



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:23 PM UTC

PDB ID : 1GZ4 / pdb_00001gz4
Title : molecular mechanism of the regulation of human mitochondrial NAD(P)⁺-dependent malic enzyme by ATP and fumarate
Authors : Yang, Z.; Lanks, C.W.; Tong, L.
Deposited on : 2002-05-15
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 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

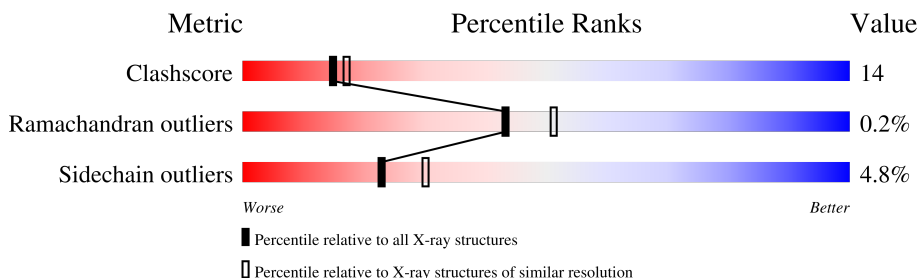
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	551	73% 25% .
1	B	551	70% 28% .
1	C	551	71% 26% .
1	D	551	72% 25% .

2 Entry composition [i](#)

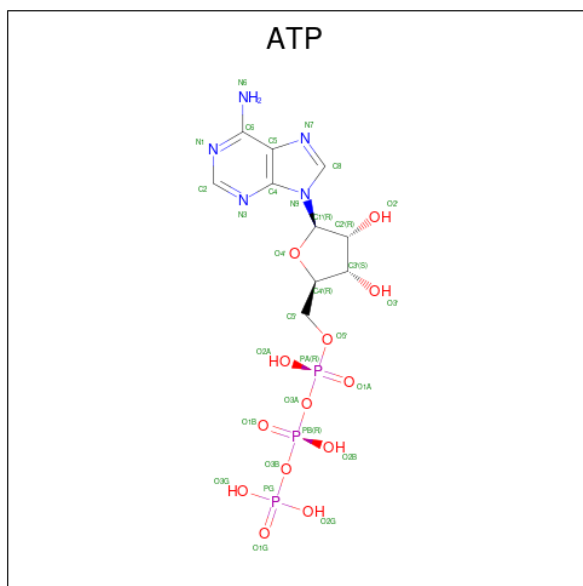
There are 6 unique types of molecules in this entry. The entry contains 18289 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NAD-DEPENDENT MALIC ENZYME.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	Se	0	0	0
			4350	2784	741	802	9	14			
1	B	551	Total	C	N	O	S	Se	0	0	0
			4350	2784	741	802	9	14			
1	C	551	Total	C	N	O	S	Se	0	0	0
			4350	2784	741	802	9	14			
1	D	551	Total	C	N	O	S	Se	0	0	0
			4351	2784	741	803	9	14			

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



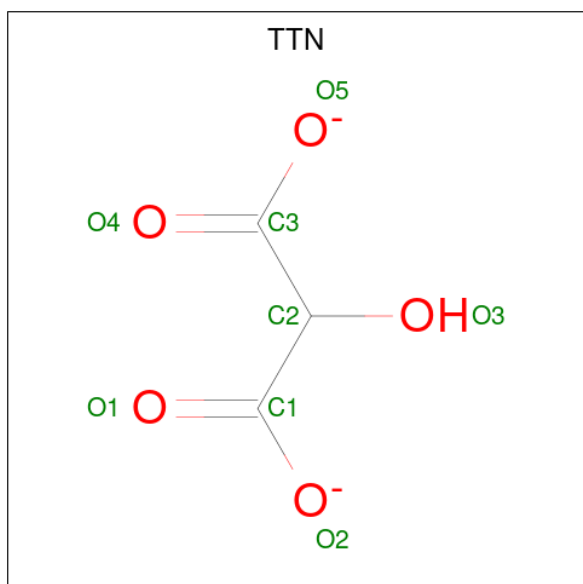
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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

- Molecule 3 is TARTRONATE (CCD ID: TTN) (formula: $C_3H_2O_5$).

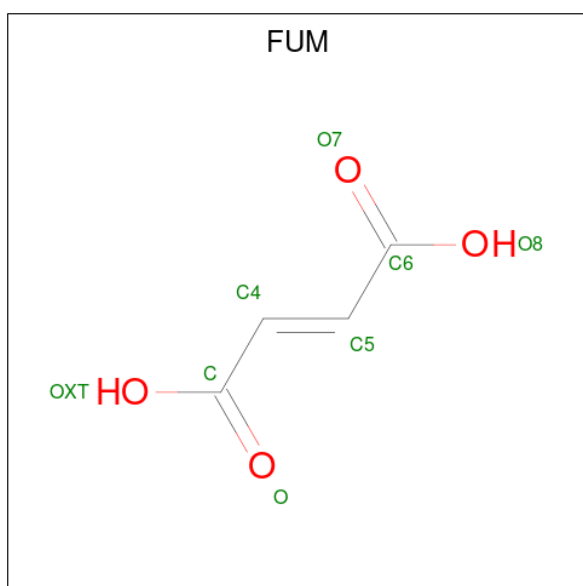


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	3	5		
3	B	1	Total	C	O	0	0
			8	3	5		
3	C	1	Total	C	O	0	0
			8	3	5		
3	D	1	Total	C	O	0	0
			8	3	5		

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mn 1 1	0	0
4	B	1	Total Mn 1 1	0	0
4	C	1	Total Mn 1 1	0	0
4	D	1	Total Mn 1 1	0	0

- Molecule 5 is FUMARIC ACID (CCD ID: FUM) (formula: $C_4H_4O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 8 4 4	0	0
5	B	1	Total C O 8 4 4	0	0
5	C	1	Total C O 8 4 4	0	0
5	D	1	Total C O 8 4 4	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	150	Total O 150 150	0	0
6	B	142	Total O 142 142	0	0

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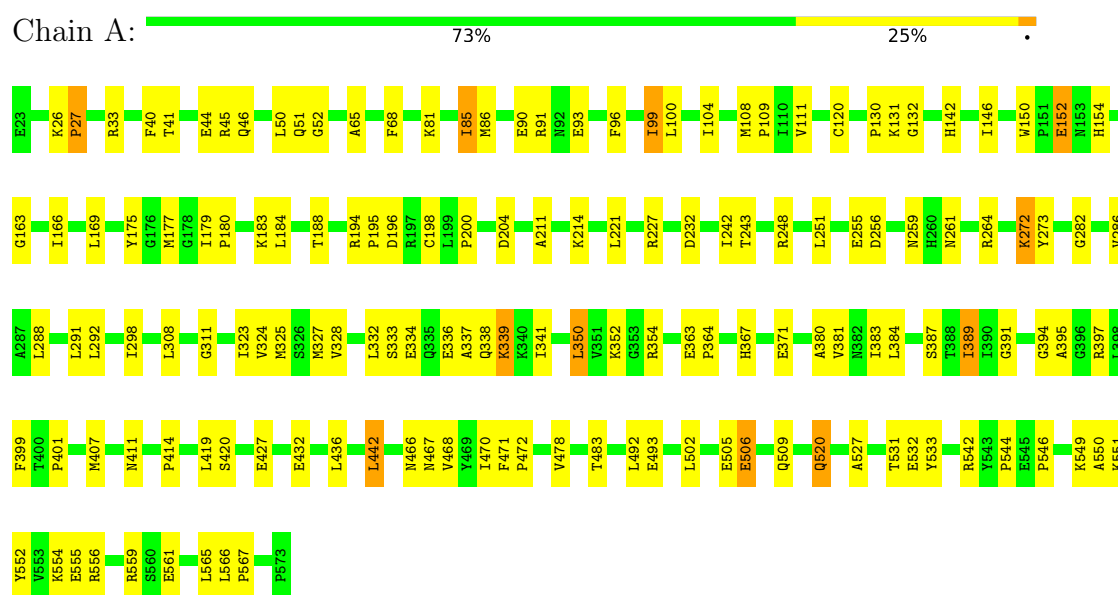
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	130	Total 130	O 130	0	0
6	D	150	Total 150	O 150	0	0

3 Residue-property plots

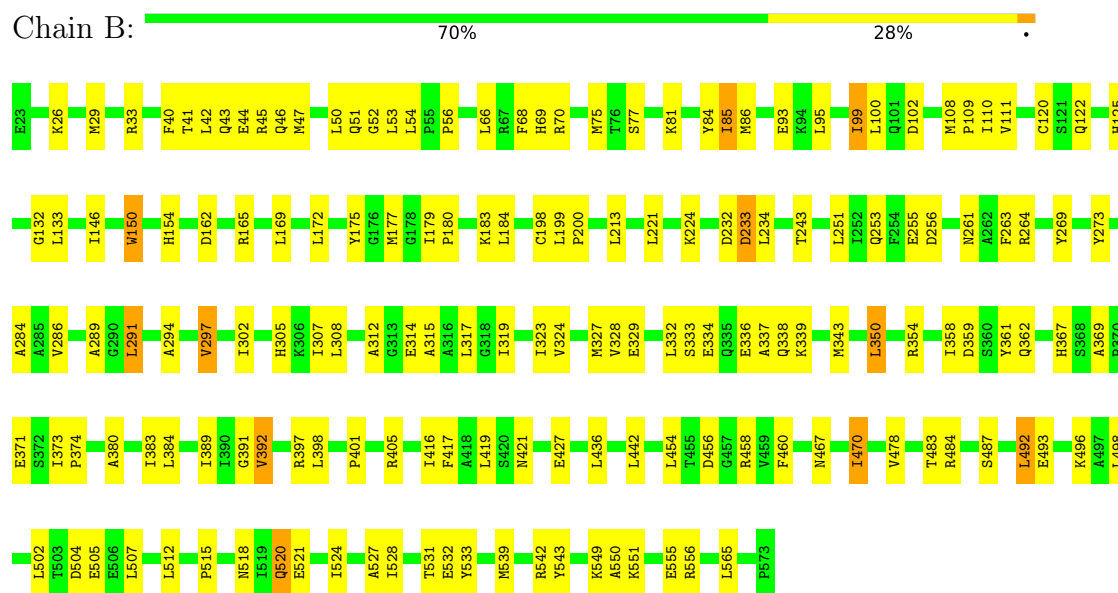
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

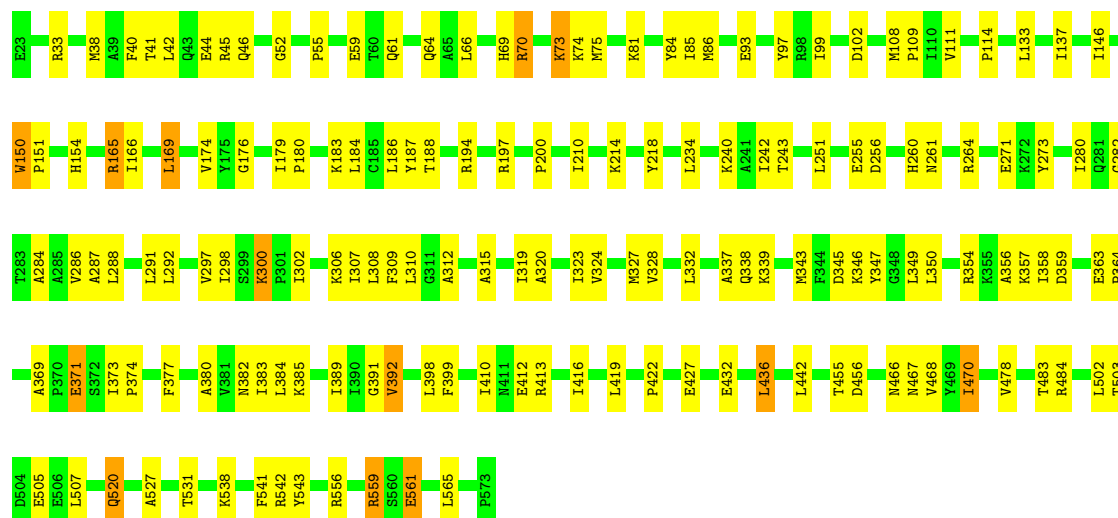


• Molecule 1: NAD-DEPENDENT MALIC ENZYME



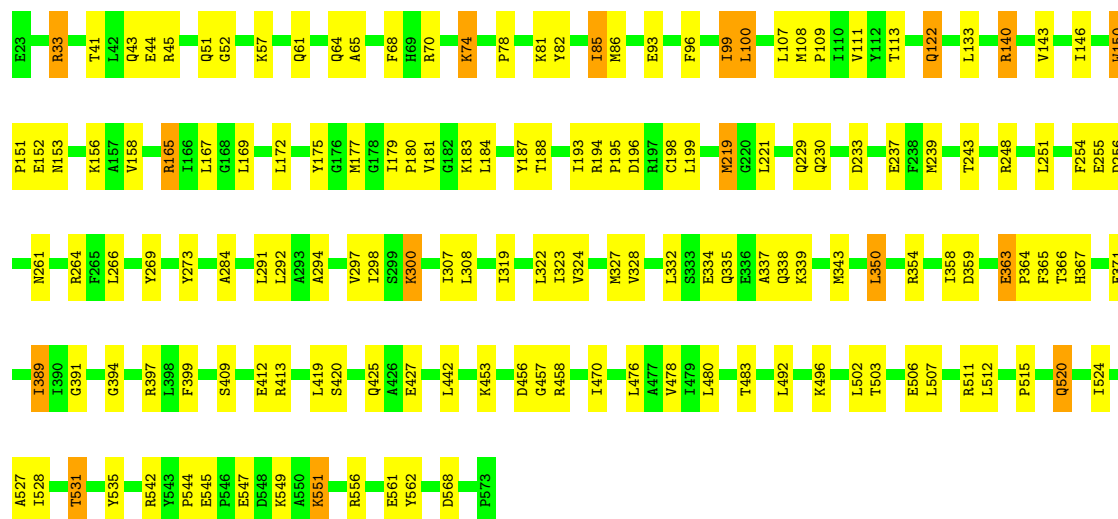
• Molecule 1: NAD-DEPENDENT MALIC ENZYME

Chain C:  71% 26%



• Molecule 1: NAD-DEPENDENT MALIC ENZYME

Chain D:  72% 25%



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	224.94Å 117.45Å 111.61Å 90.00° 109.33° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20	Depositor
% Data completeness (in resolution range)	95.0 (20.00-2.20)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.209 , 0.245	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18289	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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: FUM, ATP, TTN, MN

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	0.43	0/4430	0.87	7/5976 (0.1%)
1	B	0.43	0/4430	0.89	7/5976 (0.1%)
1	C	0.44	1/4430 (0.0%)	0.88	5/5976 (0.1%)
1	D	0.43	0/4431	0.88	6/5976 (0.1%)
All	All	0.43	1/17721 (0.0%)	0.88	25/23904 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	55	PRO	CA-C	5.25	1.54	1.51

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	470	ILE	N-CA-C	10.47	120.56	111.56
1	C	470	ILE	N-CA-C	8.50	119.47	111.48
1	B	470	ILE	N-CA-C	8.18	118.60	111.56
1	B	150	TRP	CA-C-N	8.16	127.73	119.24
1	B	150	TRP	C-N-CA	8.16	127.73	119.24
1	D	150	TRP	CA-C-N	7.26	127.11	119.05
1	D	150	TRP	C-N-CA	7.26	127.11	119.05
1	C	150	TRP	CA-C-N	7.07	126.90	119.05
1	C	150	TRP	C-N-CA	7.07	126.90	119.05
1	B	419	LEU	N-CA-C	6.34	120.75	112.89
1	A	419	LEU	N-CA-C	6.31	120.98	113.28
1	A	311	GLY	N-CA-C	-6.12	106.14	111.95
1	D	256	ASP	N-CA-C	5.93	119.75	111.74
1	D	419	LEU	N-CA-C	5.92	120.57	113.23
1	B	256	ASP	N-CA-C	5.91	119.58	111.54
1	A	256	ASP	N-CA-C	5.77	119.35	111.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	TRP	CA-C-N	5.75	125.44	119.05
1	A	150	TRP	C-N-CA	5.75	125.44	119.05
1	B	269	TYR	N-CA-C	5.60	120.39	113.50
1	C	419	LEU	N-CA-C	5.50	119.99	113.28
1	B	162	ASP	N-CA-C	-5.19	106.34	113.30
1	A	442	LEU	N-CA-C	-5.16	98.86	107.99
1	D	167	LEU	CB-CA-C	-5.15	110.62	116.54
1	C	256	ASP	N-CA-C	5.11	118.67	111.52
1	A	259	ASN	N-CA-C	5.04	117.16	111.11

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	4350	0	4383	110	0
1	B	4350	0	4383	137	0
1	C	4350	0	4383	129	0
1	D	4351	0	4383	124	0
2	A	62	0	24	0	0
2	B	62	0	24	1	0
2	C	62	0	24	1	0
2	D	62	0	24	0	0
3	A	8	0	1	1	0
3	B	8	0	1	1	0
3	C	8	0	1	1	0
3	D	8	0	1	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	8	0	1	1	0
5	B	8	0	1	0	0
5	C	8	0	1	0	0
5	D	8	0	1	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	150	0	0	6	0
6	B	142	0	0	3	0
6	C	130	0	0	3	0
6	D	150	0	0	4	0
All	All	18289	0	17636	489	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 14.

All (489) 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:B:29:MSE:HE2	1:B:50:LEU:HD22	1.28	1.15
1:B:315:ALA:HB3	1:B:392:VAL:HG21	1.25	1.10
1:A:381:VAL:HG13	1:A:407:MSE:HE3	1.38	1.06
1:C:286:VAL:HG21	1:C:467:ASN:HA	1.39	1.04
1:D:343:MSE:HE2	1:D:365:PHE:HB2	1.41	0.98
1:B:323:ILE:HG22	1:B:327:MSE:HE2	1.42	0.97
1:D:327:MSE:HE3	1:D:337:ALA:HB1	1.46	0.95
1:C:323:ILE:HG22	1:C:327:MSE:HE2	1.49	0.95
1:B:374:PRO:HG3	1:B:383:ILE:HD12	1.49	0.95
1:D:177:MSE:HE2	1:D:181:VAL:HG23	1.47	0.94
1:B:43:GLN:HG2	1:B:47:MSE:HE3	1.48	0.93
1:B:286:VAL:HG21	1:B:467:ASN:HA	1.51	0.92
1:D:140:ARG:HH22	1:D:233:ASP:HB3	1.33	0.92
1:D:177:MSE:HE1	1:D:180:PRO:HB2	1.50	0.92
1:A:286:VAL:HG21	1:A:467:ASN:HA	1.52	0.92
1:B:369:ALA:HB1	1:B:373:ILE:HD11	1.51	0.90
1:D:527:ALA:O	1:D:531:THR:HG22	1.71	0.90
1:B:315:ALA:HB3	1:B:392:VAL:CG2	2.03	0.89
1:B:26:LYS:HA	1:B:29:MSE:HE3	1.57	0.86
1:B:315:ALA:CB	1:B:392:VAL:HG21	2.05	0.86
1:D:177:MSE:CE	1:D:180:PRO:HB2	2.07	0.85
1:B:515:PRO:HG2	1:B:518:ASN:HD22	1.40	0.84
1:D:298:ILE:HG22	1:D:300:LYS:HG2	1.59	0.84
1:A:327:MSE:HE3	1:A:337:ALA:HB1	1.60	0.83
1:D:453:LYS:HZ3	1:D:457:GLY:HA2	1.44	0.82
1:B:66:LEU:HD22	1:B:70:ARG:NH1	1.92	0.82
1:A:381:VAL:CG1	1:A:407:MSE:HE3	2.09	0.82
1:C:184:LEU:HD12	1:C:200:PRO:HG3	1.61	0.82
1:B:334:GLU:O	1:B:338:GLN:HG3	1.78	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:520:GLN:H	1:B:520:GLN:HE21	1.26	0.81
1:B:492:LEU:HD22	1:B:496:LYS:HE3	1.61	0.80
1:A:407:MSE:HA	1:A:407:MSE:HE2	1.63	0.80
1:C:73:LYS:HE3	1:C:73:LYS:HA	1.64	0.80
1:D:323:ILE:HG22	1:D:327:MSE:HE2	1.62	0.79
1:A:371:GLU:H	1:A:371:GLU:CD	1.91	0.79
1:C:286:VAL:CG2	1:C:467:ASN:HA	2.13	0.79
1:B:527:ALA:O	1:B:531:THR:HG23	1.83	0.78
1:A:323:ILE:HG22	1:A:327:MSE:HE2	1.66	0.77
1:C:327:MSE:HE3	1:C:337:ALA:HB1	1.67	0.77
1:D:453:LYS:NZ	1:D:457:GLY:HA2	1.99	0.77
1:B:520:GLN:H	1:B:520:GLN:NE2	1.83	0.76
1:C:527:ALA:O	1:C:531:THR:HG23	1.86	0.76
1:C:183:LYS:HE2	1:C:255:GLU:CD	2.10	0.75
1:A:544:PRO:HD3	1:D:248:ARG:NH1	2.02	0.75
1:C:392:VAL:HG13	1:C:392:VAL:O	1.86	0.74
1:D:177:MSE:HE3	1:D:177:MSE:O	1.88	0.73
1:B:29:MSE:HE2	1:B:50:LEU:CD2	2.15	0.73
1:C:369:ALA:HB1	1:C:373:ILE:HD11	1.70	0.73
1:B:29:MSE:HE1	1:B:53:LEU:HD12	1.71	0.72
1:B:29:MSE:HE1	1:B:53:LEU:CD1	2.20	0.71
1:D:183:LYS:HE3	1:D:255:GLU:CD	2.15	0.71
1:C:520:GLN:H	1:C:520:GLN:HE21	1.35	0.71
1:A:85:ILE:HD12	1:A:96:PHE:HE1	1.56	0.70
1:D:194:ARG:HG2	1:D:194:ARG:HH11	1.55	0.70
1:C:338:GLN:NE2	1:C:364:PRO:HB3	2.06	0.70
1:D:308:LEU:HB3	1:D:389:ILE:HD12	1.75	0.69
1:B:392:VAL:O	1:B:392:VAL:HG22	1.91	0.69
1:C:371:GLU:H	1:C:371:GLU:CD	1.99	0.69
1:D:520:GLN:H	1:D:520:GLN:HE21	1.41	0.68
1:C:520:GLN:H	1:C:520:GLN:NE2	1.90	0.68
1:C:315:ALA:CB	1:C:392:VAL:HG21	2.24	0.68
1:C:354:ARG:CZ	1:C:356:ALA:HB3	2.24	0.68
1:D:456:ASP:OD1	1:D:458:ARG:HD3	1.94	0.68
1:A:81:LYS:O	1:A:85:ILE:HG23	1.92	0.68
1:C:41:THR:OG1	1:C:44:GLU:HG3	1.94	0.67
1:A:183:LYS:HE3	1:A:255:GLU:CD	2.20	0.67
1:A:179:ILE:HB	1:A:180:PRO:HD3	1.76	0.67
1:B:286:VAL:CG2	1:B:467:ASN:HA	2.25	0.67
1:D:332:LEU:HD12	1:D:332:LEU:H	1.59	0.67
1:A:211:ALA:HA	1:A:214:LYS:HE2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:ILE:HB	1:D:180:PRO:HD3	1.78	0.66
1:B:33:ARG:HD3	1:B:93:GLU:OE2	1.96	0.66
1:D:248:ARG:HG2	1:D:248:ARG:HH11	1.60	0.65
1:A:493:GLU:HG3	1:A:533:TYR:CD1	2.32	0.65
1:B:350:LEU:HD22	1:B:354:ARG:CZ	2.26	0.65
1:C:383:ILE:HG22	1:C:384:LEU:HD12	1.79	0.65
1:C:315:ALA:HB3	1:C:392:VAL:HG21	1.79	0.65
1:B:85:ILE:HD11	1:B:111:VAL:HG22	1.78	0.65
1:A:520:GLN:HE21	1:A:520:GLN:H	1.44	0.64
1:A:532:GLU:HG2	1:A:549:LYS:HG3	1.78	0.64
1:D:68:PHE:CD2	1:D:99:ILE:HG13	2.32	0.64
1:C:243:THR:HG21	1:C:273:TYR:CD2	2.33	0.64
1:D:81:LYS:O	1:D:85:ILE:HG23	1.96	0.64
1:D:298:ILE:HD11	1:D:442:LEU:HD12	1.80	0.64
1:D:358:ILE:HD13	1:D:366:THR:HG21	1.80	0.64
1:B:85:ILE:HD12	1:B:85:ILE:C	2.23	0.63
1:D:239:MSE:HE1	1:D:254:PHE:HZ	1.61	0.63
1:B:308:LEU:HB3	1:B:389:ILE:HD12	1.80	0.63
1:C:286:VAL:HG21	1:C:467:ASN:CA	2.23	0.63
1:D:300:LYS:NZ	1:D:300:LYS:HB3	2.13	0.63
1:D:308:LEU:HD23	1:D:389:ILE:HD11	1.81	0.63
1:B:154:HIS:HD2	6:B:2058:HOH:O	1.81	0.63
1:A:350:LEU:HD22	1:A:354:ARG:NH1	2.12	0.63
1:B:85:ILE:HD11	1:B:86:MSE:SE	2.48	0.62
1:B:391:GLY:HA3	1:B:427:GLU:HG2	1.81	0.62
1:B:308:LEU:HD23	1:B:389:ILE:HD11	1.80	0.62
1:A:286:VAL:CG2	1:A:467:ASN:HA	2.27	0.62
1:C:346:LYS:HE2	1:C:347:TYR:CZ	2.33	0.62
1:C:264:ARG:HG3	6:C:2075:HOH:O	2.00	0.62
1:C:324:VAL:HA	1:C:327:MSE:HE3	1.81	0.62
1:C:300:LYS:NZ	1:C:300:LYS:HB3	2.14	0.62
1:D:33:ARG:HD2	1:D:93:GLU:OE1	2.00	0.61
1:D:334:GLU:O	1:D:338:GLN:HG3	2.01	0.61
1:B:68:PHE:CD2	1:B:99:ILE:HG12	2.35	0.61
1:C:310:LEU:HD21	1:C:398:LEU:HB2	1.83	0.61
1:A:551:LYS:HG2	1:A:555:GLU:OE2	2.01	0.61
1:C:154:HIS:HD2	6:C:2072:HOH:O	1.84	0.60
1:C:538:LYS:N	1:C:538:LYS:HD2	2.16	0.60
1:C:179:ILE:HB	1:C:180:PRO:HD3	1.82	0.60
1:A:108:MSE:HB3	1:A:109:PRO:HD3	1.84	0.59
1:C:346:LYS:HE2	1:C:347:TYR:CE1	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:528:ILE:O	1:D:531:THR:HG23	2.02	0.59
1:B:179:ILE:HB	1:B:180:PRO:HD3	1.84	0.59
1:D:140:ARG:NH2	1:D:233:ASP:HB3	2.11	0.59
1:A:352:LYS:HE3	6:A:2093:HOH:O	2.03	0.59
1:B:286:VAL:HG22	1:B:470:ILE:HG12	1.83	0.59
1:B:493:GLU:HG3	1:B:533:TYR:CD1	2.38	0.59
1:B:324:VAL:HA	1:B:327:MSE:HE3	1.85	0.59
1:B:504:ASP:HA	1:B:507:LEU:HD12	1.84	0.59
1:C:52:GLY:HA3	1:D:146:ILE:HG23	1.83	0.59
1:B:551:LYS:HE2	1:B:555:GLU:OE1	2.03	0.59
1:C:298:ILE:HD11	1:C:442:LEU:HD12	1.84	0.59
1:D:298:ILE:CG2	1:D:300:LYS:HG2	2.31	0.59
1:C:354:ARG:NE	1:C:356:ALA:HB3	2.17	0.59
1:D:86:MSE:HE1	1:D:111:VAL:HG23	1.85	0.59
1:D:327:MSE:CE	1:D:337:ALA:HB1	2.27	0.59
1:A:163:GLY:HA2	1:A:166:ILE:HD11	1.84	0.58
1:C:371:GLU:OE1	1:C:371:GLU:N	2.32	0.58
1:A:132:GLY:CA	1:A:200:PRO:HG2	2.34	0.58
1:B:359:ASP:OD2	1:B:362:GLN:HG3	2.03	0.58
1:C:382:ASN:O	1:C:385:LYS:HD2	2.03	0.58
1:B:183:LYS:HE3	1:B:255:GLU:CD	2.29	0.58
1:A:327:MSE:CE	1:A:337:ALA:HB1	2.33	0.58
1:D:239:MSE:HE3	1:D:269:TYR:CE1	2.38	0.58
1:D:140:ARG:HD2	6:D:2042:HOH:O	2.03	0.57
1:A:41:THR:O	1:A:45:ARG:HG3	2.04	0.57
1:A:380:ALA:O	1:A:384:LEU:HD13	2.03	0.57
1:D:520:GLN:H	1:D:520:GLN:NE2	2.03	0.57
1:A:33:ARG:HD3	1:A:93:GLU:OE2	2.04	0.57
1:A:152:GLU:HG2	1:A:196:ASP:O	2.05	0.57
1:A:333:SER:OG	1:A:336:GLU:HG2	2.04	0.57
1:B:122:GLN:HG2	1:B:125:HIS:HB2	1.87	0.56
1:A:41:THR:OG1	1:A:44:GLU:HG3	2.06	0.56
1:B:327:MSE:HE3	1:B:337:ALA:HB1	1.86	0.56
1:B:456:ASP:OD1	1:B:458:ARG:HD3	2.05	0.56
1:B:41:THR:O	1:B:45:ARG:HG3	2.06	0.56
1:B:478:VAL:HG13	1:B:483:THR:HB	1.87	0.56
1:B:556:ARG:HG3	1:B:556:ARG:HH11	1.70	0.56
1:D:65:ALA:HA	1:D:99:ILE:HD11	1.85	0.56
1:D:70:ARG:O	1:D:74:LYS:HE3	2.04	0.56
1:C:327:MSE:CE	1:C:337:ALA:HB1	2.36	0.56
1:D:350:LEU:HD22	1:D:354:ARG:NH1	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:528:ILE:O	1:B:532:GLU:HG3	2.05	0.56
1:A:232:ASP:CG	1:A:264:ARG:HH22	2.14	0.56
1:A:520:GLN:H	1:A:520:GLN:NE2	2.03	0.56
1:B:315:ALA:HB2	6:B:2132:HOH:O	2.06	0.56
1:B:524:ILE:O	1:B:528:ILE:HG13	2.05	0.55
1:B:261:ASN:HD22	1:B:264:ARG:HH11	1.53	0.55
1:A:85:ILE:HG13	1:A:86:MSE:N	2.20	0.55
1:A:334:GLU:O	1:A:338:GLN:HG3	2.05	0.55
1:A:391:GLY:HA3	1:A:427:GLU:HG2	1.88	0.55
1:C:42:LEU:O	1:C:46:GLN:HG3	2.07	0.55
1:A:384:LEU:N	1:A:384:LEU:HD12	2.22	0.54
1:D:343:MSE:HE3	1:D:350:LEU:HD12	1.89	0.54
1:D:307:ILE:HD13	1:D:323:ILE:HD13	1.90	0.54
1:D:335:GLN:O	1:D:339:LYS:HG2	2.07	0.54
1:A:177:MSE:O	1:A:180:PRO:HD2	2.08	0.54
1:C:286:VAL:HG22	1:C:470:ILE:HG12	1.89	0.54
1:A:272:LYS:HD2	1:A:273:TYR:CE1	2.41	0.54
1:D:41:THR:O	1:D:45:ARG:HG3	2.07	0.54
1:D:177:MSE:CE	1:D:181:VAL:HG23	2.30	0.54
1:C:300:LYS:HB3	1:C:300:LYS:HZ2	1.73	0.54
1:C:384:LEU:HD12	1:C:384:LEU:N	2.23	0.54
1:A:527:ALA:O	1:A:531:THR:HG23	2.07	0.54
1:D:551:LYS:NZ	1:D:551:LYS:HB3	2.22	0.54
1:A:132:GLY:HA2	1:A:200:PRO:HG2	1.90	0.54
1:C:183:LYS:HE2	1:C:255:GLU:OE2	2.07	0.54
1:C:385:LYS:HG3	1:C:410:ILE:HD13	1.89	0.54
1:D:248:ARG:NH1	1:D:248:ARG:HG2	2.23	0.53
1:C:243:THR:HG21	1:C:273:TYR:HD2	1.73	0.53
1:C:338:GLN:HE22	1:C:364:PRO:HB3	1.73	0.53
1:D:108:MSE:HB3	1:D:109:PRO:HD3	1.91	0.53
1:C:86:MSE:SE	1:C:111:VAL:HG23	2.58	0.53
1:D:184:LEU:HD13	1:D:198:CYS:HB3	1.89	0.53
1:D:332:LEU:H	1:D:332:LEU:CD1	2.22	0.53
1:D:61:GLN:HA	1:D:64:GLN:HE21	1.73	0.53
1:B:502:LEU:HD11	1:B:512:LEU:C	2.34	0.53
1:B:333:SER:H	1:B:336:GLU:HG2	1.73	0.53
1:D:300:LYS:HB3	1:D:300:LYS:HZ3	1.72	0.53
1:A:363:GLU:HB3	1:A:364:PRO:HD3	1.90	0.53
1:C:302:ILE:HD13	1:C:332:LEU:HD13	1.91	0.53
1:B:46:GLN:HG2	1:B:51:GLN:HG3	1.91	0.52
1:C:194:ARG:NH1	1:C:197:ARG:NH2	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:GLY:CA	1:B:200:PRO:HG2	2.39	0.52
1:C:357:LYS:O	1:C:358:ILE:HD13	2.08	0.52
1:D:177:MSE:HE3	1:D:180:PRO:HB2	1.91	0.52
1:B:108:MSE:HB3	1:B:109:PRO:HD3	1.91	0.52
1:D:339:LYS:HA	1:D:367:HIS:CE1	2.43	0.52
1:A:286:VAL:HG22	1:A:470:ILE:HG12	1.90	0.52
1:A:227:ARG:HH11	1:A:227:ARG:HG2	1.74	0.52
1:D:391:GLY:HA3	1:D:427:GLU:HG2	1.92	0.52
1:C:33:ARG:HD3	1:C:93:GLU:OE2	2.10	0.52
1:D:33:ARG:NH2	1:D:196:ASP:HA	2.23	0.52
1:B:315:ALA:O	1:B:319:ILE:HG13	2.10	0.52
1:C:288:LEU:O	1:C:292:LEU:HD13	2.09	0.52
1:C:306:LYS:HE3	1:C:384:LEU:O	2.10	0.51
1:D:86:MSE:CE	1:D:111:VAL:HG23	2.40	0.51
1:D:96:PHE:O	1:D:100:LEU:HD22	2.10	0.51
1:B:339:LYS:HA	1:B:367:HIS:CE1	2.46	0.51
1:B:69:HIS:HE1	1:B:102:ASP:OD2	1.93	0.51
1:B:41:THR:OG1	1:B:44:GLU:HG3	2.10	0.51
1:A:478:VAL:HG13	1:A:483:THR:HB	1.92	0.51
1:B:421:ASN:ND2	3:B:603:TTN:O4	2.43	0.51
1:C:307:ILE:N	1:C:307:ILE:HD12	2.25	0.51
1:D:177:MSE:HE2	1:D:181:VAL:CG2	2.30	0.51
1:D:339:LYS:HE3	6:D:2100:HOH:O	2.10	0.51
1:B:150:TRP:CE2	1:B:199:LEU:HD13	2.45	0.51
1:D:140:ARG:HH22	1:D:233:ASP:CB	2.16	0.51
1:D:107:LEU:O	1:D:111:VAL:HG12	2.11	0.51
1:D:261:ASN:HD22	1:D:264:ARG:HE	1.59	0.51
1:B:165:ARG:NH1	2:B:601:ATP:O2B	2.43	0.51
1:C:260:HIS:CD2	1:C:264:ARG:HH21	2.29	0.51
1:C:287:ALA:O	1:C:291:LEU:HD22	2.10	0.51
1:B:184:LEU:HD22	1:B:198:CYS:HB3	1.93	0.51
1:D:51:GLN:HE21	1:D:51:GLN:HA	1.76	0.51
1:C:308:LEU:HB3	1:C:389:ILE:HD12	1.94	0.50
1:A:286:VAL:HG22	1:A:470:ILE:CG1	2.41	0.50
1:A:506:GLU:HA	1:A:509:GLN:NE2	2.27	0.50
1:B:243:THR:HG21	1:B:273:TYR:CD2	2.47	0.50
1:C:380:ALA:O	1:C:384:LEU:HD13	2.11	0.50
1:D:175:TYR:HE2	1:D:219:MSE:HG2	1.77	0.50
1:D:308:LEU:HB3	1:D:389:ILE:CD1	2.39	0.50
1:A:471:PHE:CG	1:A:472:PRO:HD3	2.47	0.50
1:C:108:MSE:HB3	1:C:109:PRO:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:VAL:HG22	1:B:470:ILE:CG1	2.42	0.50
1:D:243:THR:HG21	1:D:273:TYR:CD2	2.47	0.50
1:B:43:GLN:HG2	1:B:47:MSE:CE	2.32	0.49
1:B:332:LEU:H	1:B:332:LEU:CD1	2.25	0.49
1:B:232:ASP:OD1	1:B:264:ARG:NH2	2.44	0.49
1:B:302:ILE:HD12	1:B:305:HIS:ND1	2.26	0.49
1:B:350:LEU:HD22	1:B:354:ARG:NH2	2.26	0.49
1:C:41:THR:O	1:C:45:ARG:HG3	2.12	0.49
1:D:478:VAL:HG13	1:D:483:THR:HB	1.93	0.49
1:A:328:VAL:HA	1:A:332:LEU:O	2.13	0.49
1:B:518:ASN:HB3	1:B:521:GLU:CD	2.37	0.49
1:D:284:ALA:HA	1:D:319:ILE:HG12	1.95	0.49
1:A:389:ILE:HG23	1:A:399:PHE:CZ	2.47	0.49
1:A:466:ASN:ND2	3:A:603:TTN:O4	2.45	0.49
1:B:492:LEU:CD2	1:B:496:LYS:HE3	2.37	0.49
1:C:40:PHE:HE2	1:C:565:LEU:HD12	1.76	0.49
1:C:502:LEU:HD23	1:C:503:THR:O	2.12	0.49
1:A:65:ALA:HA	1:A:99:ILE:HD11	1.94	0.49
1:C:282:GLY:O	1:C:286:VAL:HG23	2.13	0.48
1:C:315:ALA:HB3	1:C:392:VAL:CG2	2.42	0.48
1:A:184:LEU:HD22	1:A:198:CYS:HB3	1.94	0.48
1:C:184:LEU:O	1:C:187:TYR:HB2	2.13	0.48
1:C:312:ALA:HB1	1:C:343:MSE:CE	2.43	0.48
1:D:476:LEU:O	1:D:480:LEU:HG	2.13	0.48
1:D:528:ILE:HA	1:D:531:THR:CG2	2.44	0.48
1:B:42:LEU:O	1:B:46:GLN:HG3	2.13	0.48
1:C:392:VAL:O	1:C:392:VAL:CG1	2.58	0.48
1:A:544:PRO:HD3	1:D:248:ARG:HH12	1.77	0.48
1:C:478:VAL:HG13	1:C:483:THR:HB	1.96	0.48
1:C:302:ILE:CD1	1:C:332:LEU:HD13	2.44	0.48
1:B:75:MSE:HE1	1:B:84:TYR:CD2	2.48	0.48
1:B:85:ILE:HD12	1:B:86:MSE:N	2.29	0.48
1:C:391:GLY:HA3	1:C:427:GLU:HG2	1.96	0.48
1:D:520:GLN:O	1:D:524:ILE:HG12	2.14	0.48
1:A:339:LYS:HB2	1:A:339:LYS:NZ	2.28	0.47
1:C:338:GLN:NE2	1:C:364:PRO:CB	2.75	0.47
1:D:503:THR:OG1	1:D:506:GLU:HG3	2.13	0.47
1:D:194:ARG:HG2	1:D:194:ARG:NH1	2.28	0.47
1:A:395:ALA:HB1	6:A:2097:HOH:O	2.13	0.47
1:C:319:ILE:O	1:C:323:ILE:HG13	2.15	0.47
1:D:319:ILE:O	1:D:323:ILE:HG13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:SER:H	1:A:336:GLU:CG	2.26	0.47
1:A:384:LEU:N	1:A:384:LEU:CD1	2.77	0.47
1:C:432:GLU:O	1:C:436:LEU:HB2	2.14	0.47
1:B:81:LYS:O	1:B:85:ILE:HG23	2.13	0.47
1:B:484:ARG:HG2	1:C:543:TYR:CZ	2.49	0.47
1:A:40:PHE:HE2	1:A:565:LEU:HD12	1.80	0.47
1:A:389:ILE:HG23	1:A:399:PHE:CE1	2.49	0.47
1:C:286:VAL:HG22	1:C:470:ILE:CG1	2.44	0.47
1:B:556:ARG:HG3	1:B:556:ARG:NH1	2.29	0.47
1:D:143:VAL:HB	1:D:237:GLU:HG2	1.96	0.47
1:D:492:LEU:HD22	1:D:496:LYS:HE2	1.96	0.47
1:A:130:PRO:HG3	1:B:54:LEU:HD23	1.96	0.47
1:B:312:ALA:HB1	1:B:343:MSE:HE3	1.98	0.47
1:B:505:GLU:CD	1:B:505:GLU:H	2.23	0.47
1:C:137:ILE:HA	1:C:234:LEU:HD22	1.97	0.47
1:D:156:LYS:HE3	6:D:2079:HOH:O	2.15	0.47
1:C:384:LEU:N	1:C:384:LEU:CD1	2.78	0.46
1:B:502:LEU:HD13	1:B:507:LEU:CD2	2.45	0.46
1:C:556:ARG:HG3	1:C:556:ARG:HH11	1.80	0.46
1:A:288:LEU:O	1:A:292:LEU:HD23	2.16	0.46
1:A:407:MSE:HA	1:A:407:MSE:CE	2.39	0.46
1:D:187:TYR:CD2	1:D:193:ILE:HD12	2.50	0.46
1:B:369:ALA:HB1	1:B:373:ILE:CD1	2.36	0.46
1:C:389:ILE:HG23	1:C:399:PHE:CE1	2.50	0.46
1:D:332:LEU:HD12	1:D:332:LEU:N	2.27	0.46
1:A:325:MSE:HA	1:A:328:VAL:HG22	1.96	0.46
1:C:261:ASN:ND2	1:C:264:ARG:NH2	2.63	0.46
1:D:64:GLN:NE2	1:D:562:TYR:OH	2.44	0.46
1:D:82:TYR:CE1	1:D:86:MSE:HE3	2.51	0.46
1:B:389:ILE:HG22	1:B:416:ILE:HA	1.97	0.46
1:D:239:MSE:HE1	1:D:254:PHE:CZ	2.47	0.46
1:A:550:ALA:O	1:A:554:LYS:HG3	2.15	0.46
1:B:520:GLN:HE21	1:B:520:GLN:N	2.04	0.46
1:C:280:ILE:O	1:C:284:ALA:HB2	2.14	0.46
1:D:535:TYR:CD2	1:D:545:GLU:HG3	2.50	0.46
1:A:146:ILE:HG23	1:B:52:GLY:HA3	1.98	0.46
1:C:261:ASN:ND2	1:C:264:ARG:HH22	2.13	0.46
1:D:502:LEU:HD11	1:D:512:LEU:C	2.41	0.46
1:B:332:LEU:N	1:B:332:LEU:HD12	2.31	0.46
1:B:502:LEU:HD13	1:B:507:LEU:HD21	1.98	0.46
1:A:214:LYS:HG3	6:A:2062:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:LEU:CD1	1:B:332:LEU:N	2.80	0.46
1:B:354:ARG:NE	1:B:358:ILE:HD11	2.31	0.46
1:C:328:VAL:HA	1:C:332:LEU:O	2.15	0.46
1:A:166:ILE:HG23	1:A:179:ILE:HG13	1.97	0.45
1:A:154:HIS:HD2	6:A:2073:HOH:O	1.98	0.45
1:B:233:ASP:CG	1:B:234:LEU:N	2.75	0.45
1:D:502:LEU:HD13	1:D:507:LEU:HD21	1.98	0.45
1:C:559:ARG:HB3	1:C:561:GLU:HG2	1.99	0.45
1:D:545:GLU:OE2	1:D:549:LYS:NZ	2.49	0.45
1:B:213:LEU:HD11	1:B:224:LYS:HD3	1.99	0.45
1:B:312:ALA:HB1	1:B:343:MSE:CE	2.46	0.45
1:C:73:LYS:HA	1:C:73:LYS:CE	2.42	0.45
1:D:122:GLN:HE21	1:D:122:GLN:HB3	1.52	0.45
1:C:308:LEU:HD12	1:C:309:PHE:N	2.32	0.45
1:A:282:GLY:O	1:A:286:VAL:HG23	2.17	0.45
1:B:307:ILE:HD13	1:B:323:ILE:HD13	1.99	0.45
1:D:165:ARG:NH2	3:D:603:TTN:O1	2.47	0.45
1:A:546:PRO:O	1:A:549:LYS:HE2	2.17	0.44
1:C:315:ALA:HB1	1:C:392:VAL:HG21	1.99	0.44
1:C:349:LEU:HD22	1:C:374:PRO:HG3	1.99	0.44
1:A:46:GLN:HG2	1:A:51:GLN:HG3	2.00	0.44
1:D:188:THR:HG21	1:D:195:PRO:HG3	1.99	0.44
1:D:239:MSE:CE	1:D:254:PHE:HZ	2.28	0.44
1:D:412:GLU:O	1:D:413:ARG:HD2	2.17	0.44
1:D:556:ARG:HG3	1:D:556:ARG:HH11	1.83	0.44
1:A:552:TYR:CE1	1:A:556:ARG:CZ	3.00	0.44
1:C:320:ALA:O	1:C:324:VAL:HG23	2.16	0.44
1:D:322:LEU:HA	1:D:322:LEU:HD12	1.82	0.44
1:B:284:ALA:HA	1:B:319:ILE:HG12	1.99	0.44
1:B:308:LEU:HB3	1:B:389:ILE:CD1	2.47	0.44
1:C:210:ILE:O	1:C:214:LYS:HG3	2.17	0.44
1:C:166:ILE:HD12	1:C:179:ILE:HG13	1.99	0.44
1:D:158:VAL:HG22	1:D:199:LEU:HB3	2.00	0.44
1:D:172:LEU:O	1:D:175:TYR:HB2	2.16	0.44
1:D:183:LYS:HE3	1:D:255:GLU:OE2	2.17	0.44
1:D:506:GLU:OE2	1:D:515:PRO:HD3	2.18	0.44
1:A:33:ARG:NH1	1:A:93:GLU:OE1	2.49	0.44
1:A:120:CYS:O	1:A:175:TYR:HB3	2.17	0.44
1:A:325:MSE:O	1:A:328:VAL:HG22	2.17	0.44
1:A:520:GLN:HB2	6:A:2126:HOH:O	2.16	0.44
1:C:218:TYR:O	1:D:57:LYS:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:MSE:HE1	1:B:53:LEU:HD13	1.98	0.44
1:B:110:ILE:N	1:B:110:ILE:HD12	2.33	0.44
1:D:85:ILE:HG13	1:D:86:MSE:N	2.27	0.44
1:A:204:ASP:OD2	1:B:56:PRO:HG2	2.18	0.44
1:B:77:SER:HB2	6:B:2015:HOH:O	2.18	0.44
1:B:329:GLU:O	1:B:329:GLU:HG2	2.18	0.44
1:C:377:PHE:CZ	1:C:389:ILE:HD11	2.53	0.44
1:A:308:LEU:HD23	1:A:389:ILE:HD11	2.00	0.44
1:B:261:ASN:ND2	1:B:264:ARG:HH11	2.15	0.44
1:B:333:SER:H	1:B:336:GLU:CG	2.30	0.44
1:B:515:PRO:CG	1:B:518:ASN:HD22	2.21	0.44
1:C:484:ARG:NH2	1:C:541:PHE:CD2	2.85	0.44
1:B:297:VAL:CG2	1:B:442:LEU:HD11	2.47	0.43
1:B:317:LEU:HD13	1:B:361:TYR:HB3	2.00	0.43
1:C:81:LYS:O	1:C:85:ILE:HG23	2.18	0.43
1:A:387:SER:HA	1:A:411:ASN:OD1	2.19	0.43
1:B:327:MSE:CE	1:B:337:ALA:HB1	2.48	0.43
1:D:78:PRO:HD2	6:D:2014:HOH:O	2.17	0.43
1:D:194:ARG:HA	1:D:195:PRO:HD3	1.91	0.43
1:D:492:LEU:HD23	1:D:492:LEU:O	2.19	0.43
1:B:528:ILE:HD13	1:B:550:ALA:HA	1.99	0.43
1:C:502:LEU:HD23	1:C:502:LEU:C	2.43	0.43
1:C:363:GLU:HB3	1:C:364:PRO:HD3	2.00	0.43
1:D:150:TRP:HA	1:D:151:PRO:HD3	1.78	0.43
1:A:91:ARG:HH21	5:A:605:FUM:C	2.30	0.43
1:A:542:ARG:HD3	1:A:542:ARG:C	2.43	0.43
1:B:85:ILE:CD1	1:B:86:MSE:SE	3.14	0.43
1:A:341:ILE:O	1:A:367:HIS:HE1	2.01	0.43
1:B:45:ARG:HB2	1:B:51:GLN:HE21	1.83	0.43
1:B:172:LEU:O	1:B:175:TYR:HB2	2.19	0.43
1:B:294:ALA:O	1:B:297:VAL:HG22	2.18	0.43
1:A:288:LEU:HG	1:A:292:LEU:CD2	2.49	0.43
1:A:394:GLY:HA2	1:A:420:SER:HB3	1.99	0.43
1:C:85:ILE:HD12	1:C:86:MSE:N	2.34	0.43
1:C:184:LEU:HD12	1:C:200:PRO:CG	2.41	0.43
1:C:240:LYS:HD2	6:C:2071:HOH:O	2.19	0.43
1:C:75:MSE:HE1	1:C:84:TYR:CG	2.53	0.43
1:C:111:VAL:HG22	1:C:111:VAL:O	2.19	0.43
1:C:284:ALA:HA	1:C:319:ILE:HG12	2.01	0.43
1:B:291:LEU:HD13	1:B:417:PHE:CE2	2.53	0.43
1:B:66:LEU:HD22	1:B:70:ARG:HH11	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:LEU:HD13	1:C:422:PRO:HD2	2.01	0.42
1:A:26:LYS:HB3	1:A:27:PRO:HD3	2.00	0.42
1:A:432:GLU:O	1:A:436:LEU:HD13	2.20	0.42
1:B:66:LEU:HD13	1:B:70:ARG:HH12	1.84	0.42
1:B:289:ALA:CB	1:B:498:LEU:HD23	2.49	0.42
1:B:354:ARG:HE	1:B:358:ILE:HD11	1.84	0.42
1:D:261:ASN:ND2	1:D:264:ARG:HH21	2.17	0.42
1:C:369:ALA:HB1	1:C:373:ILE:CD1	2.46	0.42
1:A:324:VAL:O	1:A:328:VAL:HG13	2.20	0.42
1:C:69:HIS:HE1	1:C:102:ASP:OD2	2.02	0.42
1:C:146:ILE:HG23	1:D:52:GLY:HA3	2.02	0.42
1:D:41:THR:OG1	1:D:44:GLU:HG3	2.19	0.42
1:B:85:ILE:CD1	1:B:111:VAL:HG22	2.48	0.42
1:B:132:GLY:HA2	1:B:200:PRO:HG2	2.02	0.42
1:B:380:ALA:O	1:B:384:LEU:HD23	2.20	0.42
1:D:394:GLY:HA2	1:D:420:SER:HB3	2.01	0.42
1:C:186:LEU:HD13	1:C:468:VAL:HG23	2.02	0.42
1:A:401:PRO:HA	1:A:436:LEU:CD2	2.50	0.42
1:B:487:SER:OG	1:B:539:MSE:HE1	2.19	0.42
1:B:520:GLN:O	1:B:524:ILE:HG12	2.19	0.42
1:C:542:ARG:HD3	1:C:542:ARG:C	2.44	0.42
1:D:551:LYS:HB3	1:D:551:LYS:HZ2	1.83	0.42
1:A:273:TYR:HB3	6:A:2074:HOH:O	2.20	0.42
1:A:308:LEU:HB3	1:A:389:ILE:HD12	2.01	0.42
1:B:532:GLU:HG2	1:B:549:LYS:HG2	2.01	0.42
1:C:38:MSE:HE3	1:C:59:GLU:OE1	2.19	0.42
1:A:108:MSE:N	1:A:109:PRO:CD	2.82	0.42
1:A:566:LEU:HA	1:A:567:PRO:HD3	1.95	0.42
1:B:263:PHE:CZ	1:B:314:GLU:HA	2.55	0.42
1:C:261:ASN:HD22	1:C:264:ARG:NH2	2.17	0.42
1:A:90:GLU:OE1	1:A:131:LYS:HE2	2.20	0.42
1:B:95:LEU:HG	1:B:99:ILE:HD12	2.01	0.42
1:B:328:VAL:HA	1:B:332:LEU:O	2.20	0.42
1:C:505:GLU:CD	1:C:505:GLU:H	2.27	0.42
1:D:324:VAL:O	1:D:328:VAL:HG23	2.19	0.42
1:D:542:ARG:HH12	1:D:544:PRO:HD2	1.85	0.42
1:A:104:ILE:HG13	1:A:108:MSE:HE2	2.02	0.41
1:A:227:ARG:HG2	1:A:227:ARG:NH1	2.34	0.41
1:B:493:GLU:HG3	1:B:533:TYR:CE1	2.55	0.41
1:A:142:HIS:HD1	1:D:568:ASP:CG	2.28	0.41
1:C:85:ILE:HD12	1:C:85:ILE:C	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:HA	1:A:50:LEU:HB2	2.02	0.41
1:A:86:MSE:SE	1:A:111:VAL:HG23	2.71	0.41
1:C:70:ARG:O	1:C:74:LYS:HD3	2.20	0.41
1:D:140:ARG:NH2	1:D:230:GLN:O	2.54	0.41
1:D:389:ILE:HG23	1:D:399:PHE:CE1	2.55	0.41
1:A:68:PHE:CD2	1:A:99:ILE:HG13	2.55	0.41
1:A:188:THR:HG21	1:A:195:PRO:HG3	2.01	0.41
1:A:194:ARG:HA	1:A:195:PRO:HD3	1.91	0.41
1:B:253:GLN:NE2	1:B:255:GLU:OE2	2.51	0.41
1:C:154:HIS:O	1:C:197:ARG:HD2	2.20	0.41
1:C:350:LEU:HD12	1:C:358:ILE:HD12	2.01	0.41
1:C:271:GLU:OE2	1:C:271:GLU:HA	2.19	0.41
1:C:466:ASN:ND2	3:C:603:TTN:O4	2.52	0.41
1:A:261:ASN:HD22	1:A:264:ARG:HE	1.68	0.41
1:D:328:VAL:HA	1:D:332:LEU:O	2.21	0.41
1:B:75:MSE:HE1	1:B:84:TYR:CG	2.56	0.41
1:B:454:LEU:CD1	1:B:460:PHE:HE2	2.33	0.41
1:A:383:ILE:HG22	1:A:384:LEU:HD12	2.01	0.41
1:B:108:MSE:N	1:B:109:PRO:CD	2.84	0.41
1:B:542:ARG:HD3	1:B:543:TYR:N	2.36	0.41
1:C:165:ARG:NH1	2:C:601:ATP:O2B	2.52	0.41
1:D:506:GLU:O	1:D:511:ARG:HB2	2.20	0.41
1:B:177:MSE:O	1:B:180:PRO:HD2	2.21	0.41
1:B:401:PRO:O	1:B:405:ARG:HG3	2.21	0.41
1:C:264:ARG:HG2	1:C:264:ARG:HH11	1.86	0.41
1:C:369:ALA:CB	1:C:373:ILE:HD11	2.47	0.41
1:C:389:ILE:HG22	1:C:416:ILE:HA	2.03	0.41
1:C:442:LEU:HD23	1:C:442:LEU:HA	1.95	0.41
1:D:109:PRO:HA	1:D:113:THR:O	2.21	0.41
1:D:294:ALA:O	1:D:297:VAL:HG22	2.21	0.41
1:A:52:GLY:HA3	1:B:146:ILE:HG23	2.02	0.41
1:A:242:ILE:HD13	1:A:242:ILE:HA	1.95	0.41
1:A:468:VAL:HA	1:A:471:PHE:CE2	2.57	0.41
1:C:174:VAL:C	1:C:176:GLY:N	2.79	0.41
1:C:345:ASP:OD1	1:C:345:ASP:C	2.64	0.41
1:A:411:ASN:HB2	1:A:414:PRO:HB3	2.03	0.40
1:D:363:GLU:HB2	1:D:364:PRO:HD3	2.02	0.40
1:A:243:THR:HG21	1:A:273:TYR:HD2	1.86	0.40
1:C:150:TRP:HA	1:C:151:PRO:HD3	1.86	0.40
1:C:412:GLU:O	1:C:413:ARG:HD2	2.22	0.40
1:C:456:ASP:OD1	1:C:456:ASP:C	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:PHE:HE2	1:B:565:LEU:HD12	1.86	0.40
1:A:298:ILE:HD11	1:A:442:LEU:HD12	2.04	0.40
1:C:61:GLN:HA	1:C:64:GLN:HE21	1.86	0.40
1:D:359:ASP:OD2	1:D:359:ASP:C	2.63	0.40
1:A:177:MSE:C	1:A:180:PRO:HD2	2.46	0.40
1:B:120:CYS:O	1:B:175:TYR:HB3	2.22	0.40
1:C:97:TYR:CE2	1:C:188:THR:HB	2.56	0.40
1:C:154:HIS:O	1:C:197:ARG:CD	2.70	0.40
1:D:33:ARG:HH21	1:D:152:GLU:HG3	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	549/551 (100%)	531 (97%)	17 (3%)	1 (0%)	43	51
1	B	549/551 (100%)	530 (96%)	17 (3%)	2 (0%)	30	34
1	C	549/551 (100%)	528 (96%)	20 (4%)	1 (0%)	43	51
1	D	549/551 (100%)	527 (96%)	21 (4%)	1 (0%)	43	51
All	All	2196/2204 (100%)	2116 (96%)	75 (3%)	5 (0%)	43	51

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	397	ARG
1	B	397	ARG
1	D	397	ARG
1	C	392	VAL
1	B	392	VAL

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	467/453 (103%)	446 (96%)	21 (4%)	24	33
1	B	467/453 (103%)	451 (97%)	16 (3%)	32	44
1	C	467/453 (103%)	446 (96%)	21 (4%)	24	33
1	D	467/453 (103%)	436 (93%)	31 (7%)	15	18
All	All	1868/1812 (103%)	1779 (95%)	89 (5%)	23	30

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	PRO
1	A	85	ILE
1	A	99	ILE
1	A	100	LEU
1	A	152	GLU
1	A	169	LEU
1	A	221	LEU
1	A	248	ARG
1	A	251	LEU
1	A	272	LYS
1	A	291	LEU
1	A	339	LYS
1	A	350	LEU
1	A	389	ILE
1	A	492	LEU
1	A	502	LEU
1	A	505	GLU
1	A	506	GLU
1	A	520	GLN
1	A	559	ARG
1	A	561	GLU
1	B	85	ILE
1	B	99	ILE
1	B	100	LEU

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Mol	Chain	Res	Type
1	B	133	LEU
1	B	169	LEU
1	B	221	LEU
1	B	233	ASP
1	B	251	LEU
1	B	291	LEU
1	B	297	VAL
1	B	350	LEU
1	B	371	GLU
1	B	398	LEU
1	B	436	LEU
1	B	492	LEU
1	B	520	GLN
1	C	66	LEU
1	C	70	ARG
1	C	73	LYS
1	C	99	ILE
1	C	114	PRO
1	C	133	LEU
1	C	165	ARG
1	C	169	LEU
1	C	242	ILE
1	C	251	LEU
1	C	297	VAL
1	C	300	LYS
1	C	339	LYS
1	C	359	ASP
1	C	371	GLU
1	C	436	LEU
1	C	455	THR
1	C	507	LEU
1	C	520	GLN
1	C	559	ARG
1	C	561	GLU
1	D	33	ARG
1	D	43	GLN
1	D	74	LYS
1	D	85	ILE
1	D	99	ILE
1	D	100	LEU
1	D	122	GLN
1	D	133	LEU

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Mol	Chain	Res	Type
1	D	140	ARG
1	D	153	ASN
1	D	165	ARG
1	D	169	LEU
1	D	219	MSE
1	D	221	LEU
1	D	229	GLN
1	D	251	LEU
1	D	266	LEU
1	D	291	LEU
1	D	292	LEU
1	D	300	LYS
1	D	350	LEU
1	D	363	GLU
1	D	371	GLU
1	D	389	ILE
1	D	409	SER
1	D	425	GLN
1	D	520	GLN
1	D	531	THR
1	D	547	GLU
1	D	551	LYS
1	D	561	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	64	GLN
1	A	154	HIS
1	A	230	GLN
1	A	261	ASN
1	A	330	ASN
1	A	338	GLN
1	A	425	GLN
1	A	482	ASN
1	A	520	GLN
1	B	43	GLN
1	B	51	GLN
1	B	64	GLN
1	B	69	HIS
1	B	154	HIS

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Mol	Chain	Res	Type
1	B	229	GLN
1	B	230	GLN
1	B	261	ASN
1	B	335	GLN
1	B	482	ASN
1	B	518	ASN
1	B	520	GLN
1	C	35	ASN
1	C	64	GLN
1	C	69	HIS
1	C	122	GLN
1	C	154	HIS
1	C	229	GLN
1	C	230	GLN
1	C	261	ASN
1	C	305	HIS
1	C	338	GLN
1	C	509	GLN
1	C	520	GLN
1	D	51	GLN
1	D	64	GLN
1	D	69	HIS
1	D	89	GLN
1	D	122	GLN
1	D	230	GLN
1	D	261	ASN
1	D	425	GLN
1	D	482	ASN
1	D	520	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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$
5	FUM	A	605	-	7,7,7	1.68	2 (28%)	8,8,8	0.56	0
2	ATP	D	601	-	32,33,33	1.65	9 (28%)	48,52,52	2.03	9 (18%)
3	TTN	A	603	4	5,7,7	1.42	2 (40%)	3,9,9	1.69	1 (33%)
2	ATP	B	602	-	32,33,33	1.73	8 (25%)	48,52,52	1.99	9 (18%)
3	TTN	B	603	4	5,7,7	1.45	2 (40%)	3,9,9	1.73	1 (33%)
2	ATP	B	601	-	32,33,33	1.79	6 (18%)	48,52,52	2.03	9 (18%)
3	TTN	D	603	4	5,7,7	1.45	2 (40%)	3,9,9	1.70	1 (33%)
5	FUM	C	605	-	7,7,7	1.56	2 (28%)	8,8,8	0.93	0
2	ATP	A	602	-	32,33,33	1.64	6 (18%)	48,52,52	2.01	8 (16%)
2	ATP	C	602	-	32,33,33	1.67	6 (18%)	48,52,52	2.02	9 (18%)
3	TTN	C	603	4	5,7,7	1.46	2 (40%)	3,9,9	1.71	1 (33%)
5	FUM	D	605	-	7,7,7	1.58	2 (28%)	8,8,8	0.58	0
2	ATP	D	602	-	32,33,33	1.61	7 (21%)	48,52,52	2.01	8 (16%)
2	ATP	A	601	-	32,33,33	1.64	9 (28%)	48,52,52	2.04	9 (18%)
2	ATP	C	601	-	32,33,33	1.65	7 (21%)	48,52,52	2.04	9 (18%)
5	FUM	B	605	-	7,7,7	1.56	2 (28%)	8,8,8	0.65	0

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
5	FUM	A	605	-	-	2/5/5/5	-
2	ATP	D	601	-	-	2/22/38/38	0/3/3/3
3	TTN	A	603	4	-	2/8/8/8	-
2	ATP	B	602	-	-	2/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TTN	B	603	4	-	0/8/8/8	-
2	ATP	B	601	-	-	2/22/38/38	0/3/3/3
3	TTN	D	603	4	-	2/8/8/8	-
5	FUM	C	605	-	-	0/5/5/5	-
2	ATP	A	602	-	-	2/22/38/38	0/3/3/3
2	ATP	C	602	-	-	2/22/38/38	0/3/3/3
3	TTN	C	603	4	-	2/8/8/8	-
5	FUM	D	605	-	-	2/5/5/5	-
2	ATP	D	602	-	-	2/22/38/38	0/3/3/3
2	ATP	A	601	-	-	5/22/38/38	0/3/3/3
2	ATP	C	601	-	-	3/22/38/38	0/3/3/3
5	FUM	B	605	-	-	2/5/5/5	-

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	ATP	PA-O3A	4.83	1.64	1.59
2	D	602	ATP	C5-N7	-4.51	1.30	1.39
2	B	601	ATP	C5-N7	-4.40	1.31	1.39
2	A	602	ATP	C5-N7	-4.36	1.31	1.39
2	C	602	ATP	C5-N7	-4.36	1.31	1.39
2	D	601	ATP	C5-N7	-4.30	1.31	1.39
2	C	601	ATP	C5-N7	-4.26	1.31	1.39
2	A	601	ATP	C5-N7	-4.18	1.31	1.39
2	B	602	ATP	C5-N7	-4.15	1.31	1.39
2	B	602	ATP	PB-O3B	3.32	1.63	1.59
2	B	601	ATP	C5-C4	-3.25	1.33	1.39
2	C	602	ATP	C5-C4	-3.20	1.33	1.39
2	C	601	ATP	C5-C4	-3.14	1.33	1.39
2	D	601	ATP	C5-C4	-3.11	1.33	1.39
2	A	602	ATP	PB-O3B	3.05	1.62	1.59
2	A	602	ATP	C5-C4	-2.90	1.33	1.39
2	A	601	ATP	C5-C4	-2.86	1.34	1.39
5	C	605	FUM	C5-C4	2.84	1.41	1.33
5	A	605	FUM	C4-C	2.78	1.55	1.48
2	B	602	ATP	PB-O3A	2.73	1.62	1.59
2	C	602	ATP	PB-O3A	2.72	1.62	1.59
2	C	602	ATP	PB-O3B	2.71	1.62	1.59
2	B	602	ATP	C8-N7	2.68	1.36	1.31
2	B	602	ATP	C5-C4	-2.64	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	ATP	PA-O3A	2.64	1.62	1.59
2	C	601	ATP	PB-O3B	2.60	1.62	1.59
2	D	602	ATP	C2-N1	2.59	1.38	1.33
2	D	602	ATP	C5-C4	-2.59	1.34	1.39
2	A	601	ATP	C4-N9	-2.59	1.32	1.37
2	C	601	ATP	C4-N9	-2.54	1.32	1.37
2	D	602	ATP	C8-N7	2.50	1.36	1.31
5	D	605	FUM	C4-C	2.49	1.54	1.48
5	B	605	FUM	C4-C	2.49	1.54	1.48
2	C	601	ATP	PA-O3A	2.45	1.62	1.59
2	D	602	ATP	C4-N9	-2.44	1.32	1.37
2	A	601	ATP	C2-N1	2.41	1.38	1.33
2	D	601	ATP	C4-N9	-2.38	1.32	1.37
2	B	601	ATP	C4-N9	-2.37	1.32	1.37
2	A	601	ATP	C8-N7	2.35	1.36	1.31
2	A	601	ATP	PA-O3A	2.34	1.62	1.59
5	D	605	FUM	C5-C4	2.34	1.40	1.33
5	B	605	FUM	C5-C4	2.34	1.40	1.33
2	A	601	ATP	PB-O3B	2.33	1.62	1.59
2	A	602	ATP	C2-N1	2.31	1.38	1.33
5	A	605	FUM	C5-C4	2.30	1.40	1.33
2	A	602	ATP	C8-N7	2.30	1.36	1.31
2	C	602	ATP	C2-N1	2.29	1.38	1.33
2	D	602	ATP	PB-O3B	2.29	1.62	1.59
3	B	603	TTN	O2-C1	-2.29	1.23	1.30
2	D	601	ATP	PB-O3B	2.29	1.62	1.59
2	C	602	ATP	C8-N7	2.28	1.36	1.31
2	B	602	ATP	C2-N1	2.27	1.38	1.33
3	C	603	TTN	O2-C1	-2.23	1.23	1.30
2	A	602	ATP	O4'-C1'	2.23	1.47	1.42
3	D	603	TTN	O5-C3	-2.20	1.23	1.30
2	B	601	ATP	C8-N7	2.20	1.35	1.31
3	A	603	TTN	O2-C1	-2.20	1.23	1.30
2	B	602	ATP	C4-N9	-2.19	1.33	1.37
2	D	601	ATP	C2-N1	2.19	1.37	1.33
2	D	601	ATP	PB-O3A	2.17	1.61	1.59
3	D	603	TTN	O2-C1	-2.17	1.23	1.30
3	C	603	TTN	O5-C3	-2.15	1.23	1.30
2	D	601	ATP	C8-N7	2.15	1.35	1.31
2	C	601	ATP	C2-N1	2.15	1.37	1.33
5	C	605	FUM	C4-C	2.12	1.53	1.48
2	A	601	ATP	PB-O3A	2.12	1.61	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	ATP	PA-O3A	2.11	1.61	1.59
3	B	603	TTN	O5-C3	-2.10	1.24	1.30
2	C	601	ATP	C8-N7	2.10	1.35	1.31
2	D	601	ATP	O4'-C1'	2.06	1.46	1.42
3	A	603	TTN	O5-C3	-2.05	1.24	1.30
2	B	601	ATP	PB-O3A	2.05	1.61	1.59
2	A	601	ATP	C2-N3	2.05	1.37	1.33
2	D	602	ATP	C2-N3	2.01	1.37	1.33

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	602	ATP	C5-C4-N3	-5.92	118.56	126.72
2	C	602	ATP	C5-C4-N3	-5.90	118.59	126.72
2	B	602	ATP	C5-C4-N3	-5.89	118.61	126.72
2	C	601	ATP	C5-C4-N3	-5.84	118.68	126.72
2	B	601	ATP	C5-C4-N3	-5.82	118.71	126.72
2	D	601	ATP	C5-C4-N3	-5.76	118.78	126.72
2	A	601	ATP	C5-C4-N3	-5.69	118.88	126.72
2	D	602	ATP	C5-C4-N3	-5.69	118.88	126.72
2	C	601	ATP	N3-C2-N1	-5.29	120.58	128.58
2	A	601	ATP	N3-C2-N1	-5.27	120.60	128.58
2	A	602	ATP	N3-C2-N1	-5.27	120.61	128.58
2	B	602	ATP	N3-C2-N1	-5.26	120.61	128.58
2	D	602	ATP	C6-C5-N7	-5.25	121.97	132.09
2	D	601	ATP	N3-C2-N1	-5.25	120.64	128.58
2	B	601	ATP	N3-C2-N1	-5.19	120.73	128.58
2	A	601	ATP	C6-C5-N7	-5.16	122.14	132.09
2	A	602	ATP	C6-C5-N7	-5.15	122.16	132.09
2	D	602	ATP	N3-C2-N1	-5.15	120.79	128.58
2	C	601	ATP	C6-C5-N7	-5.14	122.18	132.09
2	D	602	ATP	C6-C5-C4	5.10	124.14	117.18
2	C	602	ATP	N3-C2-N1	-5.09	120.88	128.58
2	C	602	ATP	C6-C5-N7	-5.08	122.30	132.09
2	D	601	ATP	C6-C5-N7	-5.06	122.34	132.09
2	B	601	ATP	C6-C5-N7	-5.06	122.34	132.09
2	C	601	ATP	C6-C5-C4	5.05	124.08	117.18
2	C	602	ATP	C6-C5-C4	5.05	124.08	117.18
2	A	602	ATP	C6-C5-C4	5.02	124.03	117.18
2	A	601	ATP	C6-C5-C4	4.98	123.98	117.18
2	B	602	ATP	C6-C5-N7	-4.96	122.53	132.09
2	D	601	ATP	C6-C5-C4	4.95	123.94	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	ATP	C6-C5-C4	4.93	123.91	117.18
2	C	602	ATP	N3-C4-N9	4.87	135.45	127.17
2	A	602	ATP	N3-C4-N9	4.85	135.42	127.17
2	B	601	ATP	N3-C4-N9	4.84	135.40	127.17
2	C	601	ATP	N3-C4-N9	4.83	135.38	127.17
2	A	601	ATP	N3-C4-N9	4.82	135.37	127.17
2	B	602	ATP	C6-C5-C4	4.82	123.76	117.18
2	D	601	ATP	N3-C4-N9	4.81	135.34	127.17
2	D	602	ATP	N3-C4-N9	4.72	135.19	127.17
2	B	602	ATP	N3-C4-N9	4.66	135.09	127.17
2	A	601	ATP	N9-C8-N7	-3.86	108.46	113.94
2	B	601	ATP	N9-C8-N7	-3.83	108.50	113.94
2	D	601	ATP	N9-C8-N7	-3.82	108.52	113.94
2	C	602	ATP	N9-C8-N7	-3.81	108.53	113.94
2	C	601	ATP	N9-C8-N7	-3.72	108.66	113.94
2	D	602	ATP	N9-C8-N7	-3.69	108.70	113.94
2	B	602	ATP	N9-C8-N7	-3.57	108.88	113.94
2	A	602	ATP	N9-C8-N7	-3.52	108.94	113.94
2	B	602	ATP	C2-N3-C4	3.28	119.84	111.83
2	A	602	ATP	C2-N3-C4	3.26	119.78	111.83
2	D	601	ATP	C2-N3-C4	3.19	119.61	111.83
2	C	602	ATP	C2-N3-C4	3.17	119.58	111.83
2	B	601	ATP	C2-N3-C4	3.14	119.50	111.83
2	C	601	ATP	C2-N3-C4	3.11	119.44	111.83
2	D	602	ATP	C2-N3-C4	3.10	119.41	111.83
2	A	601	ATP	C2-N3-C4	3.03	119.24	111.83
2	D	602	ATP	C4-C5-N7	2.90	113.89	110.58
2	A	601	ATP	C4-C5-N7	2.89	113.88	110.58
2	A	602	ATP	C4-C5-N7	2.82	113.81	110.58
2	B	601	ATP	C4-C5-N7	2.77	113.75	110.58
2	C	601	ATP	C4-C5-N7	2.76	113.73	110.58
2	D	601	ATP	C4-C5-N7	2.75	113.73	110.58
2	B	602	ATP	C4-C5-N7	2.73	113.71	110.58
2	C	602	ATP	C4-C5-N7	2.66	113.62	110.58
2	D	601	ATP	O4'-C1'-N9	2.49	112.86	108.09
2	B	601	ATP	O4'-C1'-N9	2.41	112.72	108.09
2	C	601	ATP	O4'-C1'-N9	2.39	112.69	108.09
3	B	603	TTN	O2-C1-O1	-2.34	118.78	124.08
3	D	603	TTN	O2-C1-O1	-2.27	118.93	124.08
3	C	603	TTN	O2-C1-O1	-2.22	119.04	124.08
3	A	603	TTN	O2-C1-O1	-2.22	119.04	124.08
2	B	602	ATP	C3'-C2'-C1'	2.12	105.47	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	602	ATP	C3'-C2'-C1'	2.07	105.38	101.46
2	A	601	ATP	O4'-C1'-N9	2.05	112.03	108.09

There are no chirality outliers.

All (32) torsion outliers are listed below:

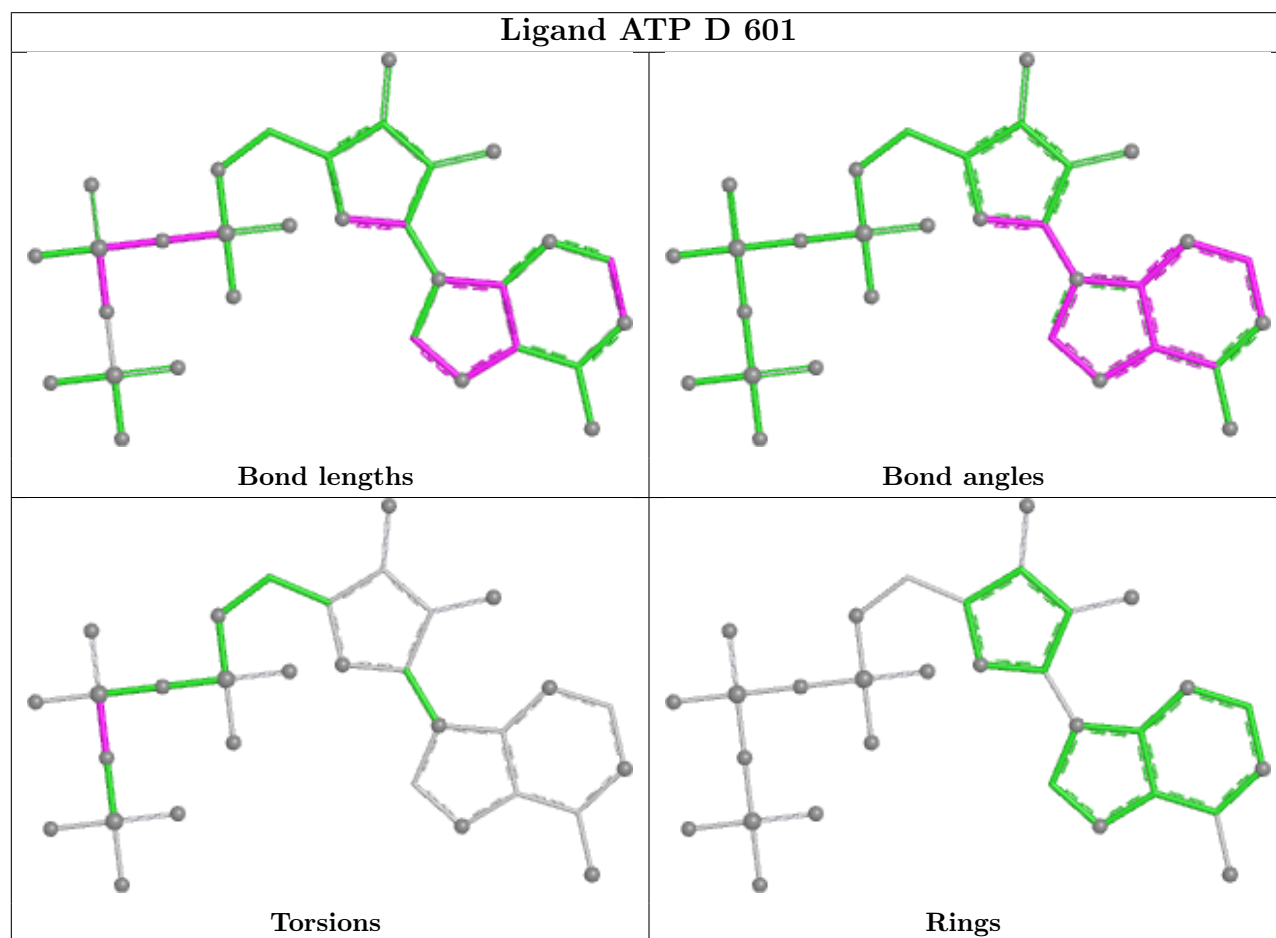
Mol	Chain	Res	Type	Atoms
3	A	603	TTN	O3-C2-C3-O4
3	A	603	TTN	O3-C2-C3-O5
3	C	603	TTN	O3-C2-C3-O4
3	C	603	TTN	O3-C2-C3-O5
2	A	602	ATP	PG-O3B-PB-O1B
2	C	602	ATP	PG-O3B-PB-O1B
3	D	603	TTN	O3-C2-C3-O4
2	B	602	ATP	PG-O3B-PB-O1B
5	D	605	FUM	C4-C5-C6-O7
5	D	605	FUM	C4-C5-C6-O8
2	A	602	ATP	PG-O3B-PB-O2B
2	B	601	ATP	PG-O3B-PB-O2B
2	B	602	ATP	PG-O3B-PB-O2B
2	C	601	ATP	PG-O3B-PB-O2B
2	C	602	ATP	PG-O3B-PB-O2B
2	D	602	ATP	PG-O3B-PB-O1B
2	D	602	ATP	PG-O3B-PB-O2B
3	D	603	TTN	O3-C2-C3-O5
5	B	605	FUM	C4-C5-C6-O8
5	B	605	FUM	C4-C5-C6-O7
2	A	601	ATP	PG-O3B-PB-O2B
2	A	601	ATP	PB-O3B-PG-O3G
2	B	601	ATP	PB-O3B-PG-O3G
2	C	601	ATP	PB-O3B-PG-O3G
2	A	601	ATP	O4'-C4'-C5'-O5'
2	D	601	ATP	PG-O3B-PB-O2B
2	C	601	ATP	O4'-C4'-C5'-O5'
5	A	605	FUM	C4-C5-C6-O8
5	A	605	FUM	C4-C5-C6-O7
2	A	601	ATP	PG-O3B-PB-O1B
2	A	601	ATP	PA-O3A-PB-O2B
2	D	601	ATP	PG-O3B-PB-O1B

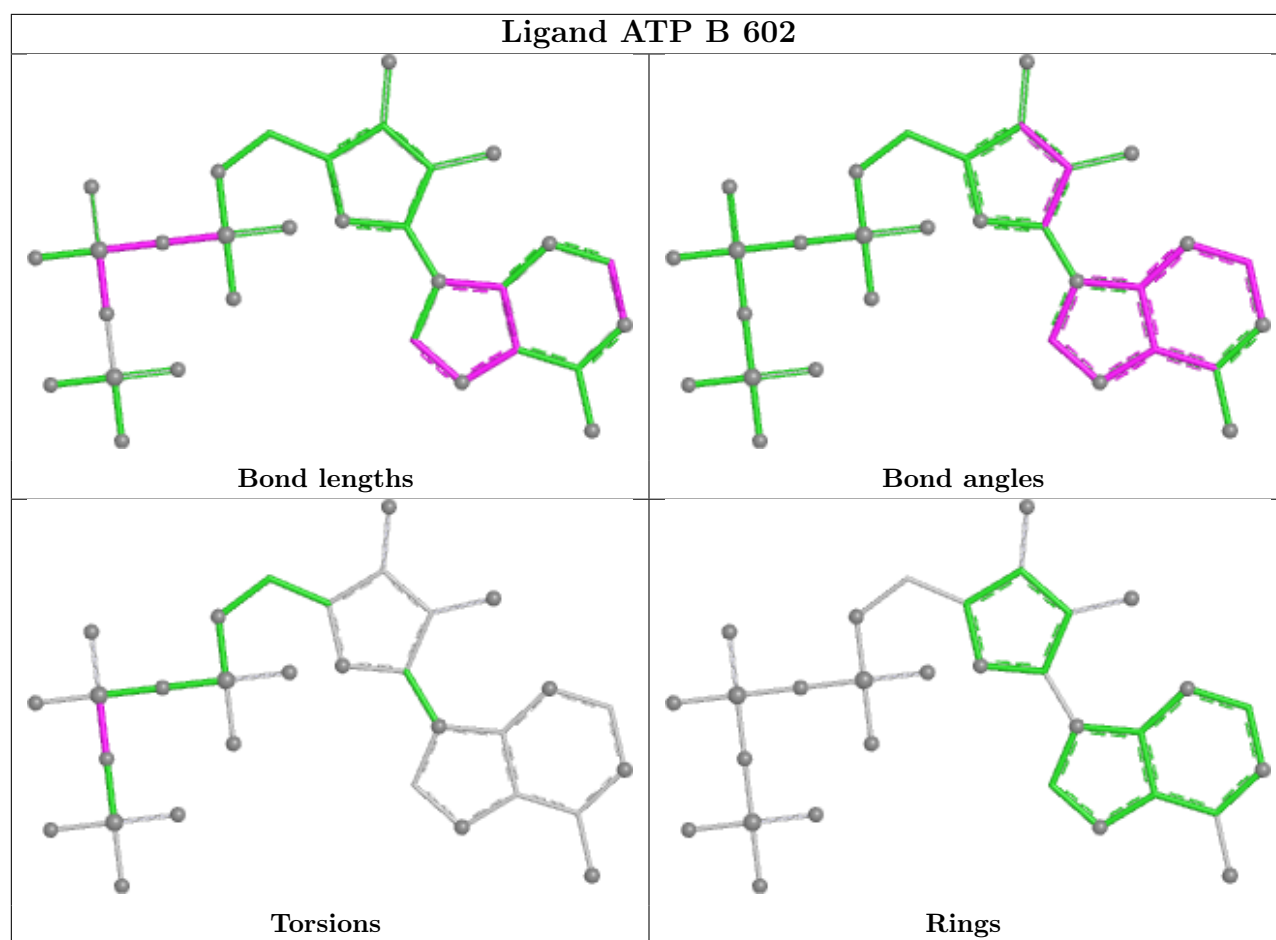
There are no ring outliers.

7 monomers are involved in 7 short contacts:

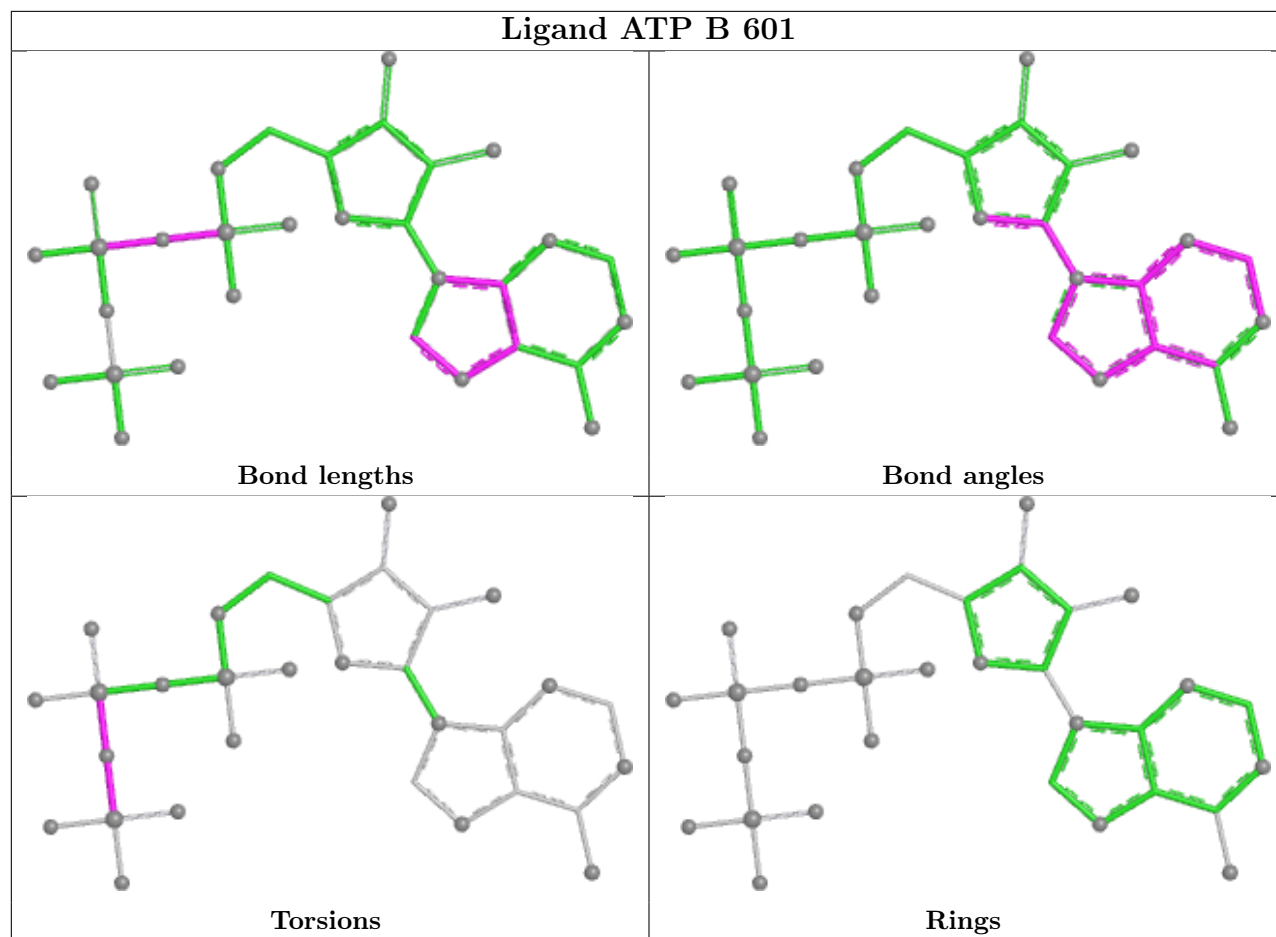
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	605	FUM	1	0
3	A	603	TTN	1	0
3	B	603	TTN	1	0
2	B	601	ATP	1	0
3	D	603	TTN	1	0
3	C	603	TTN	1	0
2	C	601	ATP	1	0

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.

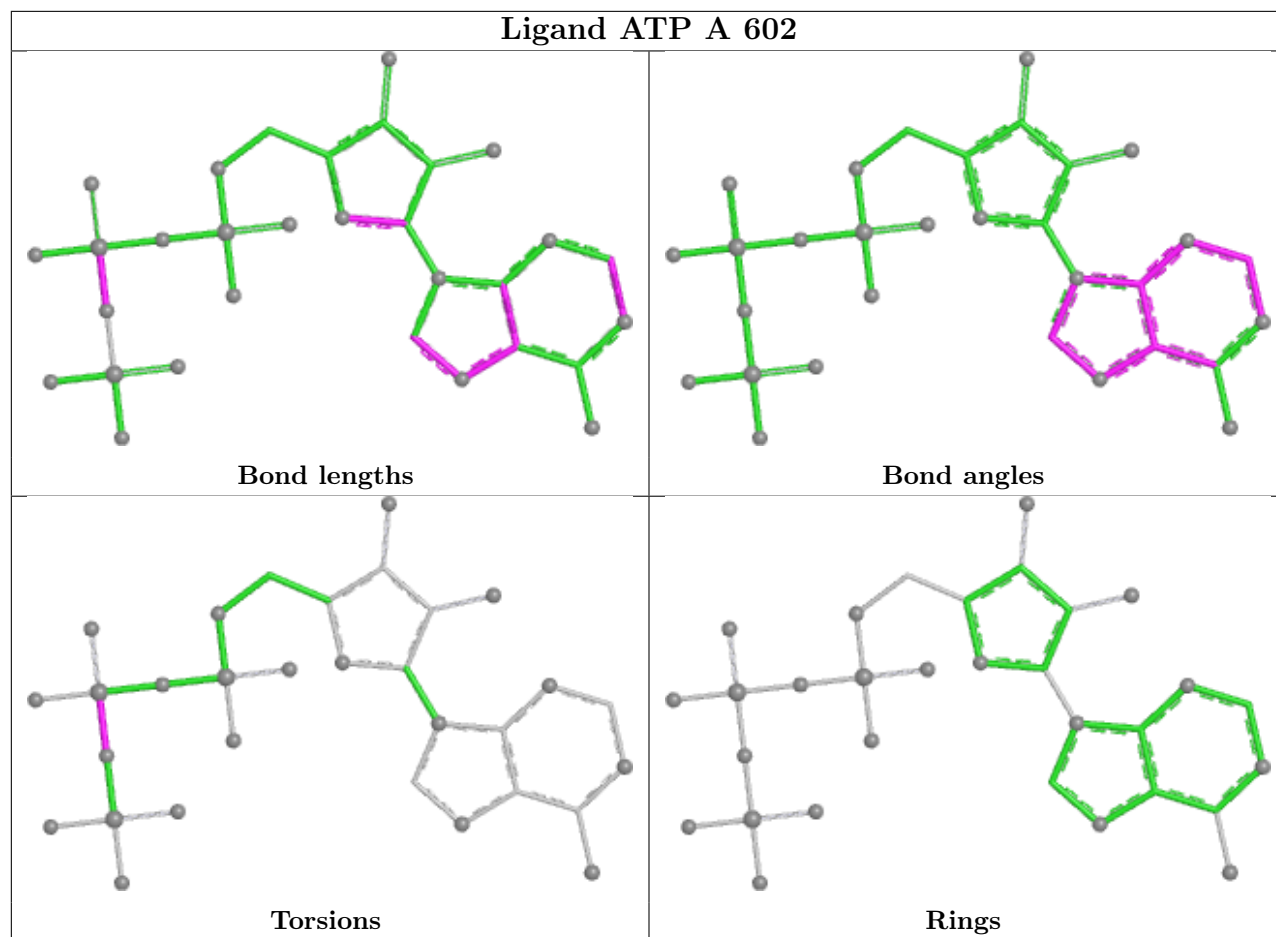


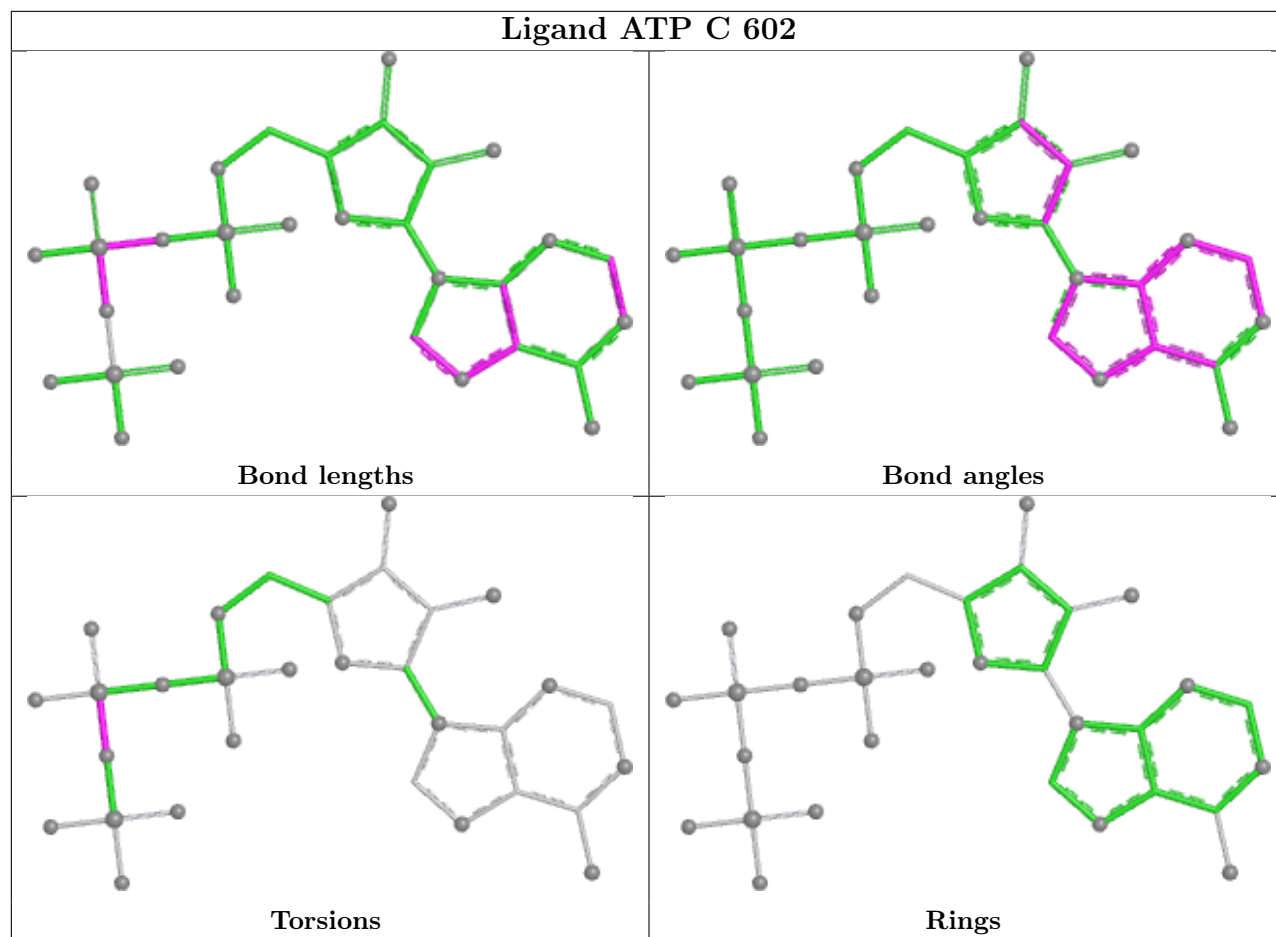


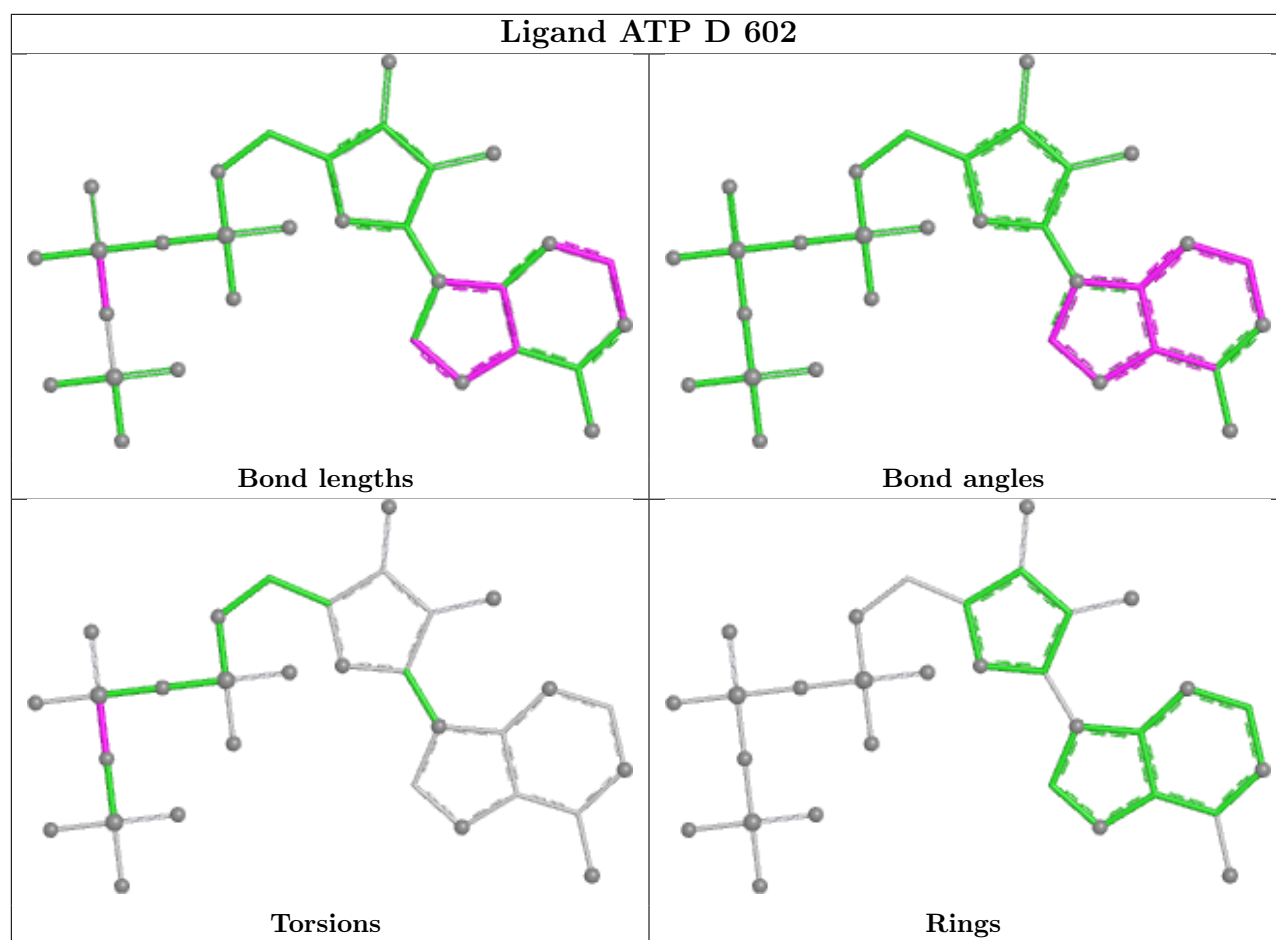
Ligand ATP B 601

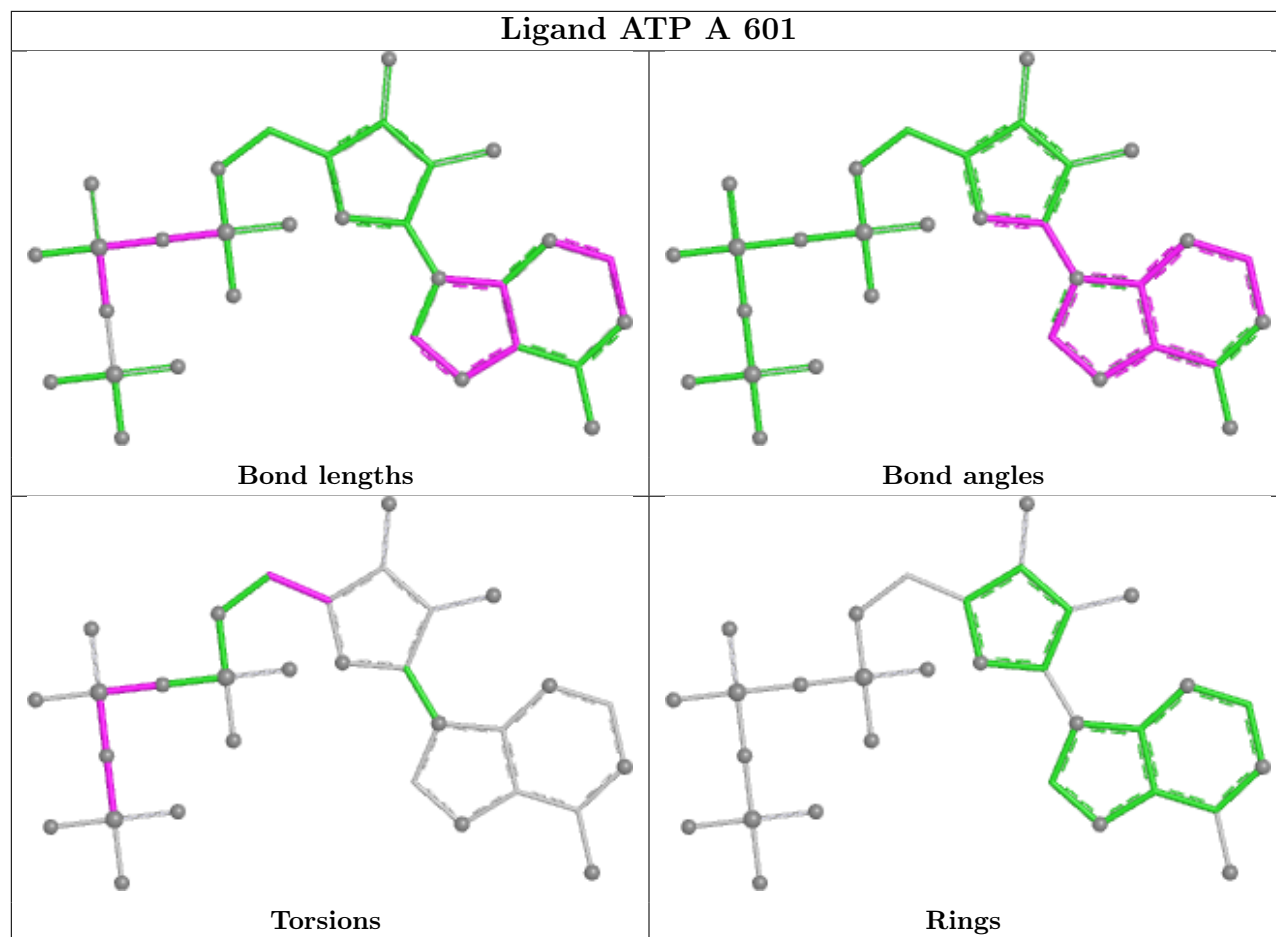


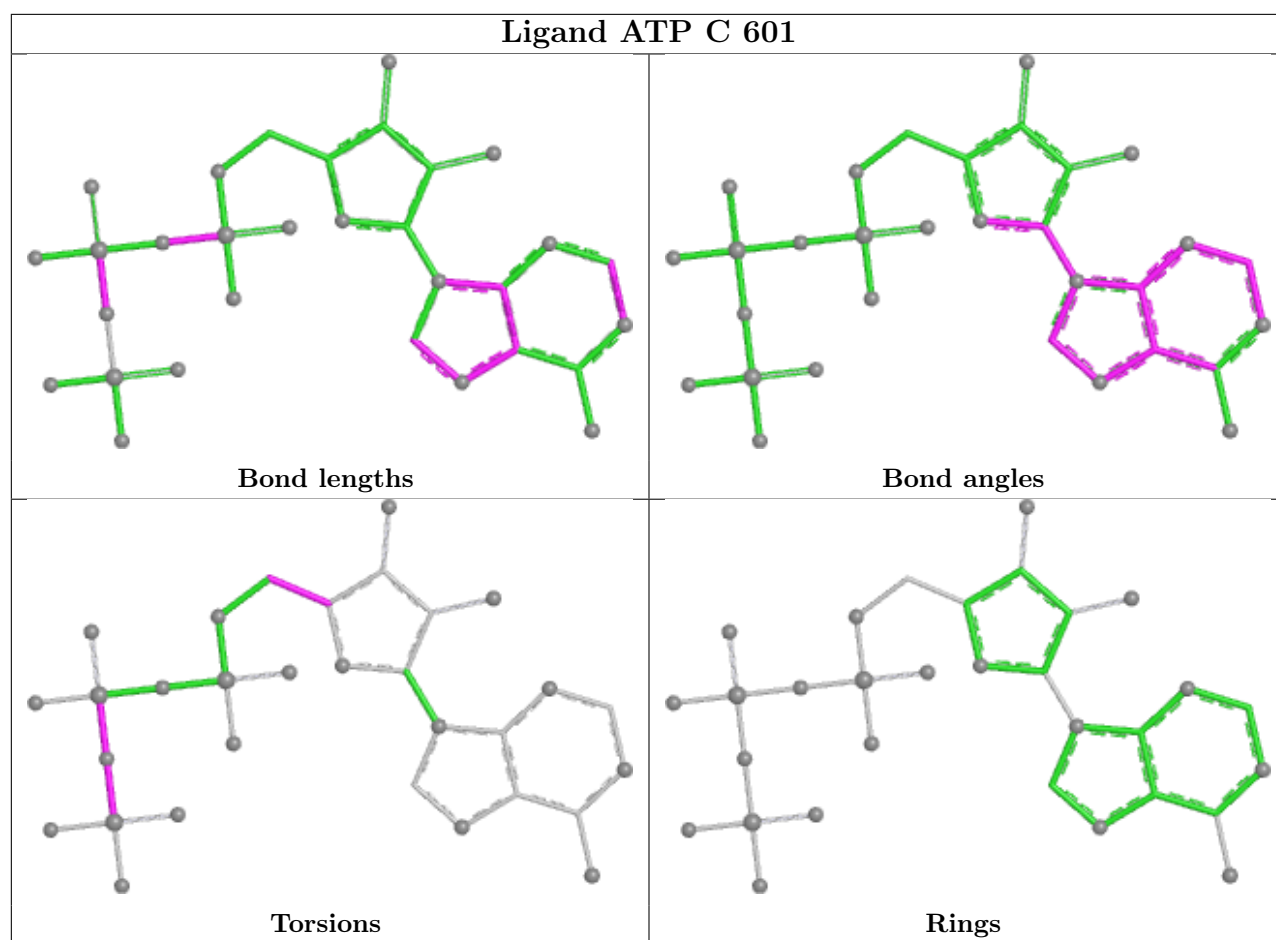
Ligand ATP A 602











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.