND2	1.96	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:D:405:VAL:CG2	1:D:578:MET:HE1	2.44	0.47
1:E:412:MET:CE	1:E:469:LEU:CB	2.93	0.47
1:E:418:LYS:NZ	4:F:800:ATP:PG	2.88	0.47
1:B:447:ALA:C	1:B:448:LEU:HD23	2.40	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:C:511:LYS:CE	1:C:516:LYS:HG3	2.45	0.47
1:B:583:ARG:CD	1:B:587:GLU:OE1	2.63	0.47
1:D:425:LYS:CE	1:D:530:GLU:HA	2.41	0.47
1:D:501:LEU:HB2	1:D:540:ARG:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:465:ILE:HG23	1:F:517:ARG:HD2	1.97	0.47
1:C:458:ASN:CG	1:D:456:ARG:HD3	2.39	0.46
1:B:334:LYS:O	1:B:337:CYS:SG	2.70	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:A:412:MET:HE2	1:A:469:LEU:HB2	1.96	0.46
1:B:425:LYS:HE3	1:B:528:MET:HE2	1.95	0.46
1:C:513:HIS:HB3	1:D:513:HIS:HD2	1.81	0.46
1:D:454:LEU:H	1:D:454:LEU:CD1	2.26	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:514:LEU:HD12	1:D:514:LEU:O	2.15	0.46
1:A:412:MET:HE2	1:A:469:LEU:HB3	1.96	0.46
1:B:459:PHE:N	1:B:459:PHE:CD2	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:300:GLU:HB2	1:F:301:MET:CE	2.41	0.46
1:F:475:VAL:CG2	1:F:528:MET:HE2	2.46	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
1:E:465:ILE:HG23	1:E:517:ARG:HD3	1.99	0.45
1:B:353:LEU:HD21	1:B:517:ARG:HH21	1.80	0.45
1:B:514:LEU:HD23	1:B:514:LEU:N	2.31	0.45
1:C:415:ASN:ND2	1:C:420:ARG:HH11	2.00	0.45
1:D:400:LYS:NZ	1:D:400:LYS:HB3	2.31	0.45
1:D:525:ILE:HG22	1:D:526:VAL:N	2.29	0.45
1:F:412:MET:HE1	1:F:420:ARG:O	2.17	0.45
1:A:612:TYR:HA	1:A:615:MET:CE	2.47	0.45
1:B:418:LYS:NZ	4:C:800:ATP:O2G	2.42	0.45
1:C:444:GLY:O	1:C:469:LEU:CD2	2.65	0.45
1:E:398:LEU:HD13	1:E:401:MET:HE1	1.98	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:A:592:ILE:HD12	1:A:592:ILE:C	2.42	0.45
1:E:269:SER:OG	1:E:272:LEU:HD13	2.15	0.45
1:E:412:MET:HE2	1:E:469:LEU:HD22	1.99	0.45
1:F:548:ARG:HG2	1:F:548:ARG:HH11	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:GLY:C	1:A:482:SER:H	2.25	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:C:349:ARG:CD	1:C:517:ARG:CZ	2.95	0.44
1:A:430:SER:N	4:A:800:ATP:O1B	2.50	0.44
1:A:602:ARG:HG3	1:A:602:ARG:HH11	1.82	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:E:412:MET:HE2	1:E:469:LEU:CD2	2.47	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:HH11	1:D:517:ARG:HG3	1.83	0.44
1:C:417:PRO:HG2	1:D:570:GLN:NE2	2.33	0.44
1:D:271:LYS:NZ	1:D:271:LYS:HB3	2.32	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:F:456:ARG:HG3	1:F:456:ARG:NH1	2.33	0.43
1:A:556:CYS:SG	1:A:625:VAL:HG13	2.57	0.43
1:A:612:TYR:HD1	1:A:615:MET:HE3	1.83	0.43
1:C:300:GLU:H	1:C:300:GLU:CD	2.26	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:HG3	1:A:567:ARG:HH11	1.83	0.43
1:C:267:GLN:H	1:C:267:GLN:CD	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:449:ASN:C	1:B:449:ASN:ND2	2.69	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:A:350:VAL:CG1	1:B:291:MET:HE3	2.49	0.43
1:A:505:VAL:HG12	1:A:506:LYS:N	2.34	0.43
1:F:440:LEU:HD21	1:F:445:GLY:C	2.44	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:C:291:MET:HE2	1:C:312:SER:OG	2.19	0.42
1:B:361:LEU:HD22	1:B:365:PHE:CE1	2.54	0.42
1:B:567:ARG:NH1	1:B:567:ARG:HG3	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:A:458:ASN:HB2	1:B:456:ARG:HE	1.85	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
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:F:278:MET:HE1	5:F:855:HOH:O	2.19	0.42
1:A:514:LEU:HB3	1:A:516:LYS:NZ	2.35	0.42
1:A:469:LEU:HD12	1:A:469:LEU:C	2.45	0.42
1:B:268:VAL:HG22	1:B:326:ILE:HG22	2.02	0.42
1:B:511:LYS:O	1:B:512:LYS:HB2	2.19	0.42
1:D:512:LYS:O	1:D:514:LEU:HG	2.20	0.42
1:F:278:MET:HE1	1:F:343:THR:HG22	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:465:ILE:CG2	1:A:517:ARG:HG3	2.50	0.41
1:A:514:LEU:HD22	1:A:516:LYS:CG	2.51	0.41
1:A:403:SER:OG	1:A:583:ARG:NH2	2.53	0.41
1:A:412:MET:CE	1:A:469:LEU:HB2	2.50	0.41
1:A:454:LEU:CB	1:B:453:PRO:HG2	2.46	0.41
1:B:388:MET:HG3	1:B:607:PHE:CE1	2.54	0.41
1:C:405:VAL:CG2	1:C:578:MET:HE1	2.51	0.41
1:C:446:LYS:HG3	1:C:463:VAL:HG12	2.02	0.41
1:F:405:VAL:HG21	1:F:578:MET:CE	2.48	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:E:528:MET:HE2	1:E:531:TYR:H	1.86	0.41
1:A:284:ASP:HB3	1:A:287:LEU:HB3	2.03	0.41
1:B:544:GLN:C	1:B:545:ILE:HD12	2.44	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:O	1:A:280:THR:CG2	2.69	0.41
1:A:286:LEU:HB2	1:F:517:ARG:HH22	1.84	0.41
1:A:350:VAL:HG22	1:B:291:MET:HE3	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:E:412:MET:HE2	1:E:469:LEU:HB2	2.03	0.41
1:E:412:MET:HE1	1:E:523:PRO:C	2.46	0.41
1:E:515:ASN:HD22	1:E:516:LYS:N	2.19	0.41
1:F:510:GLU:HG3	1:F:514:LEU:C	2.45	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:440:LEU:HD11	1:B:445:GLY:C	2.45	0.41
1:C:502:ASP:OD1	1:C:540:ARG:HD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:561:GLU:CD	1:C:561:GLU:H	2.29	0.40
1:D:284:ASP:HB3	1:D:287:LEU:HB3	2.03	0.40
1:F:480:GLY:C	1:F:482:SER:H	2.28	0.40
1:A:350:VAL:HG21	1:B:291:MET:HE3	2.04	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:405:VAL:HG21	1:C:578:MET:HE1	2.03	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:D:550:LYS:HB2	1:D:553:LEU:HD12	2.03	0.40
1:A:415:ASN:HB3	1:B:567:ARG:HH21	1.86	0.40
1:B:412:MET:HE2	1:B:469:LEU:HB2	1.98	0.40
1:C:344:VAL:O	1:C:348:LYS:HG2	2.21	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%)	21	11
1	B	360/377 (96%)	347 (96%)	12 (3%)	1 (0%)	36	30
1	C	361/377 (96%)	349 (97%)	12 (3%)	0	100	100
1	D	360/377 (96%)	349 (97%)	8 (2%)	3 (1%)	16	7
1	E	360/377 (96%)	350 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	361/377 (96%)	351 (97%)	9 (2%)	1 (0%)	36	30
All	All	2162/2262 (96%)	2094 (97%)	61 (3%)	7 (0%)	36	30

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 [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	323/336 (96%)	317 (98%)	6 (2%)	50	40
1	B	322/336 (96%)	313 (97%)	9 (3%)	38	25
1	C	324/336 (96%)	312 (96%)	12 (4%)	30	16
1	D	323/336 (96%)	311 (96%)	12 (4%)	30	16
1	E	322/336 (96%)	310 (96%)	12 (4%)	30	16
1	F	284/336 (84%)	274 (96%)	10 (4%)	32	18
All	All	1898/2016 (94%)	1837 (97%)	61 (3%)	34	20

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	288	LEU
1	A	361	LEU
1	A	440	LEU
1	A	474	ASP

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Mol	Chain	Res	Type
1	A	517	ARG
1	A	603	LEU
1	B	287	LEU
1	B	361	LEU
1	B	449	ASN
1	B	516	LYS
1	B	520	ILE
1	B	542	VAL
1	B	551	ASP
1	B	570	GLN
1	B	603	LEU
1	C	307	LYS
1	C	361	LEU
1	C	410	LYS
1	C	423	LEU
1	C	449	ASN
1	C	454	LEU
1	C	469	LEU
1	C	542	VAL
1	C	561	GLU
1	C	570	GLN
1	C	590	GLN
1	C	603	LEU
1	D	271	LYS
1	D	349	ARG
1	D	361	LEU
1	D	410	LYS
1	D	474	ASP
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	E	271	LYS
1	E	318	GLU
1	E	338	GLN
1	E	361	LEU
1	E	413	VAL
1	E	420	ARG
1	E	454	LEU

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Mol	Chain	Res	Type
1	E	491	ILE
1	E	520	ILE
1	E	542	VAL
1	E	551	ASP
1	E	603	LEU
1	F	278	MET
1	F	301	MET
1	F	338	GLN
1	F	348	LYS
1	F	361	LEU
1	F	440	LEU
1	F	542	VAL
1	F	570	GLN
1	F	590	GLN
1	F	603	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) 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	339	GLN
1	B	415	ASN
1	B	449	ASN
1	B	493	ASN
1	B	508	ASN
1	B	515	ASN
1	B	538	GLN
1	B	544	GLN
1	B	590	GLN
1	B	613	GLN
1	C	267	GLN

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Mol	Chain	Res	Type
1	C	310	GLN
1	C	333	GLN
1	C	338	GLN
1	C	339	GLN
1	C	395	HIS
1	C	415	ASN
1	C	449	ASN
1	C	458	ASN
1	C	513	HIS
1	C	515	ASN
1	C	544	GLN
1	C	570	GLN
1	C	590	GLN
1	C	613	GLN
1	D	333	GLN
1	D	338	GLN
1	D	415	ASN
1	D	467	GLN
1	D	538	GLN
1	D	544	GLN
1	D	570	GLN
1	D	593	GLN
1	E	317	HIS
1	E	323	ASN
1	E	333	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	E	538	GLN
1	E	544	GLN
1	E	613	GLN
1	F	267	GLN
1	F	310	GLN
1	F	333	GLN
1	F	338	GLN
1	F	339	GLN
1	F	395	HIS
1	F	415	ASN

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Mol	Chain	Res	Type
1	F	544	GLN
1	F	590	GLN
1	F	613	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](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 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	B	800	3	32,33,33	1.58	6 (18%)	48,52,52	3.25	19 (39%)
4	ATP	A	800	3	32,33,33	1.54	6 (18%)	48,52,52	3.22	17 (35%)
4	ATP	E	800	3	32,33,33	2.00	5 (15%)	48,52,52	2.99	16 (33%)
4	ATP	C	800	3	32,33,33	1.70	5 (15%)	48,52,52	3.04	16 (33%)
4	ATP	F	800	3	32,33,33	1.83	5 (15%)	48,52,52	3.00	16 (33%)
4	ATP	D	800	3	32,33,33	1.74	4 (12%)	48,52,52	3.10	16 (33%)

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	B	800	3	-	5/22/38/38	0/3/3/3
4	ATP	A	800	3	-	5/22/38/38	0/3/3/3
4	ATP	E	800	3	-	2/22/38/38	0/3/3/3
4	ATP	C	800	3	-	1/22/38/38	0/3/3/3
4	ATP	F	800	3	-	2/22/38/38	0/3/3/3
4	ATP	D	800	3	-	4/22/38/38	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	800	ATP	PB-O3A	7.13	1.67	1.59
4	E	800	ATP	PA-O3A	6.13	1.66	1.59
4	F	800	ATP	PB-O3A	6.09	1.66	1.59
4	C	800	ATP	PB-O3A	5.92	1.65	1.59
4	D	800	ATP	PB-O3A	5.77	1.65	1.59
4	F	800	ATP	PA-O3A	5.55	1.65	1.59
4	A	800	ATP	PB-O3A	5.13	1.65	1.59
4	D	800	ATP	PA-O3A	4.98	1.64	1.59
4	B	800	ATP	PB-O3A	4.62	1.64	1.59
4	C	800	ATP	PA-O3A	4.41	1.64	1.59
4	B	800	ATP	PA-O3A	3.36	1.63	1.59
4	A	800	ATP	PA-O3A	2.84	1.62	1.59
4	B	800	ATP	C2-N3	2.78	1.38	1.33
4	E	800	ATP	C2-N3	2.67	1.38	1.33
4	A	800	ATP	C2-N3	2.65	1.38	1.33
4	F	800	ATP	C2-N1	2.61	1.38	1.33
4	D	800	ATP	C2-N3	2.58	1.38	1.33
4	F	800	ATP	C2-N3	2.57	1.38	1.33
4	A	800	ATP	C2-N1	2.52	1.38	1.33
4	C	800	ATP	C2-N1	2.48	1.38	1.33
4	B	800	ATP	C2-N1	2.46	1.38	1.33
4	C	800	ATP	C2-N3	2.44	1.38	1.33
4	B	800	ATP	C1'-N9	2.43	1.53	1.46
4	F	800	ATP	C4-N3	2.35	1.38	1.34
4	D	800	ATP	C2-N1	2.32	1.38	1.33
4	E	800	ATP	C2-N1	2.25	1.37	1.33
4	A	800	ATP	C1'-N9	2.15	1.52	1.46
4	E	800	ATP	C4-N3	2.12	1.38	1.34
4	C	800	ATP	C4-N3	2.10	1.38	1.34
4	A	800	ATP	C4-N3	2.05	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	800	ATP	C4-N3	2.00	1.38	1.34

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	800	ATP	O3A-PB-O1B	-13.56	69.91	110.70
4	C	800	ATP	O3A-PB-O1B	-13.17	71.09	110.70
4	B	800	ATP	O3A-PB-O1B	-12.95	71.75	110.70
4	F	800	ATP	O3A-PB-O1B	-12.90	71.90	110.70
4	A	800	ATP	O3A-PB-O1B	-12.69	72.52	110.70
4	E	800	ATP	O3A-PB-O1B	-12.50	73.09	110.70
4	D	800	ATP	O2B-PB-O3A	-7.23	87.74	107.27
4	B	800	ATP	O2B-PB-O3A	-7.20	87.82	107.27
4	C	800	ATP	O2B-PB-O3A	-7.15	87.94	107.27
4	E	800	ATP	O2B-PB-O3A	-6.99	88.39	107.27
4	A	800	ATP	O2B-PB-O3A	-6.88	88.68	107.27
4	F	800	ATP	O2B-PB-O3A	-6.70	89.15	107.27
4	A	800	ATP	O5'-PA-O1A	-6.62	82.70	108.94
4	B	800	ATP	O5'-PA-O1A	-6.51	83.15	108.94
4	F	800	ATP	N3-C2-N1	-5.75	119.88	128.58
4	C	800	ATP	N3-C2-N1	-5.65	120.03	128.58
4	A	800	ATP	N3-C2-N1	-5.58	120.14	128.58
4	B	800	ATP	N3-C2-N1	-5.53	120.21	128.58
4	D	800	ATP	N3-C2-N1	-5.50	120.25	128.58
4	E	800	ATP	N3-C2-N1	-5.47	120.31	128.58
4	E	800	ATP	C5-N7-C8	5.34	111.84	103.45
4	B	800	ATP	C5-N7-C8	5.15	111.54	103.45
4	D	800	ATP	C5-N7-C8	5.13	111.52	103.45
4	C	800	ATP	O2B-PB-O3B	5.13	121.13	107.27
4	E	800	ATP	O2B-PB-O3B	5.08	121.01	107.27
4	F	800	ATP	O2B-PB-O3B	5.07	120.98	107.27
4	A	800	ATP	C5-N7-C8	5.07	111.42	103.45
4	C	800	ATP	C5-N7-C8	5.07	111.41	103.45
4	F	800	ATP	C5-N7-C8	5.06	111.41	103.45
4	D	800	ATP	O2B-PB-O3B	4.81	120.27	107.27
4	D	800	ATP	C4-C5-N7	-4.79	105.11	110.58
4	E	800	ATP	C4-C5-N7	-4.69	105.22	110.58
4	E	800	ATP	N9-C8-N7	-4.68	107.30	113.94
4	D	800	ATP	N9-C8-N7	-4.61	107.39	113.94
4	C	800	ATP	C4-C5-N7	-4.60	105.33	110.58
4	F	800	ATP	N9-C8-N7	-4.59	107.42	113.94
4	A	800	ATP	O2A-PA-O5'	-4.57	86.87	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	800	ATP	C4-C5-N7	-4.54	105.39	110.58
4	B	800	ATP	O2A-PA-O5'	-4.52	87.10	107.57
4	C	800	ATP	N9-C8-N7	-4.49	107.56	113.94
4	A	800	ATP	C4-C5-N7	-4.49	105.45	110.58
4	B	800	ATP	O2B-PB-O3B	4.47	119.36	107.27
4	B	800	ATP	C4-C5-N7	-4.46	105.49	110.58
4	A	800	ATP	O2B-PB-O3B	4.29	118.87	107.27
4	A	800	ATP	N9-C8-N7	-4.16	108.04	113.94
4	B	800	ATP	N9-C8-N7	-4.00	108.25	113.94
4	F	800	ATP	C2'-C1'-N9	3.54	122.09	113.30
4	E	800	ATP	C2'-C1'-N9	3.43	121.83	113.30
4	A	800	ATP	C2'-C1'-N9	3.40	121.74	113.30
4	B	800	ATP	O2A-PA-O1A	3.38	128.18	112.44
4	B	800	ATP	C2'-C1'-N9	3.38	121.69	113.30
4	D	800	ATP	C2'-C1'-N9	3.34	121.61	113.30
4	A	800	ATP	O2A-PA-O1A	3.31	127.84	112.44
4	B	800	ATP	C5-C4-N3	-3.22	122.28	126.72
4	C	800	ATP	C2'-C1'-N9	3.21	121.27	113.30
4	A	800	ATP	C5-C4-N3	-3.12	122.42	126.72
4	E	800	ATP	C5-C4-N3	-3.08	122.47	126.72
4	D	800	ATP	C2-N3-C4	3.04	119.26	111.83
4	D	800	ATP	C5-C4-N3	-3.00	122.58	126.72
4	E	800	ATP	C2-N3-C4	2.98	119.11	111.83
4	A	800	ATP	C2-N3-C4	2.97	119.07	111.83
4	C	800	ATP	C2-N3-C4	2.95	119.05	111.83
4	D	800	ATP	C6-C5-N7	2.95	137.78	132.09
4	C	800	ATP	C5-C4-N3	-2.94	122.67	126.72
4	F	800	ATP	C2-N3-C4	2.92	118.96	111.83
4	D	800	ATP	O2B-PB-O1B	2.92	126.01	112.44
4	B	800	ATP	C2-N3-C4	2.91	118.94	111.83
4	F	800	ATP	O2A-PA-O3A	2.87	115.04	107.27
4	D	800	ATP	O2A-PA-O3A	2.86	115.00	107.27
4	F	800	ATP	C5-C4-N3	-2.81	122.85	126.72
4	C	800	ATP	O2B-PB-O1B	2.79	125.42	112.44
4	E	800	ATP	C6-C5-N7	2.79	137.46	132.09
4	F	800	ATP	C6-C5-N7	2.77	137.43	132.09
4	A	800	ATP	O4'-C1'-N9	-2.74	102.82	108.09
4	C	800	ATP	C6-C5-N7	2.74	137.37	132.09
4	C	800	ATP	O2A-PA-O3A	2.73	114.66	107.27
4	E	800	ATP	O2A-PA-O3A	2.70	114.57	107.27
4	A	800	ATP	O2B-PB-O1B	2.69	124.97	112.44
4	B	800	ATP	O2B-PB-O1B	2.69	124.96	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	800	ATP	O2B-PB-O1B	2.67	124.88	112.44
4	A	800	ATP	C6-C5-N7	2.64	137.18	132.09
4	C	800	ATP	O2G-PG-O3B	2.56	113.20	104.64
4	B	800	ATP	O4'-C1'-N9	-2.53	103.23	108.09
4	F	800	ATP	O2B-PB-O1B	2.51	124.14	112.44
4	B	800	ATP	C6-C5-N7	2.50	136.90	132.09
4	D	800	ATP	O2G-PG-O3B	2.46	112.89	104.64
4	F	800	ATP	C4-N9-C8	2.46	108.32	105.74
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	D	800	ATP	C4-N9-C8	2.40	108.26	105.74
4	E	800	ATP	C4-N9-C8	2.35	108.21	105.74
4	B	800	ATP	O2G-PG-O3B	2.34	112.47	104.64
4	C	800	ATP	C4-N9-C8	2.32	108.18	105.74
4	A	800	ATP	O2G-PG-O3B	2.32	112.42	104.64
4	B	800	ATP	O3A-PA-O1A	2.18	117.26	110.70
4	B	800	ATP	C5'-C4'-C3'	-2.11	107.61	115.21
4	E	800	ATP	O3A-PA-O1A	-2.08	104.45	110.70
4	D	800	ATP	O4'-C4'-C5'	2.03	115.84	109.33
4	F	800	ATP	O3A-PA-O1A	-2.03	104.60	110.70
4	C	800	ATP	O3A-PA-O1A	-2.00	104.68	110.70

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	800	ATP	C5'-O5'-PA-O2A
4	D	800	ATP	C5'-O5'-PA-O3A
4	F	800	ATP	C5'-O5'-PA-O3A
4	B	800	ATP	C3'-C4'-C5'-O5'
4	B	800	ATP	O4'-C4'-C5'-O5'
4	A	800	ATP	C3'-C4'-C5'-O5'
4	A	800	ATP	O4'-C4'-C5'-O5'
4	A	800	ATP	C5'-O5'-PA-O1A
4	B	800	ATP	C5'-O5'-PA-O1A
4	D	800	ATP	C5'-O5'-PA-O1A
4	E	800	ATP	C5'-O5'-PA-O3A
4	A	800	ATP	PA-O3A-PB-O2B
4	B	800	ATP	PA-O3A-PB-O2B
4	C	800	ATP	PA-O3A-PB-O2B
4	D	800	ATP	PA-O3A-PB-O2B
4	E	800	ATP	PA-O3A-PB-O2B

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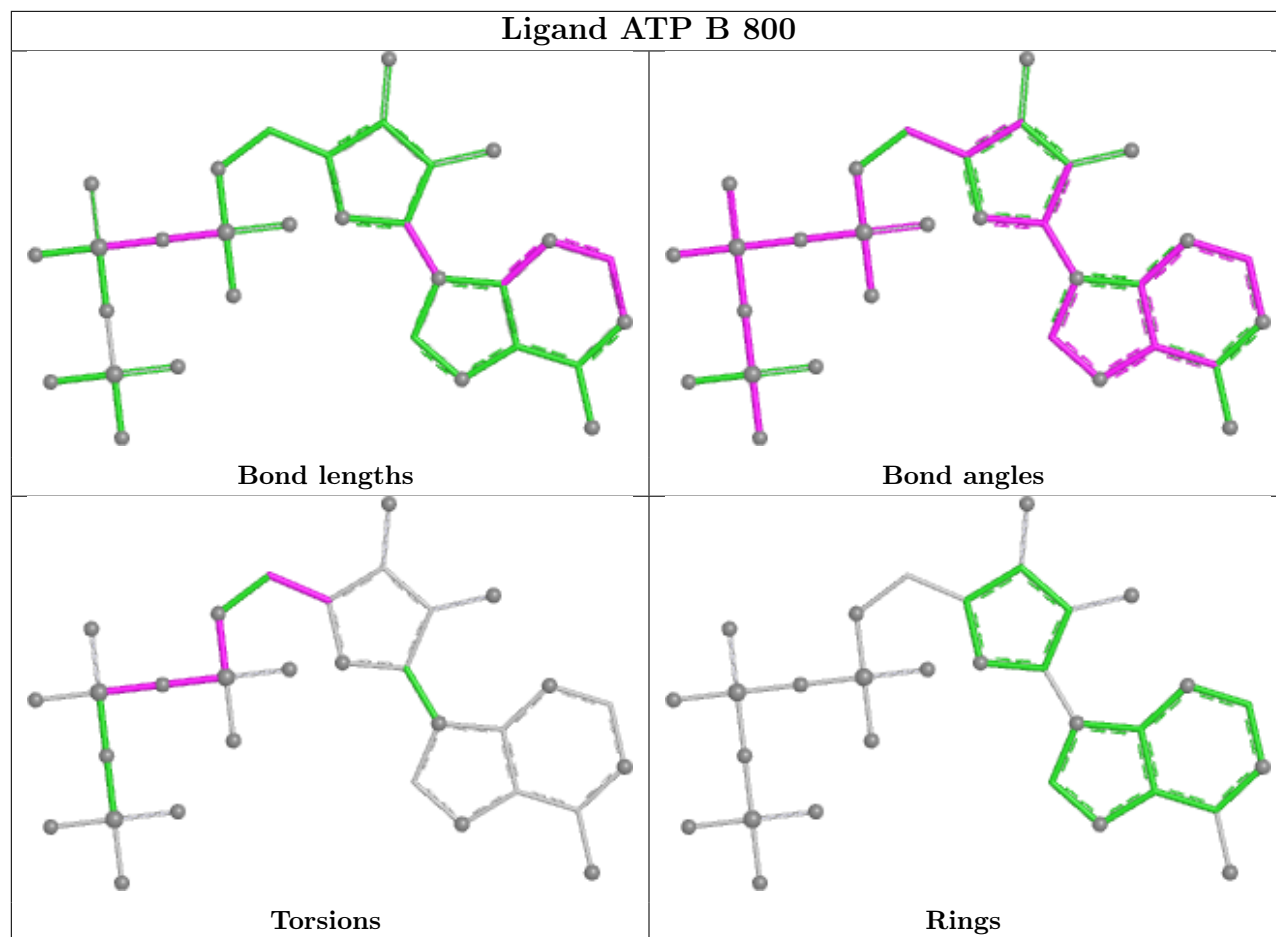
Mol	Chain	Res	Type	Atoms
4	F	800	ATP	PA-O3A-PB-O2B
4	B	800	ATP	PB-O3A-PA-O1A
4	A	800	ATP	PB-O3A-PA-O1A

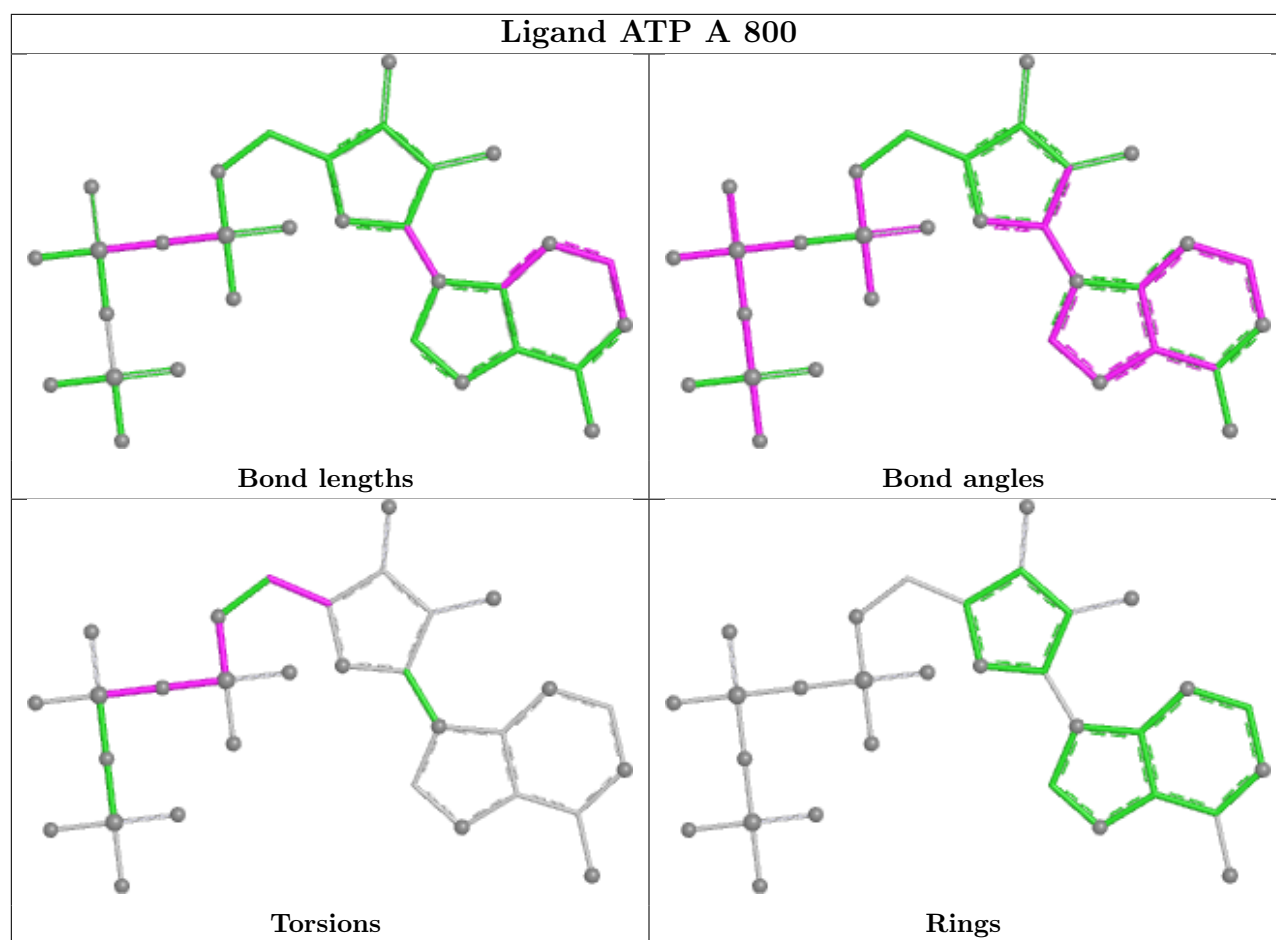
There are no ring outliers.

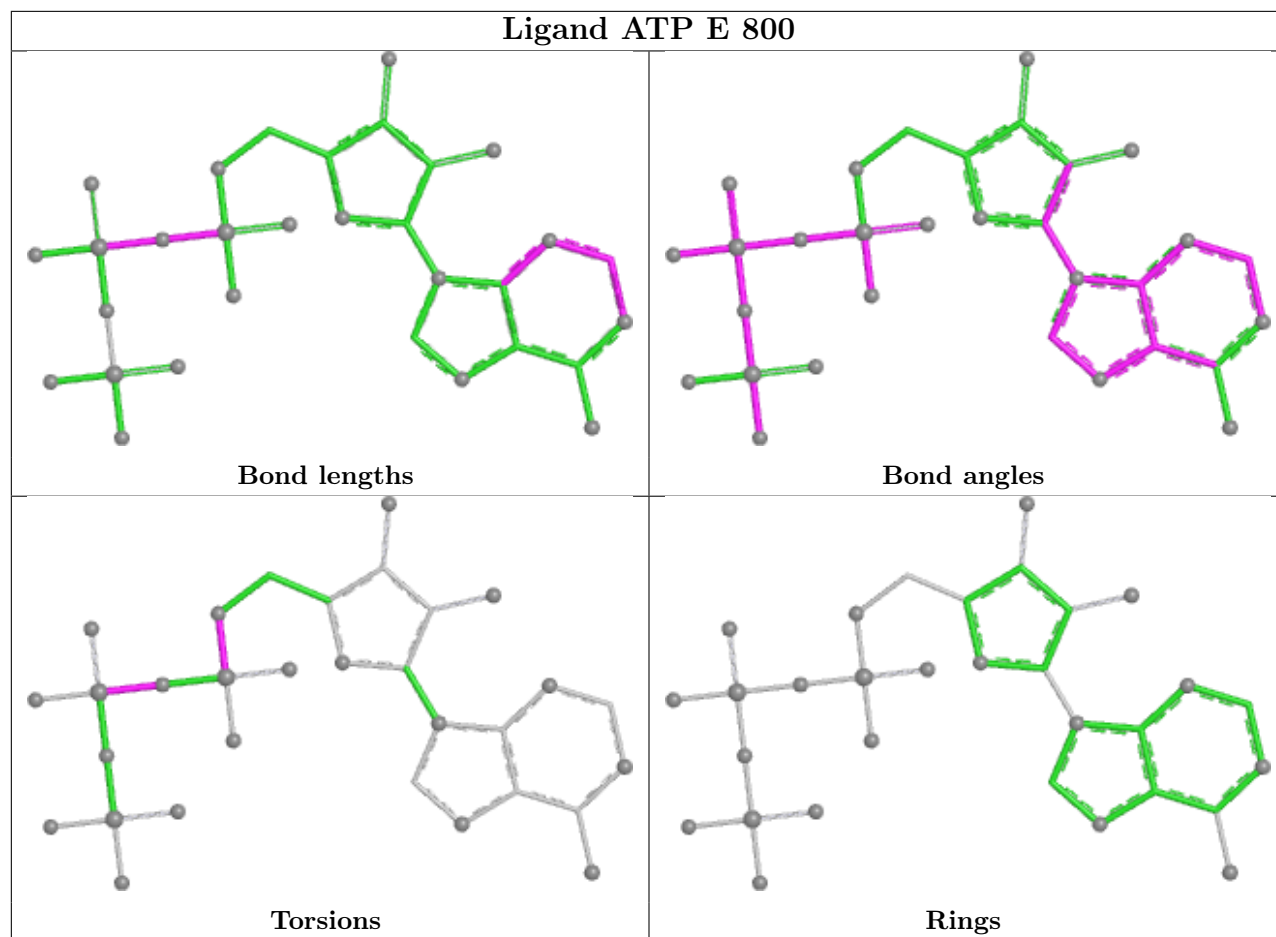
5 monomers are involved in 9 short contacts:

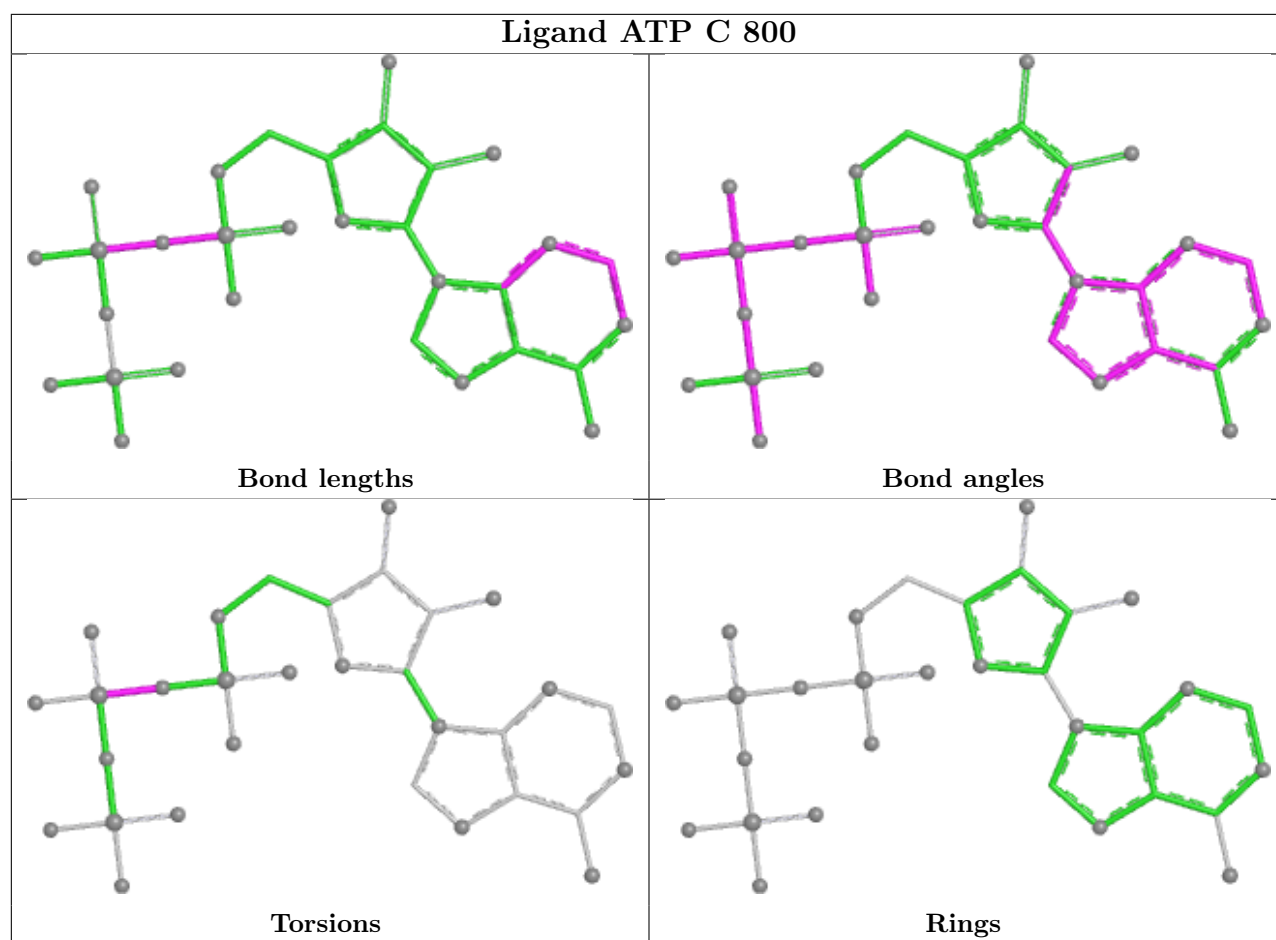
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	800	ATP	1	0
4	E	800	ATP	3	0
4	C	800	ATP	1	0
4	F	800	ATP	3	0
4	D	800	ATP	1	0

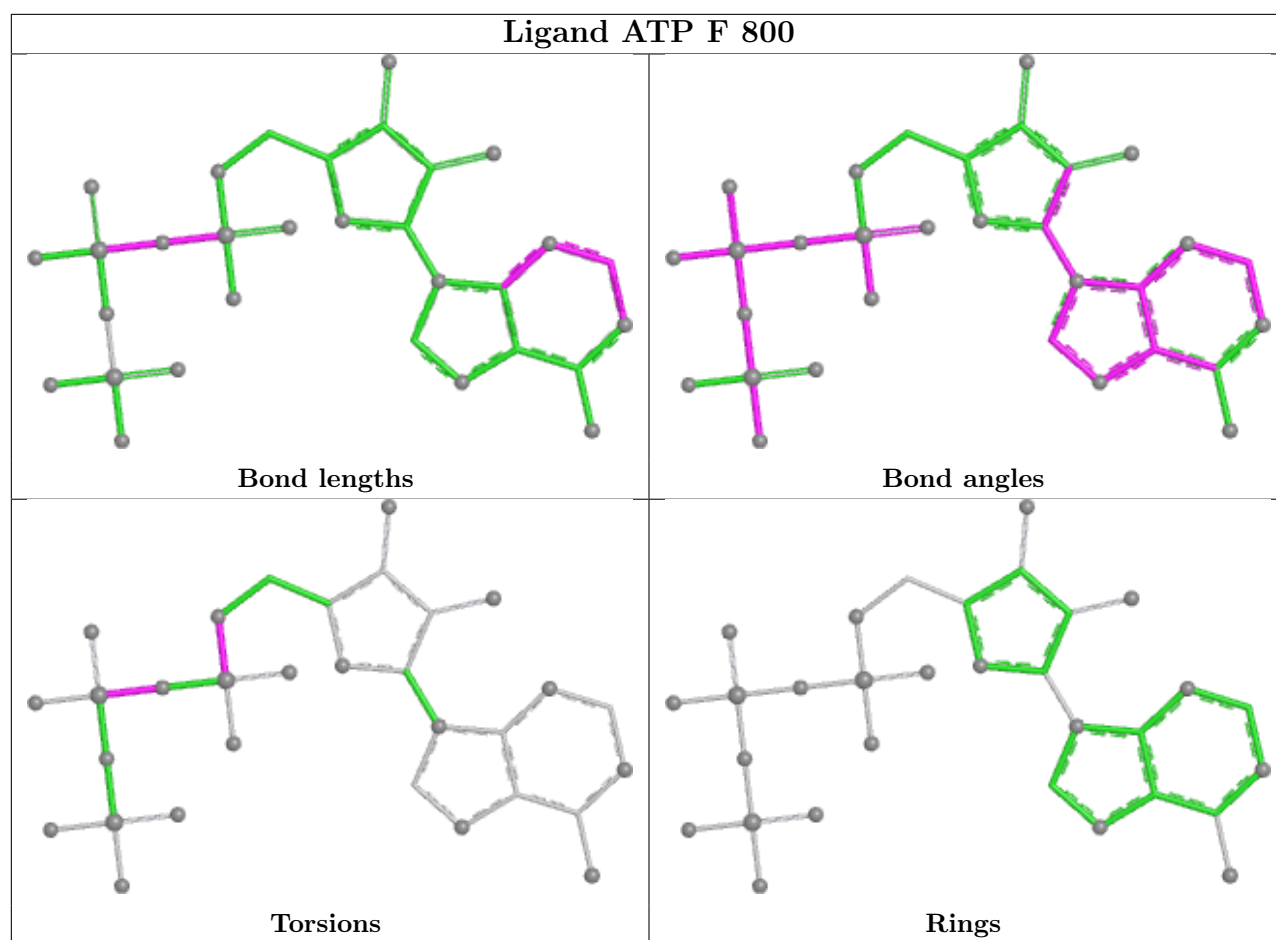
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

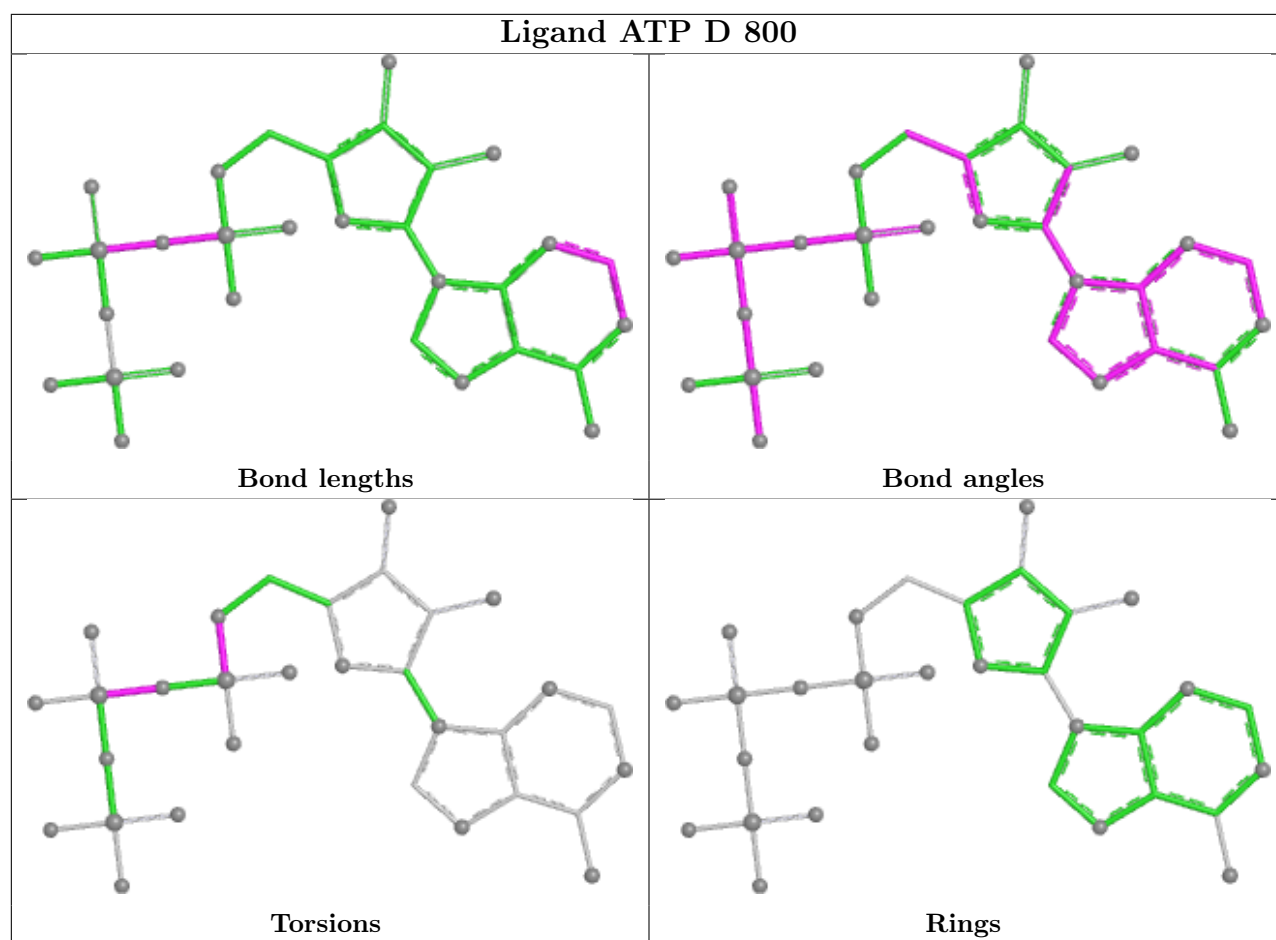












5.7 Other polymers [i](#)

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.