



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:10 PM UTC

PDB ID : 1PJ4 / pdb_00001pj4
Title : Crystal structure of human mitochondrial NAD(P)+-dependent malic enzyme in a pentary complex with natural substrate malate, ATP, Mn⁺⁺, and allosteric activator fumarate.
Authors : Tao, X.; Yang, Z.; Tong, L.
Deposited on : 2003-05-31
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

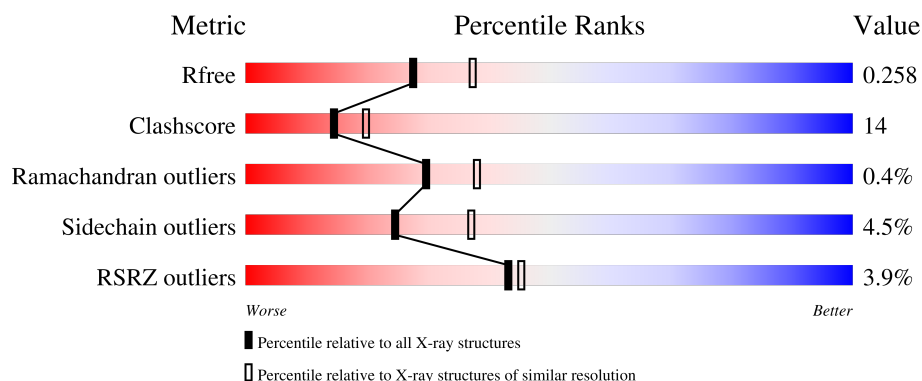
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	564	 3% 72% 23% ..
1	B	564	 5% 68% 27% ..
1	C	564	 4% 70% 26% ..
1	D	564	 3% 72% 23% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MLT	A	701	X	-	-	-
2	MLT	B	1701	X	-	-	-
2	MLT	C	2701	X	-	-	-
2	MLT	D	3701	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18442 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, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	Se	0	0	0
			4359	2790	743	803	9	14			
1	B	552	Total	C	N	O	S	Se	0	0	0
			4359	2790	743	803	9	14			
1	C	552	Total	C	N	O	S	Se	0	0	0
			4359	2790	743	803	9	14			
1	D	552	Total	C	N	O	S	Se	0	0	0
			4359	2790	743	803	9	14			

There are 56 discrepancies between the modelled and reference sequences:

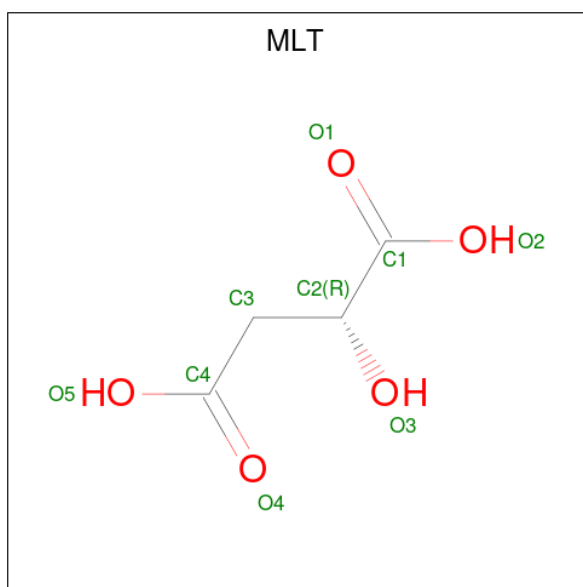
Chain	Residue	Modelled	Actual	Comment	Reference
A	29	MSE	MET	modified residue	UNP P23368
A	38	MSE	MET	modified residue	UNP P23368
A	47	MSE	MET	modified residue	UNP P23368
A	75	MSE	MET	modified residue	UNP P23368
A	86	MSE	MET	modified residue	UNP P23368
A	108	MSE	MET	modified residue	UNP P23368
A	177	MSE	MET	modified residue	UNP P23368
A	219	MSE	MET	modified residue	UNP P23368
A	239	MSE	MET	modified residue	UNP P23368
A	325	MSE	MET	modified residue	UNP P23368
A	327	MSE	MET	modified residue	UNP P23368
A	343	MSE	MET	modified residue	UNP P23368
A	407	MSE	MET	modified residue	UNP P23368
A	539	MSE	MET	modified residue	UNP P23368
B	1029	MSE	MET	modified residue	UNP P23368
B	1038	MSE	MET	modified residue	UNP P23368
B	1047	MSE	MET	modified residue	UNP P23368
B	1075	MSE	MET	modified residue	UNP P23368
B	1086	MSE	MET	modified residue	UNP P23368
B	1108	MSE	MET	modified residue	UNP P23368
B	1177	MSE	MET	modified residue	UNP P23368

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1219	MSE	MET	modified residue	UNP P23368
B	1239	MSE	MET	modified residue	UNP P23368
B	1325	MSE	MET	modified residue	UNP P23368
B	1327	MSE	MET	modified residue	UNP P23368
B	1343	MSE	MET	modified residue	UNP P23368
B	1407	MSE	MET	modified residue	UNP P23368
B	1539	MSE	MET	modified residue	UNP P23368
C	2029	MSE	MET	modified residue	UNP P23368
C	2038	MSE	MET	modified residue	UNP P23368
C	2047	MSE	MET	modified residue	UNP P23368
C	2075	MSE	MET	modified residue	UNP P23368
C	2086	MSE	MET	modified residue	UNP P23368
C	2108	MSE	MET	modified residue	UNP P23368
C	2177	MSE	MET	modified residue	UNP P23368
C	2219	MSE	MET	modified residue	UNP P23368
C	2239	MSE	MET	modified residue	UNP P23368
C	2325	MSE	MET	modified residue	UNP P23368
C	2327	MSE	MET	modified residue	UNP P23368
C	2343	MSE	MET	modified residue	UNP P23368
C	2407	MSE	MET	modified residue	UNP P23368
C	2539	MSE	MET	modified residue	UNP P23368
D	3029	MSE	MET	modified residue	UNP P23368
D	3038	MSE	MET	modified residue	UNP P23368
D	3047	MSE	MET	modified residue	UNP P23368
D	3075	MSE	MET	modified residue	UNP P23368
D	3086	MSE	MET	modified residue	UNP P23368
D	3108	MSE	MET	modified residue	UNP P23368
D	3177	MSE	MET	modified residue	UNP P23368
D	3219	MSE	MET	modified residue	UNP P23368
D	3239	MSE	MET	modified residue	UNP P23368
D	3325	MSE	MET	modified residue	UNP P23368
D	3327	MSE	MET	modified residue	UNP P23368
D	3343	MSE	MET	modified residue	UNP P23368
D	3407	MSE	MET	modified residue	UNP P23368
D	3539	MSE	MET	modified residue	UNP P23368

- Molecule 2 is D-MALATE (CCD ID: MLT) (formula: C₄H₆O₅).

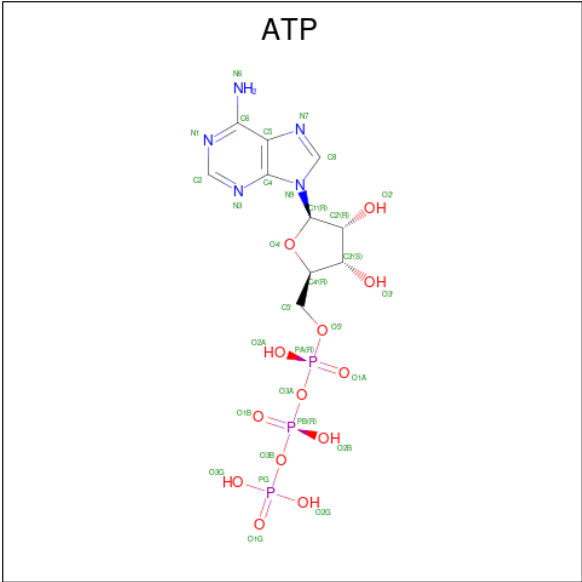


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			9	4	5		
2	B	1	Total	C	O	0	0
			9	4	5		
2	C	1	Total	C	O	0	0
			9	4	5		
2	D	1	Total	C	O	0	0
			9	4	5		

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

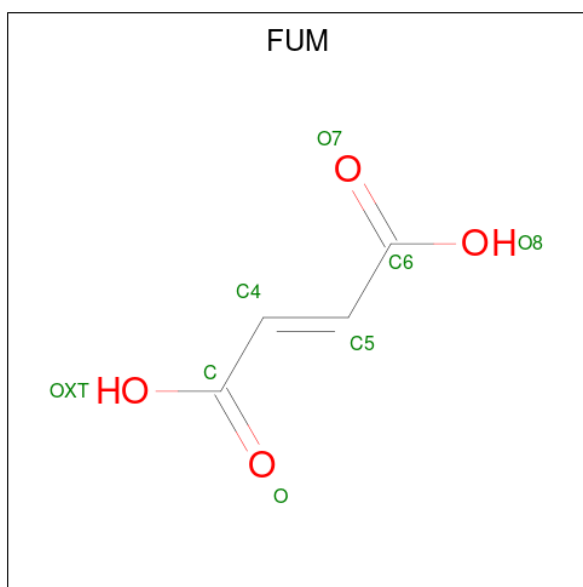
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 5 is FUMARIC ACID (CCD ID: FUM) (formula: C₄H₄O₄).



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

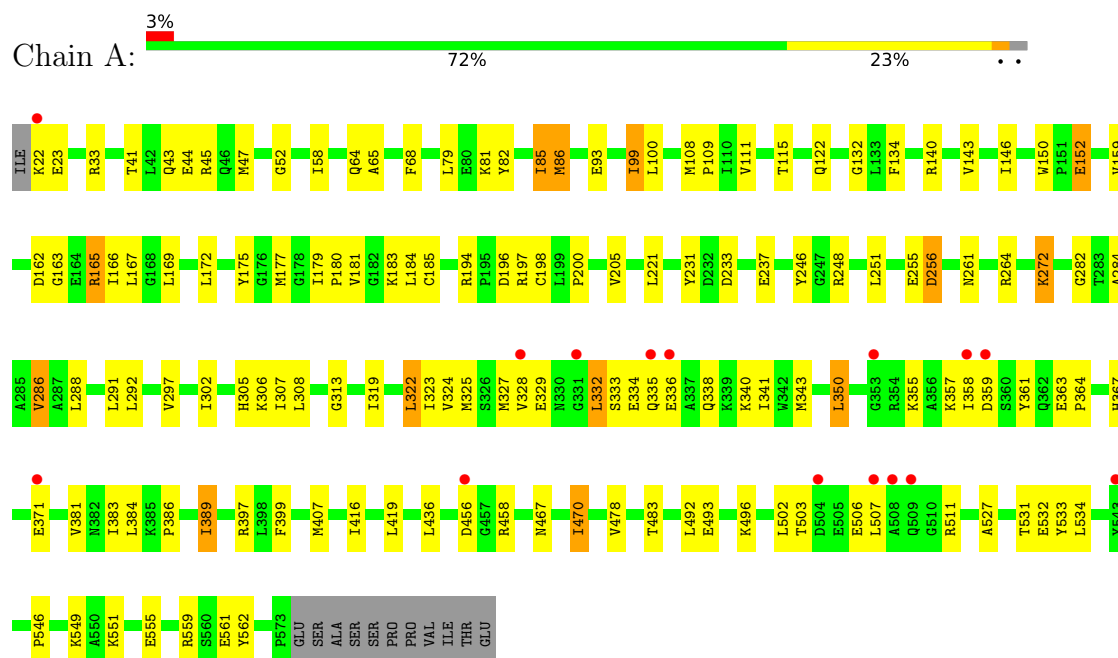
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	165	Total	O	0	0
			165	165		
6	B	176	Total	O	0	0
			176	176		
6	C	169	Total	O	0	0
			169	169		
6	D	176	Total	O	0	0
			176	176		

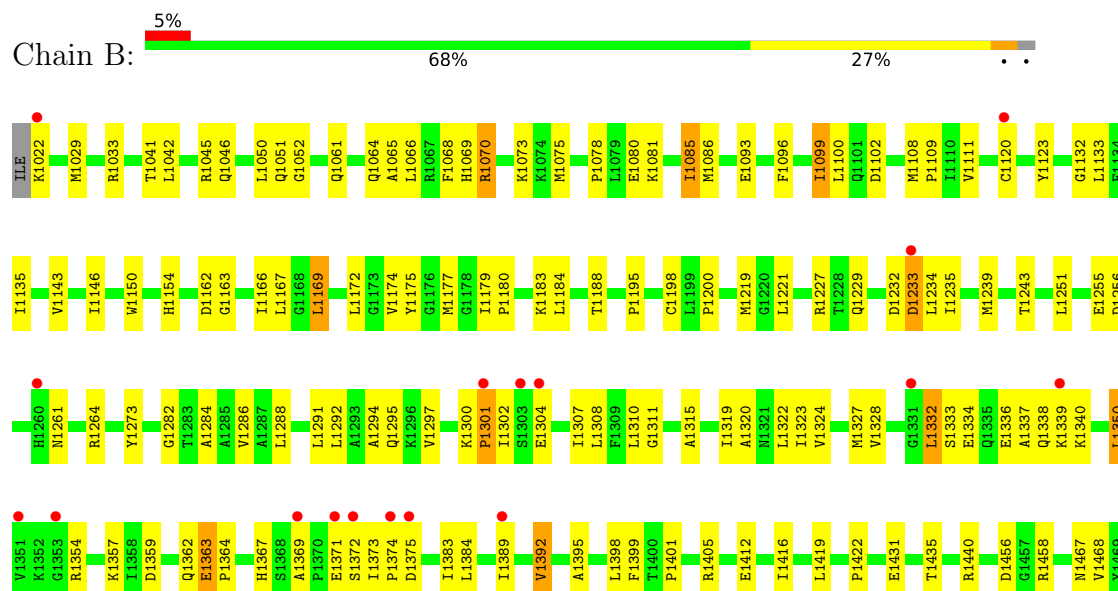
3 Residue-property plots

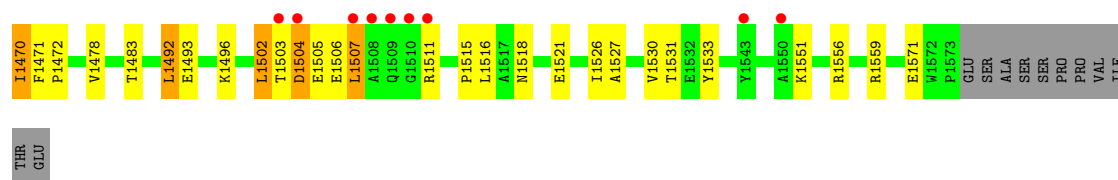
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: NAD-dependent malic enzyme, mitochondrial

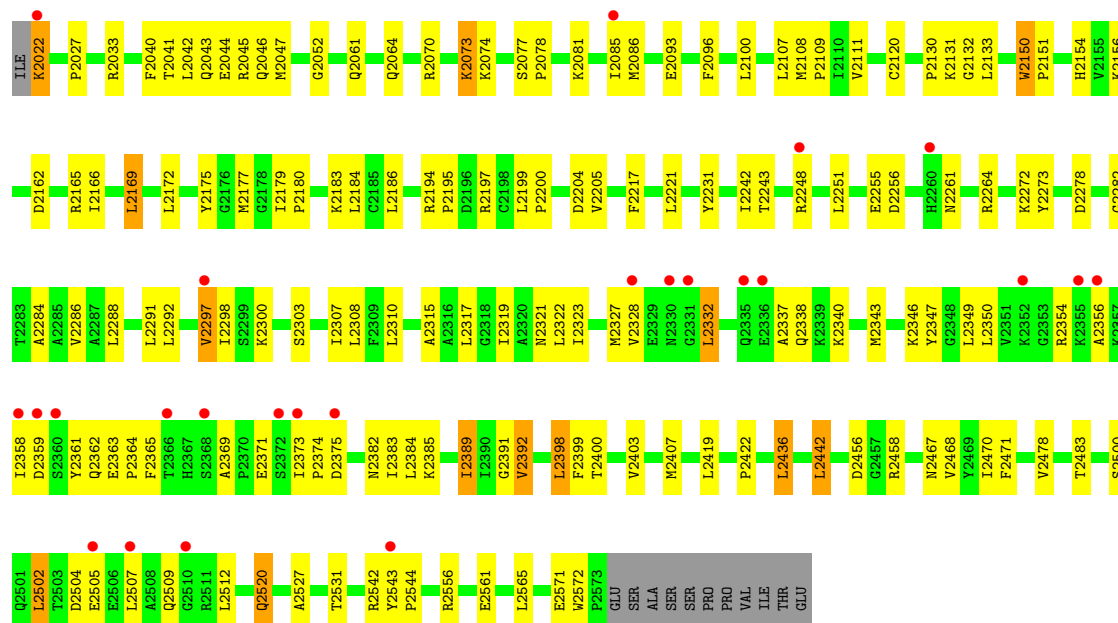


- Molecule 1: NAD-dependent malic enzyme, mitochondrial

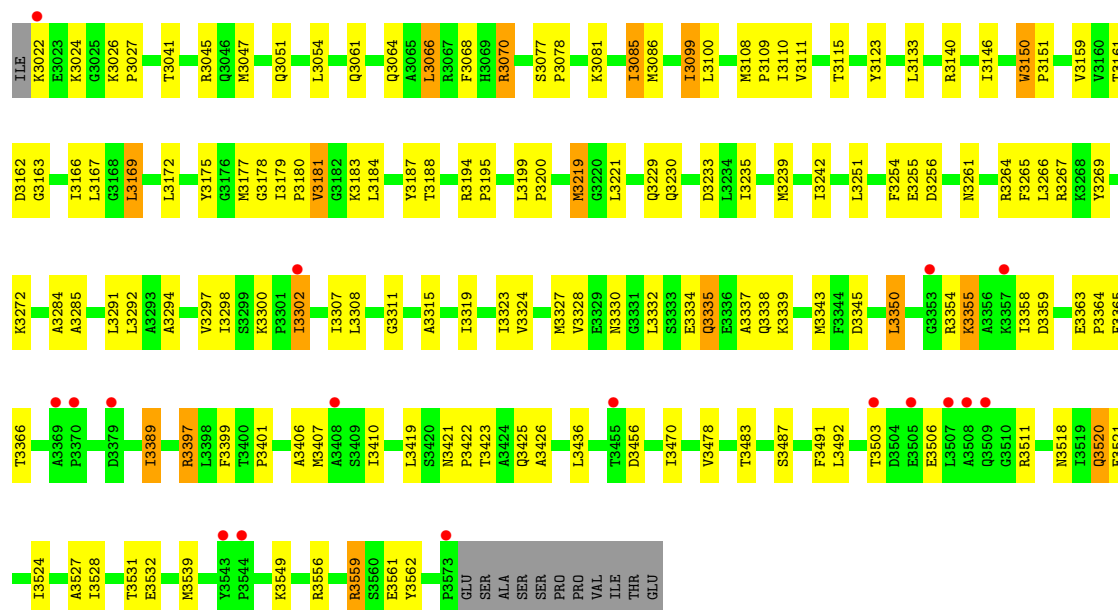




- Molecule 1: NAD-dependent malic enzyme, mitochondrial



- Molecule 1: NAD-dependent malic enzyme, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	226.05Å 117.34Å 111.31Å 90.00° 109.00° 90.00°	Depositor
Resolution (Å)	19.94 – 2.30 19.94 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.7 (19.94-2.30) 97.4 (19.94-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.93 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.211 , 0.252 0.217 , 0.258	Depositor DCC
R_{free} test set	8990 reflections (7.52%)	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	18442	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, MLT, MN, FUM

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	0.44	0/4439	0.90	10/5987 (0.2%)
1	B	0.44	0/4439	0.92	10/5987 (0.2%)
1	C	0.44	0/4439	0.90	6/5987 (0.1%)
1	D	0.44	0/4439	0.90	11/5987 (0.2%)
All	All	0.44	0/17756	0.90	37/23948 (0.2%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3470	ILE	N-CA-C	10.25	120.37	111.56
1	B	1470	ILE	N-CA-C	9.38	119.63	111.56
1	A	470	ILE	N-CA-C	8.43	119.40	111.48
1	D	3150	TRP	CA-C-N	7.85	127.76	119.05
1	D	3150	TRP	C-N-CA	7.85	127.76	119.05
1	D	3419	LEU	N-CA-C	7.66	122.45	113.18
1	A	419	LEU	N-CA-C	7.45	122.19	113.18
1	B	1150	TRP	CA-C-N	7.37	127.23	119.05
1	B	1150	TRP	C-N-CA	7.37	127.23	119.05
1	C	2150	TRP	CA-C-N	6.96	126.78	119.05
1	C	2150	TRP	C-N-CA	6.96	126.78	119.05
1	B	1419	LEU	N-CA-C	6.34	121.01	113.28
1	A	115	THR	N-CA-C	6.11	117.94	111.28
1	C	2419	LEU	N-CA-C	5.96	120.55	113.28
1	B	1311	GLY	N-CA-C	-5.90	105.68	112.29
1	D	3167	LEU	CB-CA-C	-5.90	109.76	116.54
1	B	1162	ASP	N-CA-C	-5.86	104.67	112.94
1	A	162	ASP	N-CA-C	-5.74	105.00	113.61
1	D	3470	ILE	CB-CA-C	-5.73	106.00	111.44
1	C	2162	ASP	N-CA-C	-5.70	104.91	112.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	TRP	CA-C-N	5.65	125.50	119.28
1	A	150	TRP	C-N-CA	5.65	125.50	119.28
1	B	1167	LEU	CB-CA-C	-5.54	110.17	116.54
1	B	1395	ALA	N-CA-C	5.53	119.19	111.56
1	A	256	ASP	N-CA-C	5.47	118.94	111.39
1	A	167	LEU	CB-CA-C	-5.46	110.27	116.54
1	D	3115	THR	N-CA-C	5.40	117.92	111.71
1	C	2442	LEU	N-CA-C	-5.37	99.65	108.41
1	D	3311	GLY	N-CA-C	-5.32	106.90	111.95
1	D	3187	TYR	N-CA-C	-5.30	105.40	111.07
1	D	3256	ASP	N-CA-C	5.29	118.69	111.39
1	B	1507	LEU	N-CA-C	-5.29	105.42	111.07
1	C	2256	ASP	N-CA-C	5.28	118.91	111.52
1	A	470	ILE	CB-CA-C	-5.25	107.25	111.71
1	A	246	TYR	N-CA-C	5.20	119.77	113.38
1	B	1310	LEU	N-CA-C	-5.09	99.49	108.20
1	D	3162	ASP	N-CA-C	-5.02	105.86	112.94

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4359	0	4396	113	0
1	B	4359	0	4396	140	0
1	C	4359	0	4396	136	0
1	D	4359	0	4396	114	0
2	A	9	0	3	0	0
2	B	9	0	3	0	0
2	C	9	0	3	0	0
2	D	9	0	3	1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	62	0	24	1	0
4	B	62	0	24	1	0
4	C	62	0	24	1	0
4	D	62	0	24	1	0
5	A	8	0	1	0	0
5	B	8	0	1	0	0
5	C	8	0	1	0	0
5	D	8	0	1	0	0
6	A	165	0	0	2	0
6	B	176	0	0	7	0
6	C	169	0	0	8	0
6	D	176	0	0	4	0
All	All	18442	0	17696	496	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 (496) 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:1315:ALA:HB3	1:B:1392:VAL:HG21	1.25	1.14
1:D:3177:MSE:HE1	1:D:3200:PRO:HB2	1.14	1.07
1:C:2286:VAL:HG21	1:C:2467:ASN:HA	1.38	1.05
1:B:1323:ILE:HG22	1:B:1327:MSE:HE2	1.40	1.03
1:C:2132:GLY:HA3	1:C:2177:MSE:CE	1.89	1.01
1:A:177:MSE:HE2	1:A:181:VAL:HG23	1.43	1.00
1:A:323:ILE:HG22	1:A:327:MSE:HE2	1.44	1.00
1:D:3343:MSE:HE2	1:D:3365:PHE:HB2	1.43	1.00
1:B:1286:VAL:HG21	1:B:1467:ASN:HA	1.41	0.99
1:D:3140:ARG:HH22	1:D:3233:ASP:HB3	1.29	0.94
1:D:3323:ILE:HG22	1:D:3327:MSE:HE2	1.46	0.94
1:A:177:MSE:HE1	1:A:180:PRO:HB2	1.53	0.91
1:A:286:VAL:HG21	1:A:467:ASN:HA	1.52	0.90
1:D:3177:MSE:HE1	1:D:3200:PRO:CB	2.01	0.90
1:D:3520:GLN:H	1:D:3520:GLN:HE21	1.19	0.90
1:B:1315:ALA:CB	1:B:1392:VAL:HG21	2.02	0.89
1:C:2073:LYS:HE3	1:C:2073:LYS:HA	1.53	0.88
1:A:407:MSE:HA	1:A:407:MSE:HE2	1.55	0.87
1:B:1069:HIS:O	1:B:1073:LYS:HG2	1.76	0.85
1:A:371:GLU:H	1:A:371:GLU:CD	1.83	0.84
1:C:2343:MSE:HE2	1:C:2365:PHE:HB2	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:MSE:HE1	1:A:200:PRO:HB2	1.61	0.83
1:A:177:MSE:HE3	1:A:177:MSE:O	1.77	0.83
1:B:1066:LEU:HD22	1:B:1070:ARG:NH1	1.93	0.83
1:A:478:VAL:HG13	1:A:483:THR:HB	1.61	0.81
1:C:2520:GLN:H	1:C:2520:GLN:HE21	1.27	0.81
1:B:1334:GLU:O	1:B:1338:GLN:HG3	1.80	0.81
1:B:1369:ALA:HB1	1:B:1373:ILE:HD11	1.60	0.81
1:B:1527:ALA:O	1:B:1531:THR:HG23	1.80	0.81
1:C:2343:MSE:HE3	1:C:2350:LEU:HD12	1.61	0.80
1:A:381:VAL:HG13	1:A:407:MSE:HE3	1.64	0.79
1:B:1315:ALA:HB3	1:B:1392:VAL:CG2	2.09	0.79
1:C:2323:ILE:HG22	1:C:2327:MSE:HE2	1.64	0.79
1:C:2286:VAL:HG22	1:C:2470:ILE:HG12	1.64	0.79
1:D:3123:TYR:HD2	1:D:3219:MSE:HE1	1.45	0.78
1:D:3478:VAL:HG13	1:D:3483:THR:HB	1.65	0.78
1:C:2132:GLY:HA3	1:C:2177:MSE:HE1	1.65	0.77
1:A:381:VAL:CG1	1:A:407:MSE:HE3	2.15	0.77
1:A:177:MSE:CE	1:A:180:PRO:HB2	2.13	0.76
1:C:2184:LEU:HD12	1:C:2200:PRO:HG3	1.66	0.75
1:A:551:LYS:O	1:A:555:GLU:HG3	1.88	0.74
1:D:3239:MSE:HE1	1:D:3254:PHE:HZ	1.51	0.73
1:D:3520:GLN:H	1:D:3520:GLN:NE2	1.86	0.72
1:C:2527:ALA:O	1:C:2531:THR:HG23	1.90	0.72
1:C:2286:VAL:CG2	1:C:2467:ASN:HA	2.19	0.72
1:B:1504:ASP:HA	1:B:1507:LEU:HD12	1.72	0.72
1:B:1505:GLU:CD	1:B:1505:GLU:H	1.98	0.71
1:D:3177:MSE:CE	1:D:3200:PRO:HB2	2.07	0.71
1:C:2520:GLN:H	1:C:2520:GLN:NE2	1.89	0.71
1:A:456:ASP:OD1	1:A:458:ARG:HD3	1.91	0.70
1:A:81:LYS:O	1:A:85:ILE:HG23	1.92	0.70
1:C:2327:MSE:HE3	1:C:2337:ALA:HB1	1.74	0.70
1:C:2085:ILE:HG13	1:C:2086:MSE:N	2.05	0.69
1:B:1301:PRO:HD2	1:B:1304:GLU:OE2	1.93	0.69
1:C:2354:ARG:NE	1:C:2356:ALA:HB3	2.07	0.69
1:B:1085:ILE:HD11	1:B:1111:VAL:HG22	1.75	0.69
1:C:2392:VAL:O	1:C:2392:VAL:HG13	1.92	0.69
1:D:3140:ARG:NH2	1:D:3233:ASP:HB3	2.06	0.69
1:B:1286:VAL:CG2	1:B:1467:ASN:HA	2.22	0.68
1:B:1108:MSE:HB3	1:B:1109:PRO:HD3	1.76	0.68
1:B:1085:ILE:C	1:B:1085:ILE:HD12	2.18	0.68
1:A:177:MSE:CE	1:A:200:PRO:HB2	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1075:MSE:HE2	1:B:1080:GLU:HG2	1.75	0.67
1:D:3194:ARG:HH11	1:D:3194:ARG:HG2	1.60	0.67
1:C:2338:GLN:NE2	1:C:2364:PRO:HB3	2.09	0.67
1:A:86:MSE:HE1	1:A:185:CYS:SG	2.34	0.67
1:C:2179:ILE:HB	1:C:2180:PRO:HD3	1.77	0.67
1:D:3183:LYS:HE3	1:D:3255:GLU:CD	2.21	0.66
1:D:3298:ILE:HG22	1:D:3300:LYS:HG2	1.78	0.66
1:B:1374:PRO:HG3	1:B:1383:ILE:HD12	1.77	0.66
1:C:2371:GLU:CD	1:C:2371:GLU:H	2.03	0.66
1:B:1075:MSE:HE2	1:B:1080:GLU:CD	2.21	0.65
1:D:3532:GLU:HG2	1:D:3549:LYS:HG2	1.79	0.65
1:A:108:MSE:HB3	1:A:109:PRO:HD3	1.77	0.65
1:D:3334:GLU:O	1:D:3338:GLN:HG3	1.96	0.65
1:A:288:LEU:HD22	1:A:322:LEU:HD12	1.77	0.65
1:B:1350:LEU:HD22	1:B:1354:ARG:CZ	2.27	0.65
1:B:1492:LEU:HD22	1:B:1496:LYS:HE3	1.77	0.65
1:B:1392:VAL:HG22	1:B:1392:VAL:O	1.97	0.64
1:B:1183:LYS:HE3	1:B:1255:GLU:CD	2.22	0.63
1:D:3527:ALA:O	1:D:3531:THR:HG22	1.96	0.63
1:C:2504:ASP:HA	1:C:2507:LEU:HD12	1.80	0.63
1:A:334:GLU:O	1:A:338:GLN:HG3	1.99	0.63
1:C:2315:ALA:CB	1:C:2392:VAL:HG21	2.27	0.63
1:D:3163:GLY:HA2	1:D:3166:ILE:HD11	1.81	0.63
1:A:493:GLU:HG3	1:A:533:TYR:CD1	2.34	0.63
1:D:3179:ILE:HB	1:D:3180:PRO:HD3	1.81	0.63
1:B:1041:THR:O	1:B:1045:ARG:HG3	1.98	0.62
1:A:272:LYS:HB2	1:A:272:LYS:NZ	2.15	0.62
1:C:2073:LYS:HE3	1:C:2073:LYS:CA	2.28	0.62
1:D:3081:LYS:O	1:D:3085:ILE:HG23	1.98	0.62
1:A:363:GLU:HB3	1:A:364:PRO:HD3	1.81	0.62
1:A:407:MSE:HA	1:A:407:MSE:CE	2.29	0.62
1:A:325:MSE:O	1:A:328:VAL:HG22	1.99	0.61
1:B:1286:VAL:HG22	1:B:1470:ILE:CG1	2.30	0.61
1:B:1518:ASN:HB3	1:B:1521:GLU:CD	2.25	0.61
1:B:1232:ASP:OD1	1:B:1264:ARG:NH2	2.34	0.61
1:C:2286:VAL:HG22	1:C:2470:ILE:CG1	2.29	0.61
1:B:1081:LYS:O	1:B:1085:ILE:HG23	2.00	0.61
1:D:3327:MSE:HE3	1:D:3337:ALA:HB1	1.83	0.61
1:B:1401:PRO:O	1:B:1405:ARG:HG3	2.00	0.61
1:A:302:ILE:O	1:A:340:LYS:HE2	2.01	0.61
1:A:527:ALA:O	1:A:531:THR:HG23	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1515:PRO:HG2	1:B:1518:ASN:HD22	1.66	0.60
1:A:288:LEU:CD2	1:A:322:LEU:HD12	2.31	0.60
1:A:302:ILE:HA	1:A:305:HIS:HD2	1.67	0.60
1:C:2132:GLY:HA3	1:C:2177:MSE:HE2	1.81	0.60
1:C:2243:THR:HG21	1:C:2273:TYR:CD2	2.37	0.60
1:B:1300:LYS:HG3	1:B:1304:GLU:CD	2.27	0.60
1:D:3123:TYR:CD2	1:D:3219:MSE:HE1	2.32	0.59
1:A:41:THR:OG1	1:A:44:GLU:HG3	2.03	0.59
1:B:1478:VAL:HG13	1:B:1483:THR:HB	1.85	0.59
1:C:2315:ALA:HB3	1:C:2392:VAL:HG21	1.84	0.59
1:C:2052:GLY:HA3	1:D:3146:ILE:HG23	1.84	0.59
1:B:1315:ALA:O	1:B:1319:ILE:HG13	2.03	0.58
1:C:2509:GLN:HG2	6:C:222:HOH:O	2.02	0.58
1:C:2183:LYS:HE2	1:C:2255:GLU:CD	2.28	0.58
1:A:33:ARG:HD3	1:A:93:GLU:OE2	2.03	0.58
1:A:179:ILE:HB	1:A:180:PRO:HD3	1.86	0.58
1:B:1286:VAL:HG22	1:B:1470:ILE:HG12	1.86	0.58
1:B:1493:GLU:HG3	1:B:1533:TYR:CD1	2.38	0.58
1:A:532:GLU:HG2	1:A:549:LYS:HG3	1.85	0.58
1:C:2288:LEU:HD22	1:C:2322:LEU:HG	1.86	0.58
1:B:1075:MSE:HE2	1:B:1080:GLU:CG	2.33	0.57
1:A:333:SER:OG	1:A:336:GLU:HG2	2.03	0.57
1:D:3108:MSE:HB3	1:D:3109:PRO:HD3	1.87	0.57
1:D:3406:ALA:O	1:D:3410:ILE:HG13	2.05	0.57
1:A:23:GLU:OE2	1:A:23:GLU:HA	2.04	0.57
1:A:172:LEU:O	1:A:175:TYR:HB2	2.04	0.57
1:C:2346:LYS:HE2	1:C:2347:TYR:CE1	2.39	0.57
1:B:1504:ASP:HA	1:B:1507:LEU:CD1	2.33	0.57
1:B:1556:ARG:HH11	1:B:1556:ARG:HG3	1.70	0.57
1:A:286:VAL:CG2	1:A:467:ASN:HA	2.29	0.56
1:B:1526:ILE:O	1:B:1530:VAL:HG23	2.05	0.56
1:A:261:ASN:HD22	1:A:264:ARG:HE	1.52	0.56
1:B:1179:ILE:HB	1:B:1180:PRO:HD3	1.87	0.56
1:C:2204:ASP:OD2	1:C:2221:LEU:HG	2.04	0.56
1:B:1177:MSE:O	1:B:1180:PRO:HD2	2.05	0.56
1:C:2308:LEU:HB3	1:C:2389:ILE:HD12	1.86	0.56
1:C:2363:GLU:HB3	1:C:2364:PRO:HD3	1.87	0.56
1:C:2154:HIS:O	1:C:2197:ARG:HD2	2.06	0.56
1:C:2383:ILE:HG22	1:C:2384:LEU:HD12	1.87	0.56
1:B:1169:LEU:HD13	1:B:1422:PRO:HD2	1.88	0.56
1:D:3177:MSE:O	1:D:3180:PRO:HD2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3350:LEU:HD22	1:D:3354:ARG:CZ	2.36	0.56
1:D:3492:LEU:O	1:D:3492:LEU:HD23	2.06	0.56
1:B:1261:ASN:HD22	1:B:1264:ARG:HD3	1.71	0.56
1:C:2154:HIS:HD2	6:C:231:HOH:O	1.88	0.56
1:A:86:MSE:SE	1:A:111:VAL:HG23	2.56	0.56
1:A:152:GLU:HG2	1:A:196:ASP:O	2.06	0.55
1:C:2061:GLN:HA	1:C:2064:GLN:HE21	1.70	0.55
1:D:3110:ILE:N	1:D:3110:ILE:HD12	2.21	0.55
1:C:2359:ASP:OD2	1:C:2362:GLN:HG3	2.06	0.55
1:A:22:LYS:O	1:A:22:LYS:HG2	2.06	0.55
1:A:307:ILE:HD13	1:A:323:ILE:HD13	1.89	0.55
1:C:2502:LEU:HD22	1:C:2507:LEU:HG	1.88	0.55
1:D:3068:PHE:CD2	1:D:3099:ILE:HG13	2.41	0.55
1:B:1456:ASP:OD1	1:B:1458:ARG:HD3	2.07	0.55
1:A:132:GLY:CA	1:A:200:PRO:HG2	2.37	0.55
1:A:302:ILE:HA	1:A:305:HIS:CD2	2.42	0.55
1:C:2349:LEU:HD22	1:C:2374:PRO:HG3	1.87	0.55
1:D:3307:ILE:HD13	1:D:3323:ILE:HD13	1.87	0.55
1:D:3528:ILE:O	1:D:3531:THR:CG2	2.55	0.55
1:B:1085:ILE:HD11	1:B:1086:MSE:SE	2.57	0.54
1:C:2315:ALA:O	1:C:2319:ILE:HG13	2.07	0.54
1:C:2040:PHE:HE2	1:C:2565:LEU:HD12	1.72	0.54
1:C:2297:VAL:CG2	1:C:2442:LEU:HD11	2.37	0.54
1:C:2354:ARG:CZ	1:C:2356:ALA:HB3	2.36	0.54
1:C:2500:SER:HB3	6:C:237:HOH:O	2.07	0.54
1:D:3183:LYS:HE3	1:D:3255:GLU:OE2	2.07	0.54
1:B:1559:ARG:HH11	1:B:1559:ARG:HG2	1.72	0.54
1:C:2131:LYS:O	1:C:2177:MSE:HE2	2.07	0.54
1:B:1135:ILE:HD13	1:B:1143:VAL:HG13	1.88	0.54
1:A:506:GLU:O	1:A:511:ARG:HB2	2.08	0.54
1:C:2043:GLN:NE2	1:C:2047:MSE:HE1	2.23	0.54
1:B:1363:GLU:HB3	1:B:1364:PRO:HD3	1.89	0.53
1:D:3294:ALA:O	1:D:3297:VAL:HG22	2.09	0.53
1:D:3335:GLN:O	1:D:3339:LYS:HG2	2.08	0.53
1:B:1571:GLU:HG3	6:B:670:HOH:O	2.07	0.53
1:C:2165:ARG:O	1:C:2165:ARG:HG2	2.09	0.53
1:B:1066:LEU:HD22	1:B:1070:ARG:HH11	1.70	0.53
1:C:2150:TRP:CE2	1:C:2199:LEU:HD13	2.44	0.53
1:B:1471:PHE:CG	1:B:1472:PRO:HD3	2.44	0.53
1:D:3350:LEU:HD22	1:D:3354:ARG:NH1	2.23	0.53
1:A:350:LEU:HD13	1:A:358:ILE:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3308:LEU:HB3	1:D:3389:ILE:HD12	1.91	0.53
1:A:248:ARG:HH22	1:A:272:LYS:HG3	1.74	0.53
1:B:1261:ASN:HA	1:B:1264:ARG:HD3	1.89	0.53
1:B:1327:MSE:HE3	1:B:1337:ALA:HB1	1.91	0.53
1:C:2108:MSE:HB3	1:C:2109:PRO:HD3	1.89	0.53
1:C:2166:ILE:HG23	1:C:2179:ILE:HG13	1.91	0.53
1:B:1294:ALA:O	1:B:1297:VAL:HG22	2.08	0.52
1:A:272:LYS:HB2	1:A:272:LYS:HZ2	1.73	0.52
1:C:2186:LEU:HD13	1:C:2468:VAL:CG2	2.39	0.52
1:B:1389:ILE:HG22	1:B:1416:ILE:HA	1.92	0.52
1:A:350:LEU:HD13	1:A:358:ILE:CD1	2.39	0.52
1:C:2288:LEU:O	1:C:2292:LEU:HD13	2.09	0.52
1:D:3051:GLN:HE21	1:D:3051:GLN:HA	1.75	0.52
1:B:1282:GLY:O	1:B:1286:VAL:HG23	2.09	0.52
1:B:1503:THR:OG1	1:B:1506:GLU:HG3	2.10	0.52
1:D:3169:LEU:HD13	1:D:3422:PRO:HD2	1.92	0.52
1:B:1333:SER:OG	1:B:1336:GLU:HG2	2.10	0.52
1:D:3359:ASP:HB2	6:D:465:HOH:O	2.10	0.52
1:B:1233:ASP:CG	1:B:1234:LEU:N	2.67	0.51
1:C:2307:ILE:N	1:C:2307:ILE:HD12	2.25	0.51
1:C:2328:VAL:HA	1:C:2332:LEU:O	2.10	0.51
1:D:3315:ALA:HB2	6:D:460:HOH:O	2.10	0.51
1:A:79:LEU:HD22	1:A:122:GLN:HE22	1.75	0.51
1:B:1384:LEU:N	1:B:1384:LEU:HD22	2.25	0.51
1:C:2042:LEU:O	1:C:2046:GLN:HG3	2.11	0.51
1:C:2505:GLU:CD	1:C:2505:GLU:H	2.19	0.51
1:C:2556:ARG:HH11	1:C:2556:ARG:HG3	1.76	0.51
1:B:1302:ILE:HD11	1:B:1327:MSE:HG2	1.93	0.51
1:A:82:TYR:O	1:A:86:MSE:HB2	2.11	0.51
1:A:286:VAL:HG22	1:A:470:ILE:CG1	2.41	0.50
1:A:297:VAL:CG2	1:A:507:LEU:HG	2.41	0.50
1:A:324:VAL:O	1:A:328:VAL:HG13	2.11	0.50
1:B:1132:GLY:CA	1:B:1200:PRO:HG2	2.41	0.50
1:D:3064:GLN:NE2	1:D:3562:TYR:OH	2.39	0.50
1:D:3503:THR:OG1	1:D:3506:GLU:HG3	2.11	0.50
1:B:1075:MSE:CE	1:B:1080:GLU:HG2	2.41	0.50
1:B:1320:ALA:O	1:B:1324:VAL:HG23	2.12	0.50
1:A:546:PRO:O	1:A:549:LYS:HE2	2.11	0.50
1:B:1308:LEU:HB3	1:B:1389:ILE:HD12	1.92	0.50
1:A:492:LEU:HD23	1:A:492:LEU:O	2.10	0.50
1:D:3518:ASN:HB3	1:D:3521:GLU:OE2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1506:GLU:O	1:B:1511:ARG:HB2	2.11	0.50
1:A:503:THR:OG1	1:A:506:GLU:HG3	2.11	0.50
1:D:3041:THR:O	1:D:3045:ARG:HG3	2.11	0.50
1:D:3261:ASN:ND2	1:D:3264:ARG:HH21	2.10	0.50
1:D:3556:ARG:HH11	1:D:3556:ARG:HG3	1.77	0.50
1:B:1099:ILE:HG22	1:B:1100:LEU:HD12	1.93	0.50
1:C:2315:ALA:HB3	1:C:2392:VAL:CG2	2.40	0.50
1:C:2350:LEU:HD22	1:C:2358:ILE:CD1	2.42	0.50
1:D:3332:LEU:CD1	1:D:3332:LEU:H	2.25	0.50
1:D:3528:ILE:O	1:D:3531:THR:HG22	2.12	0.50
1:B:1518:ASN:O	1:B:1521:GLU:HG2	2.12	0.50
1:C:2308:LEU:HD23	1:C:2389:ILE:HD11	1.94	0.50
1:A:183:LYS:HE3	1:A:255:GLU:CD	2.36	0.50
1:A:79:LEU:HD22	1:A:122:GLN:NE2	2.27	0.49
1:B:1332:LEU:CD1	1:B:1332:LEU:H	2.25	0.49
1:C:2361:TYR:O	1:C:2364:PRO:HD2	2.12	0.49
1:D:3086:MSE:SE	1:D:3111:VAL:HG23	2.62	0.49
1:D:3284:ALA:HA	1:D:3319:ILE:HG12	1.93	0.49
1:A:308:LEU:HB3	1:A:389:ILE:HD12	1.93	0.49
1:B:1033:ARG:HG3	1:B:1033:ARG:HH11	1.77	0.49
1:D:3172:LEU:O	1:D:3175:TYR:HB2	2.11	0.49
1:A:43:GLN:HG2	1:A:47:MSE:HE3	1.94	0.49
1:B:1096:PHE:O	1:B:1100:LEU:HD13	2.12	0.49
1:C:2041:THR:O	1:C:2045:ARG:HG3	2.12	0.49
1:D:3397:ARG:HD3	1:D:3426:ALA:O	2.12	0.49
1:A:332:LEU:HA	1:A:336:GLU:OE2	2.13	0.49
1:C:2392:VAL:HG13	6:C:120:HOH:O	2.12	0.49
1:C:2165:ARG:O	1:C:2165:ARG:NH1	2.46	0.49
1:C:2177:MSE:CE	1:C:2200:PRO:HB2	2.43	0.49
1:C:2298:ILE:HG22	1:C:2300:LYS:HB2	1.95	0.49
1:D:3520:GLN:HE21	1:D:3520:GLN:N	1.99	0.49
1:A:43:GLN:CG	1:A:47:MSE:HE3	2.42	0.48
1:A:389:ILE:HG23	1:A:399:PHE:CZ	2.48	0.48
1:B:1068:PHE:CD2	1:B:1099:ILE:HG13	2.49	0.48
1:B:1288:LEU:O	1:B:1292:LEU:HD13	2.12	0.48
1:D:3506:GLU:O	1:D:3511:ARG:HB2	2.12	0.48
1:B:1392:VAL:HG23	4:B:1601:ATP:O3G	2.14	0.48
1:C:2248:ARG:HH21	1:C:2272:LYS:HG2	1.78	0.48
1:C:2389:ILE:HG23	1:C:2399:PHE:CZ	2.49	0.48
1:A:177:MSE:O	1:A:180:PRO:HD2	2.14	0.48
1:B:1184:LEU:HD12	1:B:1200:PRO:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3188:THR:HG21	1:D:3195:PRO:HG3	1.95	0.48
1:D:3358:ILE:HD13	1:D:3366:THR:OG1	2.13	0.48
1:A:308:LEU:HD23	1:A:389:ILE:HD11	1.94	0.48
1:B:1235:ILE:O	1:B:1239:MSE:HG2	2.13	0.48
1:C:2338:GLN:HE22	1:C:2364:PRO:HB3	1.79	0.48
1:D:3324:VAL:HA	1:D:3327:MSE:HE3	1.96	0.48
1:D:3492:LEU:HD23	1:D:3492:LEU:C	2.38	0.48
1:B:1123:TYR:CD2	1:B:1219:MSE:HE1	2.49	0.48
1:B:1389:ILE:HG23	1:B:1399:PHE:CE1	2.49	0.48
1:C:2310:LEU:HD21	1:C:2398:LEU:HB2	1.96	0.48
1:C:2371:GLU:OE2	1:C:2371:GLU:N	2.39	0.48
1:D:3487:SER:OG	1:D:3539:MSE:HE1	2.13	0.48
1:B:1302:ILE:O	1:B:1340:LYS:HE3	2.13	0.48
1:A:177:MSE:CE	1:A:181:VAL:HG23	2.28	0.48
1:A:282:GLY:O	1:A:286:VAL:HG23	2.13	0.48
1:A:146:ILE:HG23	1:B:1052:GLY:HA3	1.96	0.48
1:B:1511:ARG:NH1	6:B:34:HOH:O	2.46	0.47
1:A:64:GLN:NE2	1:A:562:TYR:OH	2.39	0.47
1:A:332:LEU:H	1:A:332:LEU:CD1	2.27	0.47
1:B:1120:CYS:O	1:B:1175:TYR:HB3	2.14	0.47
1:B:1188:THR:HG21	1:B:1195:PRO:HG3	1.95	0.47
1:A:371:GLU:OE2	1:A:371:GLU:N	2.43	0.47
1:C:2081:LYS:O	1:C:2085:ILE:HG23	2.15	0.47
1:B:1468:VAL:HA	1:B:1471:PHE:CE2	2.50	0.47
1:C:2033:ARG:HD3	1:C:2093:GLU:OE2	2.14	0.47
1:A:324:VAL:HA	1:A:327:MSE:HE3	1.97	0.47
1:B:1286:VAL:HG22	1:B:1470:ILE:HG13	1.97	0.47
1:B:1350:LEU:HD22	1:B:1354:ARG:NH2	2.27	0.47
1:A:140:ARG:NH2	1:A:233:ASP:OD2	2.48	0.47
1:A:165:ARG:O	1:A:256:ASP:HB3	2.14	0.47
1:C:2177:MSE:HE1	1:C:2200:PRO:HB2	1.97	0.47
1:A:163:GLY:HA2	1:A:166:ILE:HD11	1.97	0.47
1:A:65:ALA:HA	1:A:99:ILE:HD11	1.97	0.47
1:C:2507:LEU:HB2	6:C:121:HOH:O	2.14	0.47
1:C:2556:ARG:HG3	1:C:2556:ARG:NH1	2.30	0.47
1:A:45:ARG:NH2	1:A:58:ILE:HD13	2.30	0.47
1:A:483:THR:OG1	1:A:534:LEU:HD13	2.15	0.47
1:A:492:LEU:CD2	1:A:496:LYS:HE2	2.45	0.47
1:B:1022:LYS:HD3	1:B:1022:LYS:C	2.40	0.47
1:B:1078:PRO:HD2	6:B:115:HOH:O	2.14	0.47
1:C:2346:LYS:HE2	1:C:2347:TYR:CZ	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3235:ILE:HG13	1:D:3265:PHE:CZ	2.49	0.46
1:C:2315:ALA:HB2	6:C:424:HOH:O	2.14	0.46
1:B:1229:GLN:HA	1:B:1229:GLN:NE2	2.31	0.46
1:C:2172:LEU:O	1:C:2175:TYR:HB2	2.14	0.46
1:A:286:VAL:HG22	1:A:470:ILE:HG13	1.96	0.46
1:C:2458:ARG:HD2	6:C:663:HOH:O	2.14	0.46
1:B:1029:MSE:SE	1:B:1050:LEU:HD22	2.65	0.46
1:B:1046:GLN:HG2	1:B:1051:GLN:HG3	1.97	0.46
1:B:1308:LEU:HD23	1:B:1389:ILE:HD11	1.97	0.46
1:C:2303:SER:O	1:C:2340:LYS:NZ	2.41	0.46
1:D:3140:ARG:HH22	1:D:3233:ASP:CB	2.13	0.46
1:D:3161:THR:HG22	1:D:3180:PRO:HG2	1.97	0.46
1:D:3332:LEU:N	1:D:3332:LEU:HD12	2.31	0.46
1:B:1243:THR:HG21	1:B:1273:TYR:CD2	2.51	0.46
1:B:1359:ASP:OD2	1:B:1362:GLN:HG3	2.15	0.46
1:B:1556:ARG:HG3	1:B:1556:ARG:NH1	2.30	0.46
1:C:2073:LYS:HA	1:C:2073:LYS:CE	2.36	0.46
1:B:1085:ILE:HD12	1:B:1086:MSE:N	2.31	0.46
1:B:1307:ILE:N	1:B:1307:ILE:HD12	2.31	0.46
1:C:2156:LYS:HA	1:C:2156:LYS:HE2	1.97	0.46
1:C:2369:ALA:HB1	1:C:2373:ILE:HD11	1.98	0.46
1:A:41:THR:O	1:A:45:ARG:HG3	2.16	0.45
1:A:328:VAL:HA	1:A:332:LEU:O	2.16	0.45
1:B:1284:ALA:HA	1:B:1319:ILE:HG12	1.98	0.45
1:A:22:LYS:HZ1	1:C:2027:PRO:HG2	1.80	0.45
1:A:177:MSE:O	1:A:177:MSE:CE	2.56	0.45
1:B:1261:ASN:ND2	1:B:1264:ARG:HH11	2.14	0.45
1:C:2183:LYS:HE2	1:C:2255:GLU:OE2	2.16	0.45
1:C:2350:LEU:HD23	1:C:2354:ARG:NH1	2.32	0.45
1:D:3169:LEU:HD13	1:D:3422:PRO:CD	2.47	0.45
1:D:3239:MSE:HE3	1:D:3269:TYR:CE1	2.52	0.45
1:A:306:LYS:HB3	1:A:386:PRO:HA	1.99	0.45
1:A:323:ILE:CG2	1:A:327:MSE:HE2	2.31	0.45
1:C:2315:ALA:HB1	1:C:2392:VAL:HG21	1.97	0.45
1:D:3524:ILE:O	1:D:3528:ILE:HG13	2.16	0.45
1:B:1075:MSE:HE2	1:B:1080:GLU:OE1	2.17	0.45
1:B:1172:LEU:O	1:B:1175:TYR:HB2	2.17	0.45
1:C:2310:LEU:HB3	1:C:2391:GLY:HA2	1.97	0.45
1:D:3140:ARG:HD2	6:D:637:HOH:O	2.15	0.45
1:D:3239:MSE:HE1	1:D:3254:PHE:CZ	2.40	0.45
1:A:143:VAL:HB	1:A:237:GLU:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ALA:HA	1:A:319:ILE:HG12	1.99	0.45
1:B:1328:VAL:HA	1:B:1332:LEU:O	2.16	0.45
1:C:2186:LEU:HD13	1:C:2468:VAL:HG23	1.99	0.45
1:B:1033:ARG:NH1	1:B:1093:GLU:OE2	2.49	0.45
1:C:2520:GLN:HB2	6:C:265:HOH:O	2.17	0.45
1:C:2468:VAL:HA	1:C:2471:PHE:CE2	2.52	0.45
1:C:2297:VAL:HG21	1:C:2442:LEU:HD11	1.99	0.45
1:C:2502:LEU:HD11	1:C:2512:LEU:C	2.42	0.45
1:C:2120:CYS:O	1:C:2175:TYR:HB3	2.17	0.44
1:D:3267:ARG:HD2	6:D:109:HOH:O	2.17	0.44
1:A:132:GLY:HA2	1:A:200:PRO:HG2	1.99	0.44
1:A:184:LEU:HD22	1:A:198:CYS:HB3	1.98	0.44
1:B:1061:GLN:HA	1:B:1064:GLN:HE21	1.82	0.44
1:B:1166:ILE:HG23	1:B:1179:ILE:HG13	1.98	0.44
1:D:3177:MSE:C	1:D:3180:PRO:HD2	2.42	0.44
1:A:335:GLN:HB2	6:A:4635:HOH:O	2.18	0.44
1:C:2041:THR:OG1	1:C:2044:GLU:HG3	2.16	0.44
1:C:2520:GLN:HE21	1:C:2520:GLN:N	2.05	0.44
1:D:3150:TRP:HA	1:D:3151:PRO:HD3	1.75	0.44
1:A:313:GLY:HA2	6:A:4711:HOH:O	2.17	0.44
1:B:1551:LYS:NZ	6:B:569:HOH:O	2.50	0.44
1:D:3159:VAL:HG23	1:D:3184:LEU:HD21	1.99	0.44
1:C:2478:VAL:HG13	1:C:2483:THR:HB	2.00	0.44
1:D:3194:ARG:HG2	1:D:3194:ARG:NH1	2.28	0.44
1:A:341:ILE:O	1:A:367:HIS:HE1	2.01	0.44
1:A:389:ILE:HG22	1:A:416:ILE:HA	2.00	0.44
1:B:1154:HIS:HD2	6:B:259:HOH:O	2.01	0.44
1:D:3285:ALA:HB2	1:D:3491:PHE:HB3	1.98	0.44
1:C:2022:LYS:NZ	1:C:2022:LYS:HB3	2.32	0.44
1:C:2382:ASN:O	1:C:2385:LYS:HD2	2.18	0.44
1:D:3421:ASN:ND2	2:D:3701:MLT:H32	2.33	0.44
1:A:159:VAL:HG23	1:A:184:LEU:HD21	1.99	0.44
1:A:205:VAL:HG11	1:A:231:TYR:HD1	1.81	0.44
1:C:2317:LEU:O	1:C:2321:ASN:ND2	2.51	0.44
1:D:3123:TYR:HD2	1:D:3219:MSE:CE	2.24	0.44
1:B:1132:GLY:HA3	1:B:1200:PRO:HG2	2.00	0.43
1:C:2085:ILE:CG1	1:C:2086:MSE:N	2.77	0.43
1:D:3324:VAL:O	1:D:3328:VAL:HG23	2.18	0.43
1:A:302:ILE:HD12	1:A:305:HIS:HD2	1.83	0.43
1:B:1354:ARG:HB2	6:B:653:HOH:O	2.17	0.43
1:C:2217:PHE:CZ	1:D:3066:LEU:HD23	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2571:GLU:CD	1:C:2572:TRP:H	2.26	0.43
1:B:1069:HIS:HE1	1:B:1102:ASP:OD2	2.01	0.43
1:B:1108:MSE:HE3	1:B:1516:LEU:HD11	2.00	0.43
1:B:1169:LEU:HD13	1:B:1422:PRO:CD	2.48	0.43
1:B:1350:LEU:HD22	1:B:1354:ARG:NH1	2.33	0.43
1:C:2070:ARG:O	1:C:2074:LYS:HD3	2.19	0.43
1:D:3345:ASP:HB2	4:D:3601:ATP:O2'	2.19	0.43
1:B:1065:ALA:HA	1:B:1099:ILE:HD11	2.01	0.43
1:C:2436:LEU:HD12	1:C:2436:LEU:HA	1.79	0.43
1:C:2543:TYR:HA	1:C:2544:PRO:C	2.43	0.43
1:B:1166:ILE:HA	1:B:1256:ASP:OD2	2.19	0.43
1:B:1372:SER:O	1:B:1374:PRO:HD3	2.18	0.43
1:B:1412:GLU:O	1:B:1440:ARG:NH1	2.48	0.43
1:D:3528:ILE:O	1:D:3531:THR:HG23	2.18	0.43
1:A:341:ILE:O	1:A:367:HIS:CE1	2.72	0.43
1:A:383:ILE:HG22	1:A:384:LEU:HD12	1.99	0.43
1:B:1227:ARG:HG2	1:B:1227:ARG:HH11	1.84	0.43
1:B:1300:LYS:CG	1:B:1304:GLU:HG3	2.48	0.43
1:D:3559:ARG:HE	1:D:3559:ARG:HB2	1.73	0.43
1:B:1315:ALA:HB2	6:B:272:HOH:O	2.18	0.43
1:B:1431:GLU:O	1:B:1435:THR:HG23	2.18	0.43
1:D:3363:GLU:HB2	1:D:3364:PRO:HD3	2.00	0.43
1:C:2096:PHE:O	1:C:2100:LEU:HD13	2.19	0.42
1:C:2319:ILE:O	1:C:2323:ILE:HG13	2.19	0.42
1:D:3061:GLN:HA	1:D:3064:GLN:HE21	1.84	0.42
1:B:1085:ILE:HD12	1:B:1096:PHE:HE1	1.83	0.42
1:B:1288:LEU:HD22	1:B:1322:LEU:HG	2.00	0.42
1:C:2261:ASN:ND2	1:C:2264:ARG:NH2	2.68	0.42
1:C:2363:GLU:C	1:C:2363:GLU:CD	2.87	0.42
1:D:3051:GLN:HA	1:D:3051:GLN:NE2	2.34	0.42
1:D:3140:ARG:NH2	1:D:3230:GLN:O	2.50	0.42
1:D:3315:ALA:O	1:D:3319:ILE:HG13	2.19	0.42
1:D:3397:ARG:HD3	1:D:3397:ARG:HA	1.92	0.42
1:A:492:LEU:HD23	1:A:492:LEU:C	2.44	0.42
1:B:1184:LEU:HD22	1:B:1198:CYS:HB3	2.00	0.42
1:B:1322:LEU:HD12	1:B:1322:LEU:HA	1.83	0.42
1:C:2077:SER:HA	1:C:2078:PRO:HD3	1.92	0.42
1:C:2284:ALA:HA	1:C:2319:ILE:HG12	2.00	0.42
1:D:3528:ILE:C	1:D:3531:THR:HG22	2.45	0.42
1:C:2150:TRP:HA	1:C:2151:PRO:HD3	1.83	0.42
1:C:2130:PRO:HG3	1:D:3054:LEU:HD23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2297:VAL:HG22	1:C:2442:LEU:HD11	2.02	0.42
1:D:3066:LEU:HD21	1:D:3070:ARG:HH21	1.84	0.42
1:A:194:ARG:NH1	1:A:197:ARG:NH2	2.67	0.42
1:A:328:VAL:HG23	1:A:329:GLU:N	2.34	0.42
1:D:3363:GLU:CB	1:D:3364:PRO:HD3	2.50	0.42
1:A:177:MSE:HE2	1:A:181:VAL:CG2	2.30	0.42
1:B:1085:ILE:C	1:B:1085:ILE:CD1	2.87	0.42
1:B:1046:GLN:HG2	1:B:1051:GLN:CG	2.50	0.42
1:D:3359:ASP:OD2	1:D:3359:ASP:C	2.62	0.42
1:B:1042:LEU:O	1:B:1046:GLN:HG3	2.20	0.42
1:B:1295:GLN:HA	1:B:1295:GLN:OE1	2.20	0.42
1:D:3302:ILE:HD11	1:D:3327:MSE:HG2	2.02	0.42
1:D:3389:ILE:HG23	1:D:3399:PHE:CE1	2.54	0.42
1:B:1559:ARG:HH11	1:B:1559:ARG:CG	2.32	0.41
1:D:3199:LEU:HA	1:D:3200:PRO:HD3	1.90	0.41
1:D:3308:LEU:HD23	1:D:3389:ILE:HD11	2.02	0.41
1:D:3528:ILE:HA	1:D:3531:THR:CG2	2.50	0.41
1:C:2243:THR:HG21	1:C:2273:TYR:HD2	1.82	0.41
1:C:2400:THR:OG1	1:C:2403:VAL:HG23	2.20	0.41
1:D:3051:GLN:HE21	1:D:3051:GLN:CA	2.33	0.41
1:D:3401:PRO:HA	1:D:3436:LEU:CD1	2.50	0.41
1:A:359:ASP:OD2	1:A:361:TYR:HD1	2.03	0.41
1:A:381:VAL:HG13	1:A:407:MSE:CE	2.44	0.41
1:C:2166:ILE:HD12	1:C:2179:ILE:HG13	2.02	0.41
1:C:2205:VAL:HG11	1:C:2231:TYR:HD1	1.86	0.41
1:C:2456:ASP:OD1	1:C:2458:ARG:HD3	2.21	0.41
1:D:3178:GLY:O	1:D:3181:VAL:HG13	2.20	0.41
1:D:3298:ILE:CG2	1:D:3300:LYS:HG2	2.48	0.41
1:D:3332:LEU:CD1	1:D:3332:LEU:N	2.84	0.41
1:B:1174:VAL:HG12	1:B:1174:VAL:O	2.20	0.41
1:C:2107:LEU:O	1:C:2111:VAL:HG12	2.20	0.41
1:D:3026:LYS:HB3	1:D:3027:PRO:HD3	2.02	0.41
1:C:2261:ASN:ND2	1:C:2264:ARG:HH21	2.18	0.41
1:D:3239:MSE:CE	1:D:3254:PHE:HZ	2.28	0.41
1:D:3528:ILE:HA	1:D:3531:THR:HG22	2.02	0.41
1:A:343:MSE:HE3	1:A:350:LEU:HG	2.02	0.41
1:B:1163:GLY:HA2	1:B:1166:ILE:HD11	2.01	0.41
1:C:2183:LYS:HE3	1:C:2278:ASP:OD2	2.20	0.41
1:C:2186:LEU:HD13	1:C:2468:VAL:HG21	2.02	0.41
1:D:3407:MSE:HE2	1:D:3407:MSE:HB2	1.90	0.41
1:B:1332:LEU:CD1	1:B:1332:LEU:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2389:ILE:HB	1:C:2407:MSE:HE2	2.03	0.41
1:D:3177:MSE:O	1:D:3181:VAL:HG12	2.21	0.41
1:A:389:ILE:HG23	1:A:399:PHE:CE1	2.55	0.41
1:B:1177:MSE:C	1:B:1180:PRO:HD2	2.46	0.41
1:C:2169:LEU:CD2	1:C:2422:PRO:HD3	2.51	0.41
1:D:3300:LYS:HE3	1:D:3300:LYS:HB3	1.89	0.41
1:A:134:PHE:O	1:B:1052:GLY:HA2	2.21	0.41
1:B:1357:LYS:N	1:B:1357:LYS:HD3	2.35	0.41
1:B:1502:LEU:HD13	1:B:1507:LEU:HD23	2.02	0.41
1:C:2322:LEU:HD12	1:C:2322:LEU:HA	1.87	0.41
1:B:1339:LYS:HA	1:B:1367:HIS:CE1	2.56	0.40
1:C:2154:HIS:O	1:C:2197:ARG:CD	2.69	0.40
1:D:3456:ASP:OD1	1:D:3456:ASP:C	2.64	0.40
1:A:165:ARG:NH1	4:A:4601:ATP:O1G	2.54	0.40
1:C:2194:ARG:HA	1:C:2195:PRO:HD2	1.91	0.40
1:C:2542:ARG:HD3	1:C:2542:ARG:C	2.46	0.40
1:D:3556:ARG:HG3	1:D:3556:ARG:NH1	2.36	0.40
1:D:3077:SER:HA	1:D:3078:PRO:HD3	1.91	0.40
1:D:3355:LYS:NZ	1:D:3355:LYS:HB2	2.37	0.40
1:A:52:GLY:HA3	1:B:1146:ILE:HG23	2.04	0.40
1:A:68:PHE:CD2	1:A:99:ILE:HG13	2.57	0.40
1:A:196:ASP:OD1	1:A:197:ARG:HG3	2.21	0.40
1:C:2194:ARG:HG3	4:C:2602:ATP:C6	2.57	0.40
1:C:2282:GLY:O	1:C:2286:VAL:HG23	2.21	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	550/564 (98%)	531 (96%)	16 (3%)	3 (0%)	24 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	550/564 (98%)	534 (97%)	14 (2%)	2 (0%)	30	38
1	C	550/564 (98%)	532 (97%)	16 (3%)	2 (0%)	30	38
1	D	550/564 (98%)	531 (96%)	17 (3%)	2 (0%)	30	38
All	All	2200/2256 (98%)	2128 (97%)	63 (3%)	9 (0%)	30	38

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	357	LYS
1	C	2332	LEU
1	A	397	ARG
1	B	1332	LEU
1	A	332	LEU
1	D	3397	ARG
1	B	1392	VAL
1	D	3302	ILE
1	C	2392	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	468/465 (101%)	447 (96%)	21 (4%)	24	37
1	B	468/465 (101%)	450 (96%)	18 (4%)	29	44
1	C	468/465 (101%)	453 (97%)	15 (3%)	34	51
1	D	468/465 (101%)	438 (94%)	30 (6%)	16	23
All	All	1872/1860 (101%)	1788 (96%)	84 (4%)	24	37

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	ILE
1	A	86	MSE

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Mol	Chain	Res	Type
1	A	99	ILE
1	A	100	LEU
1	A	152	GLU
1	A	165	ARG
1	A	169	LEU
1	A	221	LEU
1	A	251	LEU
1	A	272	LYS
1	A	286	VAL
1	A	291	LEU
1	A	292	LEU
1	A	322	LEU
1	A	350	LEU
1	A	355	LYS
1	A	389	ILE
1	A	436	LEU
1	A	502	LEU
1	A	559	ARG
1	A	561	GLU
1	B	1070	ARG
1	B	1085	ILE
1	B	1099	ILE
1	B	1133	LEU
1	B	1169	LEU
1	B	1221	LEU
1	B	1233	ASP
1	B	1251	LEU
1	B	1291	LEU
1	B	1301	PRO
1	B	1350	LEU
1	B	1363	GLU
1	B	1371	GLU
1	B	1375	ASP
1	B	1398	LEU
1	B	1492	LEU
1	B	1502	LEU
1	B	1504	ASP
1	C	2022	LYS
1	C	2073	LYS
1	C	2133	LEU
1	C	2169	LEU
1	C	2242	ILE

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Mol	Chain	Res	Type
1	C	2251	LEU
1	C	2291	LEU
1	C	2297	VAL
1	C	2375	ASP
1	C	2389	ILE
1	C	2398	LEU
1	C	2436	LEU
1	C	2502	LEU
1	C	2520	GLN
1	C	2561	GLU
1	D	3022	LYS
1	D	3024	LYS
1	D	3047	MSE
1	D	3066	LEU
1	D	3070	ARG
1	D	3085	ILE
1	D	3099	ILE
1	D	3100	LEU
1	D	3133	LEU
1	D	3169	LEU
1	D	3181	VAL
1	D	3219	MSE
1	D	3221	LEU
1	D	3229	GLN
1	D	3242	ILE
1	D	3251	LEU
1	D	3266	LEU
1	D	3272	LYS
1	D	3291	LEU
1	D	3292	LEU
1	D	3330	ASN
1	D	3335	GLN
1	D	3350	LEU
1	D	3355	LYS
1	D	3389	ILE
1	D	3423	THR
1	D	3425	GLN
1	D	3520	GLN
1	D	3559	ARG
1	D	3561	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	51	GLN
1	A	64	GLN
1	A	122	GLN
1	A	154	HIS
1	A	230	GLN
1	A	261	ASN
1	A	330	ASN
1	A	335	GLN
1	A	425	GLN
1	A	482	ASN
1	A	520	GLN
1	B	1064	GLN
1	B	1069	HIS
1	B	1122	GLN
1	B	1154	HIS
1	B	1229	GLN
1	B	1230	GLN
1	B	1261	ASN
1	B	1335	GLN
1	B	1482	ASN
1	B	1518	ASN
1	C	2035	ASN
1	C	2043	GLN
1	C	2051	GLN
1	C	2064	GLN
1	C	2069	HIS
1	C	2122	GLN
1	C	2154	HIS
1	C	2229	GLN
1	C	2230	GLN
1	C	2261	ASN
1	C	2338	GLN
1	C	2509	GLN
1	C	2520	GLN
1	D	3043	GLN
1	D	3051	GLN
1	D	3064	GLN
1	D	3069	HIS
1	D	3071	ASN
1	D	3122	GLN
1	D	3230	GLN
1	D	3261	ASN

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Mol	Chain	Res	Type
1	D	3330	ASN
1	D	3338	GLN
1	D	3425	GLN
1	D	3482	ASN
1	D	3520	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	$\# Z > 2$
4	ATP	A	4602	-	32,33,33	1.64	7 (21%)	48,52,52	2.00	8 (16%)
4	ATP	C	2601	-	32,33,33	1.62	6 (18%)	48,52,52	2.04	9 (18%)
5	FUM	C	2700	-	7,7,7	2.36	4 (57%)	8,8,8	1.31	1 (12%)
2	MLT	A	701	3	8,8,8	1.28	2 (25%)	10,10,10	1.63	3 (30%)
4	ATP	B	1601	-	32,33,33	1.69	8 (25%)	48,52,52	2.05	9 (18%)
4	ATP	B	1602	-	32,33,33	1.79	9 (28%)	48,52,52	2.04	9 (18%)
4	ATP	D	3602	-	32,33,33	1.67	7 (21%)	48,52,52	2.02	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FUM	A	700	-	7,7,7	2.30	5 (71%)	8,8,8	1.57	2 (25%)
5	FUM	B	1700	-	7,7,7	2.29	5 (71%)	8,8,8	1.46	1 (12%)
2	MLT	B	1701	3	8,8,8	1.38	2 (25%)	10,10,10	1.63	2 (20%)
5	FUM	D	3700	-	7,7,7	2.39	4 (57%)	8,8,8	1.73	2 (25%)
4	ATP	D	3601	-	32,33,33	1.55	7 (21%)	48,52,52	2.03	9 (18%)
2	MLT	D	3701	3	8,8,8	1.29	2 (25%)	10,10,10	1.62	3 (30%)
2	MLT	C	2701	3	8,8,8	1.31	2 (25%)	10,10,10	1.64	3 (30%)
4	ATP	C	2602	-	32,33,33	1.67	7 (21%)	48,52,52	2.03	9 (18%)
4	ATP	A	4601	-	32,33,33	1.59	7 (21%)	48,52,52	2.03	9 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	A	4602	-	-	2/22/38/38	0/3/3/3
4	ATP	C	2601	-	-	6/22/38/38	0/3/3/3
5	FUM	C	2700	-	-	0/5/5/5	-
2	MLT	A	701	3	1/1/3/3	0/8/8/8	-
4	ATP	B	1601	-	-	6/22/38/38	0/3/3/3
4	ATP	B	1602	-	-	1/22/38/38	0/3/3/3
4	ATP	D	3602	-	-	3/22/38/38	0/3/3/3
5	FUM	A	700	-	-	0/5/5/5	-
5	FUM	B	1700	-	-	0/5/5/5	-
2	MLT	B	1701	3	1/1/3/3	2/8/8/8	-
5	FUM	D	3700	-	-	0/5/5/5	-
4	ATP	D	3601	-	-	6/22/38/38	0/3/3/3
2	MLT	D	3701	3	1/1/3/3	2/8/8/8	-
2	MLT	C	2701	3	1/1/3/3	2/8/8/8	-
4	ATP	C	2602	-	-	2/22/38/38	0/3/3/3
4	ATP	A	4601	-	-	8/22/38/38	0/3/3/3

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1602	ATP	C5-N7	-4.71	1.30	1.39
4	A	4602	ATP	C5-N7	-4.54	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2602	ATP	C5-N7	-4.38	1.31	1.39
4	D	3602	ATP	C5-N7	-4.36	1.31	1.39
4	D	3601	ATP	C5-N7	-4.30	1.31	1.39
4	A	4601	ATP	C5-N7	-4.30	1.31	1.39
4	B	1601	ATP	C5-N7	-4.26	1.31	1.39
4	C	2601	ATP	PB-O3B	3.96	1.63	1.59
4	C	2601	ATP	C5-N7	-3.94	1.31	1.39
4	B	1602	ATP	PB-O3B	3.54	1.63	1.59
4	B	1601	ATP	PB-O3B	3.27	1.63	1.59
5	D	3700	FUM	OXT-C	-3.26	1.22	1.30
4	C	2601	ATP	C5-C4	-3.17	1.33	1.39
4	C	2602	ATP	PB-O3A	3.14	1.62	1.59
4	B	1601	ATP	C5-C4	-3.13	1.33	1.39
4	C	2602	ATP	C5-C4	-3.11	1.33	1.39
5	B	1700	FUM	O7-C6	3.10	1.30	1.23
4	D	3602	ATP	PB-O3B	3.04	1.62	1.59
4	B	1602	ATP	C5-C4	-3.00	1.33	1.39
5	C	2700	FUM	OXT-C	-2.97	1.22	1.30
5	A	700	FUM	OXT-C	-2.94	1.22	1.30
5	C	2700	FUM	C5-C6	2.89	1.55	1.48
5	D	3700	FUM	C5-C6	2.85	1.55	1.48
4	A	4601	ATP	PB-O3B	2.82	1.62	1.59
4	D	3602	ATP	C5-C4	-2.80	1.34	1.39
4	A	4602	ATP	PB-O3B	2.80	1.62	1.59
4	D	3601	ATP	PB-O3B	2.80	1.62	1.59
4	D	3601	ATP	C5-C4	-2.79	1.34	1.39
4	A	4602	ATP	C5-C4	-2.78	1.34	1.39
4	A	4601	ATP	C5-C4	-2.73	1.34	1.39
5	A	700	FUM	C5-C6	2.72	1.55	1.48
4	D	3602	ATP	C8-N7	2.69	1.36	1.31
5	C	2700	FUM	C5-C4	2.63	1.40	1.33
4	B	1601	ATP	PA-O3A	2.61	1.62	1.59
5	B	1700	FUM	C5-C6	2.61	1.54	1.48
4	A	4601	ATP	C8-N7	2.57	1.36	1.31
4	B	1602	ATP	C8-N7	2.55	1.36	1.31
4	B	1602	ATP	PA-O3A	2.52	1.62	1.59
4	D	3602	ATP	PB-O3A	2.51	1.62	1.59
4	B	1602	ATP	PB-O3A	2.45	1.62	1.59
4	D	3602	ATP	C2-N1	2.43	1.38	1.33
5	C	2700	FUM	O7-C6	2.41	1.28	1.23
5	D	3700	FUM	C5-C4	2.39	1.40	1.33
4	C	2601	ATP	C4-N9	-2.38	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2602	ATP	C8-N7	2.38	1.36	1.31
5	D	3700	FUM	C4-C	2.38	1.54	1.48
4	D	3601	ATP	C4-N9	-2.36	1.32	1.37
4	A	4601	ATP	C2-N1	2.35	1.38	1.33
4	B	1601	ATP	C8-N7	2.35	1.36	1.31
4	D	3601	ATP	C8-N7	2.34	1.36	1.31
4	D	3601	ATP	C2-N3	2.32	1.38	1.33
2	D	3701	MLT	O2-C1	-2.31	1.23	1.30
5	A	700	FUM	C5-C4	2.31	1.40	1.33
4	B	1601	ATP	C4-N9	-2.29	1.32	1.37
4	D	3602	ATP	O4'-C1'	2.29	1.47	1.42
5	B	1700	FUM	O8-C6	-2.28	1.24	1.30
5	B	1700	FUM	OXT-C	-2.27	1.24	1.30
4	A	4602	ATP	C8-N7	2.25	1.36	1.31
4	B	1602	ATP	C4-N9	-2.24	1.33	1.37
4	D	3601	ATP	C2-N1	2.23	1.37	1.33
5	A	700	FUM	O7-C6	2.23	1.28	1.23
4	A	4601	ATP	C4-N9	-2.23	1.33	1.37
4	A	4602	ATP	C2-N1	2.23	1.37	1.33
5	A	700	FUM	C4-C	2.21	1.53	1.48
2	A	701	MLT	O2-C1	-2.20	1.23	1.30
4	B	1601	ATP	C2-N3	2.19	1.37	1.33
4	C	2602	ATP	PA-O3A	2.18	1.61	1.59
2	D	3701	MLT	O5-C4	-2.18	1.23	1.30
5	B	1700	FUM	C5-C4	2.18	1.39	1.33
2	B	1701	MLT	O2-C1	-2.17	1.23	1.30
4	B	1601	ATP	C2-N1	2.15	1.37	1.33
4	B	1602	ATP	C2-N3	2.15	1.37	1.33
4	B	1602	ATP	C2-N1	2.14	1.37	1.33
4	A	4602	ATP	PB-O3A	2.14	1.61	1.59
4	A	4602	ATP	C4-N9	-2.13	1.33	1.37
4	C	2601	ATP	C8-N7	2.12	1.35	1.31
4	A	4601	ATP	C2-N3	2.12	1.37	1.33
4	C	2601	ATP	C2-N1	2.11	1.37	1.33
4	C	2602	ATP	C4-N9	-2.09	1.33	1.37
2	A	701	MLT	O5-C4	-2.08	1.23	1.30
4	C	2602	ATP	C2-N1	2.07	1.37	1.33
2	B	1701	MLT	O5-C4	-2.07	1.24	1.30
2	C	2701	MLT	O2-C1	-2.05	1.24	1.30
2	C	2701	MLT	O5-C4	-2.03	1.24	1.30

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2602	ATP	C5-C4-N3	-6.01	118.44	126.72
4	D	3602	ATP	C5-C4-N3	-5.92	118.57	126.72
4	A	4602	ATP	C5-C4-N3	-5.88	118.63	126.72
4	B	1601	ATP	C5-C4-N3	-5.86	118.65	126.72
4	B	1602	ATP	C5-C4-N3	-5.84	118.67	126.72
4	A	4601	ATP	C5-C4-N3	-5.83	118.69	126.72
4	D	3601	ATP	C5-C4-N3	-5.80	118.74	126.72
4	C	2601	ATP	C5-C4-N3	-5.75	118.81	126.72
4	B	1602	ATP	N3-C2-N1	-5.38	120.44	128.58
4	C	2601	ATP	N3-C2-N1	-5.32	120.53	128.58
4	D	3602	ATP	N3-C2-N1	-5.29	120.58	128.58
4	C	2602	ATP	N3-C2-N1	-5.23	120.66	128.58
4	A	4602	ATP	N3-C2-N1	-5.20	120.71	128.58
4	B	1601	ATP	C6-C5-N7	-5.19	122.09	132.09
4	B	1602	ATP	C6-C5-N7	-5.19	122.09	132.09
4	B	1601	ATP	N3-C2-N1	-5.18	120.74	128.58
4	A	4601	ATP	N3-C2-N1	-5.16	120.77	128.58
4	D	3601	ATP	N3-C2-N1	-5.15	120.79	128.58
4	A	4601	ATP	C6-C5-N7	-5.15	122.17	132.09
4	D	3601	ATP	C6-C5-N7	-5.13	122.21	132.09
4	C	2601	ATP	C6-C5-N7	-5.11	122.24	132.09
4	C	2602	ATP	C6-C5-N7	-5.10	122.26	132.09
4	B	1601	ATP	C6-C5-C4	5.10	124.14	117.18
4	D	3601	ATP	C6-C5-C4	5.06	124.08	117.18
4	B	1602	ATP	C6-C5-C4	5.05	124.07	117.18
4	A	4601	ATP	C6-C5-C4	5.05	124.07	117.18
4	A	4602	ATP	C6-C5-N7	-5.05	122.36	132.09
4	D	3602	ATP	C6-C5-N7	-5.03	122.39	132.09
4	C	2602	ATP	C6-C5-C4	5.00	124.01	117.18
4	D	3602	ATP	C6-C5-C4	4.97	123.96	117.18
4	C	2601	ATP	C6-C5-C4	4.96	123.96	117.18
4	A	4601	ATP	N3-C4-N9	4.90	135.50	127.17
4	A	4602	ATP	C6-C5-C4	4.89	123.86	117.18
4	C	2602	ATP	N3-C4-N9	4.88	135.46	127.17
4	D	3601	ATP	N3-C4-N9	4.87	135.44	127.17
4	C	2601	ATP	N3-C4-N9	4.86	135.43	127.17
4	B	1601	ATP	N3-C4-N9	4.82	135.36	127.17
4	A	4602	ATP	N3-C4-N9	4.81	135.34	127.17
4	D	3602	ATP	N3-C4-N9	4.75	135.25	127.17
4	B	1602	ATP	N3-C4-N9	4.71	135.19	127.17
4	A	4601	ATP	N9-C8-N7	-3.90	108.40	113.94
4	C	2601	ATP	N9-C8-N7	-3.82	108.52	113.94
4	B	1601	ATP	N9-C8-N7	-3.81	108.53	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	3601	ATP	N9-C8-N7	-3.78	108.57	113.94
4	B	1602	ATP	N9-C8-N7	-3.75	108.61	113.94
4	A	4602	ATP	N9-C8-N7	-3.63	108.78	113.94
2	C	2701	MLT	O2-C1-C2	3.62	120.40	112.74
2	A	701	MLT	O2-C1-C2	3.60	120.35	112.74
4	D	3602	ATP	N9-C8-N7	-3.59	108.84	113.94
2	B	1701	MLT	O2-C1-C2	3.58	120.32	112.74
4	C	2602	ATP	N9-C8-N7	-3.56	108.89	113.94
2	D	3701	MLT	O2-C1-C2	3.53	120.22	112.74
4	B	1602	ATP	C2-N3-C4	3.29	119.88	111.83
4	D	3602	ATP	C2-N3-C4	3.27	119.81	111.83
4	C	2601	ATP	C2-N3-C4	3.21	119.68	111.83
4	C	2602	ATP	C2-N3-C4	3.21	119.67	111.83
4	B	1601	ATP	C2-N3-C4	3.17	119.58	111.83
4	A	4602	ATP	C2-N3-C4	3.17	119.56	111.83
4	D	3601	ATP	C2-N3-C4	3.17	119.56	111.83
4	A	4601	ATP	C2-N3-C4	3.08	119.36	111.83
4	B	1602	ATP	C4-C5-N7	2.84	113.83	110.58
4	C	2601	ATP	C4-C5-N7	2.81	113.80	110.58
4	A	4602	ATP	C4-C5-N7	2.80	113.78	110.58
4	B	1601	ATP	C4-C5-N7	2.79	113.77	110.58
4	A	4601	ATP	C4-C5-N7	2.77	113.75	110.58
4	C	2602	ATP	C4-C5-N7	2.75	113.73	110.58
4	D	3601	ATP	C4-C5-N7	2.74	113.71	110.58
4	D	3602	ATP	C4-C5-N7	2.69	113.65	110.58
5	D	3700	FUM	O7-C6-C5	-2.54	113.27	121.06
4	B	1601	ATP	O4'-C1'-N9	2.42	112.73	108.09
5	D	3700	FUM	OXT-C-C4	2.34	124.77	116.16
4	A	4601	ATP	O4'-C1'-N9	2.29	112.49	108.09
2	B	1701	MLT	O2-C1-O1	-2.25	118.97	124.08
5	A	700	FUM	OXT-C-C4	2.25	124.43	116.16
4	D	3601	ATP	O4'-C1'-N9	2.23	112.37	108.09
5	A	700	FUM	O7-C6-C5	-2.22	114.27	121.06
4	B	1602	ATP	C3'-C2'-C1'	2.19	105.61	101.46
2	D	3701	MLT	O2-C1-O1	-2.17	119.15	124.08
4	C	2601	ATP	O4'-C1'-N9	2.14	112.21	108.09
4	C	2602	ATP	C3'-C2'-C1'	2.14	105.51	101.46
2	A	701	MLT	O2-C1-O1	-2.13	119.24	124.08
2	C	2701	MLT	O5-C4-C3	2.13	120.61	114.00
5	B	1700	FUM	OXT-C-C4	2.10	123.89	116.16
2	C	2701	MLT	O2-C1-O1	-2.10	119.32	124.08
2	A	701	MLT	O5-C4-C3	2.10	120.52	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	3602	ATP	C3'-C2'-C1'	2.09	105.42	101.46
5	C	2700	FUM	O7-C6-C5	-2.04	114.81	121.06
2	D	3701	MLT	O5-C4-C3	2.01	120.26	114.00

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	701	MLT	C2
2	B	1701	MLT	C2
2	C	2701	MLT	C2
2	D	3701	MLT	C2

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1601	ATP	PB-O3B-PG-O1G
4	D	3601	ATP	PB-O3B-PG-O1G
4	A	4601	ATP	PG-O3B-PB-O2B
4	B	1601	ATP	PG-O3B-PB-O2B
4	C	2601	ATP	PG-O3B-PB-O2B
4	D	3601	ATP	PG-O3B-PB-O2B
4	A	4601	ATP	PB-O3B-PG-O1G
4	C	2601	ATP	PB-O3B-PG-O1G
2	B	1701	MLT	C2-C3-C4-O4
2	B	1701	MLT	C2-C3-C4-O5
4	A	4602	ATP	PG-O3B-PB-O2B
4	C	2602	ATP	PG-O3B-PB-O2B
4	A	4601	ATP	PB-O3A-PA-O5'
4	A	4601	ATP	PB-O3B-PG-O2G
4	A	4601	ATP	PB-O3B-PG-O3G
4	B	1601	ATP	PB-O3B-PG-O2G
4	B	1601	ATP	PB-O3B-PG-O3G
4	C	2601	ATP	PB-O3B-PG-O2G
4	C	2601	ATP	PB-O3B-PG-O3G
4	D	3601	ATP	PB-O3B-PG-O2G
4	D	3601	ATP	PB-O3B-PG-O3G
2	C	2701	MLT	C2-C3-C4-O5
4	A	4601	ATP	O4'-C4'-C5'-O5'
4	A	4601	ATP	PG-O3B-PB-O1B
4	A	4601	ATP	PA-O3A-PB-O2B
4	B	1601	ATP	PG-O3B-PB-O1B
4	B	1602	ATP	PG-O3B-PB-O2B

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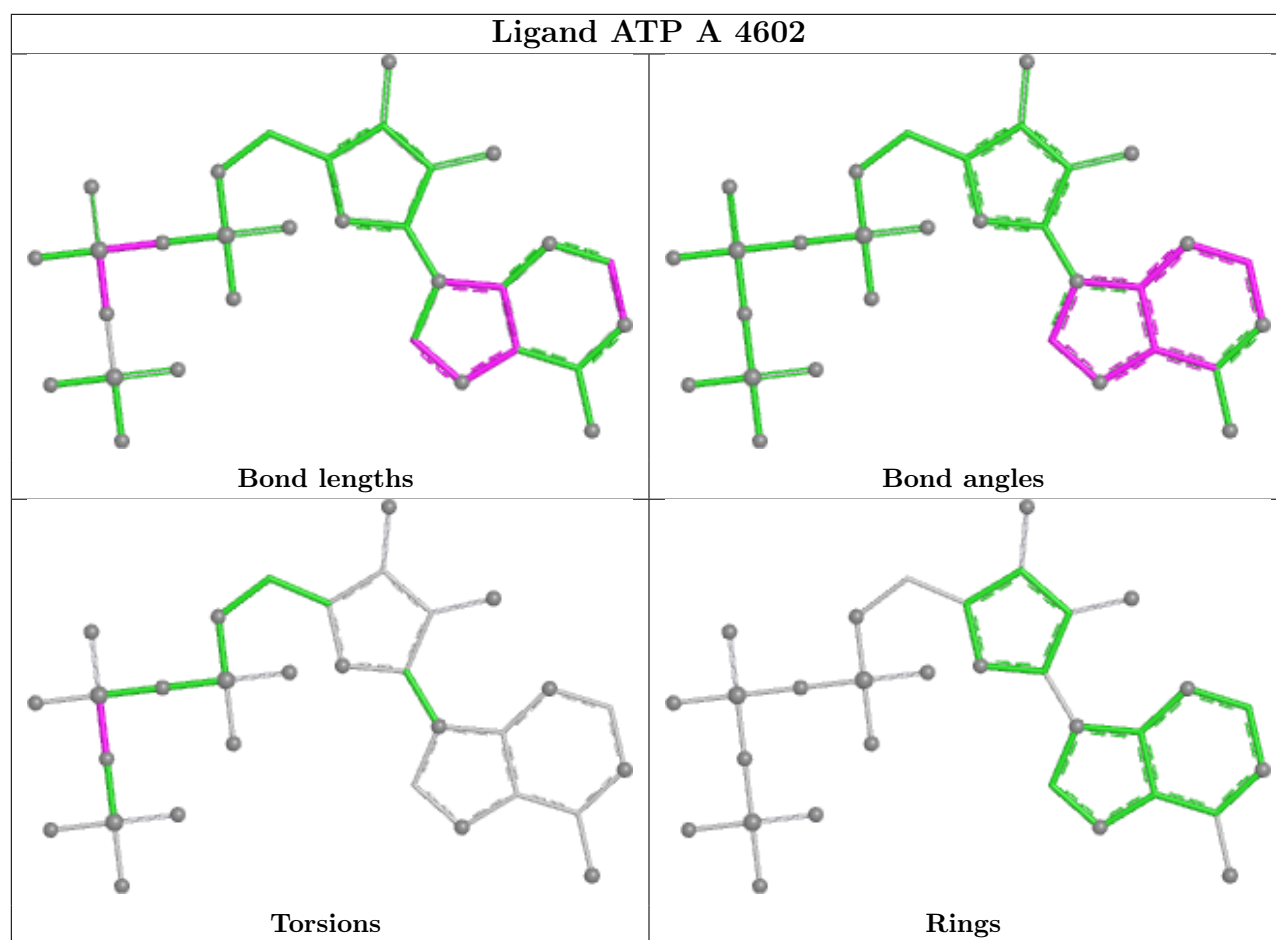
Mol	Chain	Res	Type	Atoms
4	D	3601	ATP	PG-O3B-PB-O1B
4	D	3601	ATP	PA-O3A-PB-O2B
4	D	3602	ATP	PG-O3B-PB-O2B
4	B	1601	ATP	O4'-C4'-C5'-O5'
2	C	2701	MLT	C2-C3-C4-O4
4	C	2601	ATP	O4'-C4'-C5'-O5'
2	D	3701	MLT	C2-C3-C4-O4
2	D	3701	MLT	C2-C3-C4-O5
4	A	4602	ATP	PG-O3B-PB-O1B
4	C	2601	ATP	PG-O3B-PB-O1B
4	C	2602	ATP	PG-O3B-PB-O1B
4	D	3602	ATP	PG-O3B-PB-O1B
4	D	3602	ATP	PB-O3A-PA-O1A

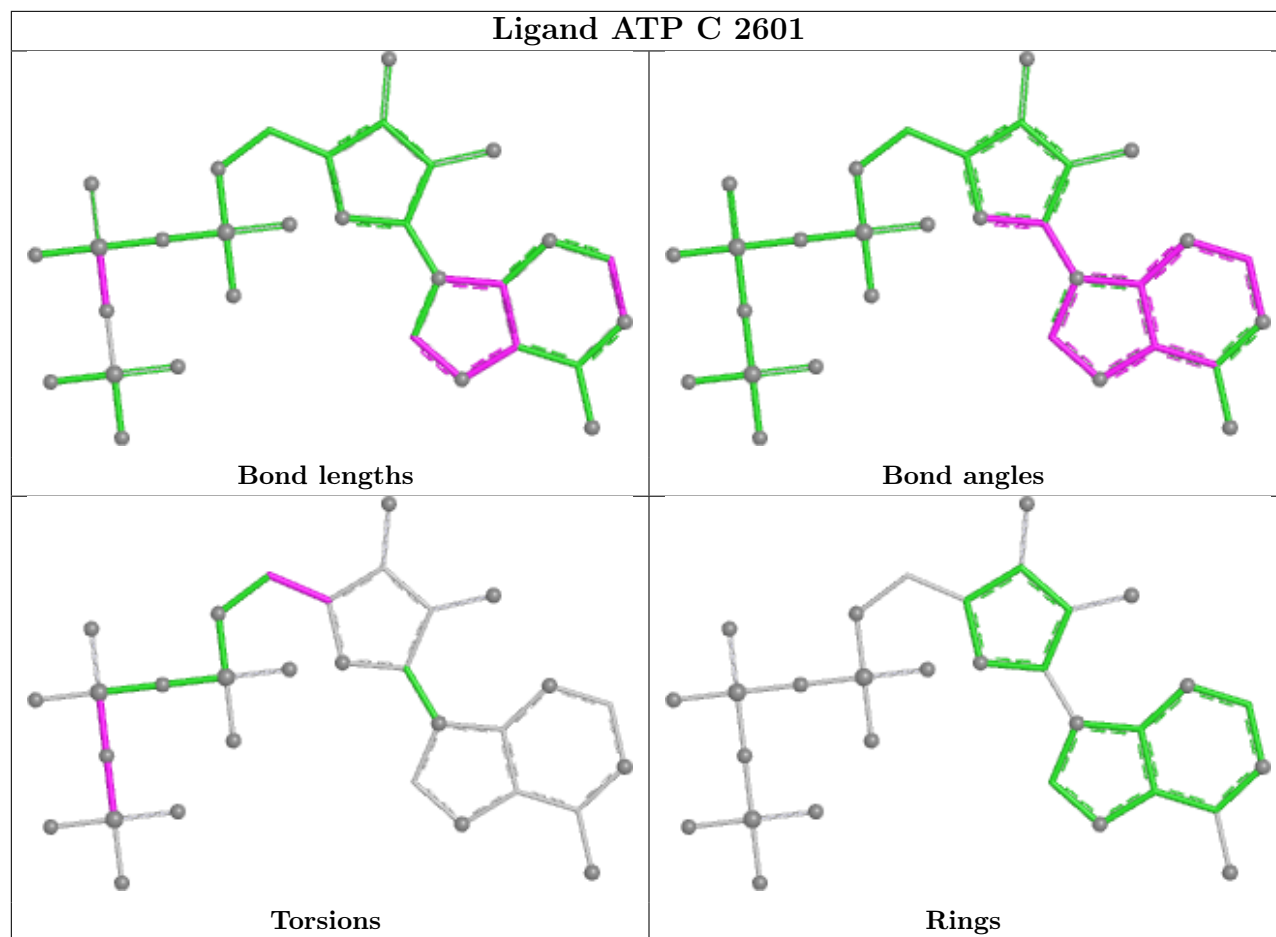
There are no ring outliers.

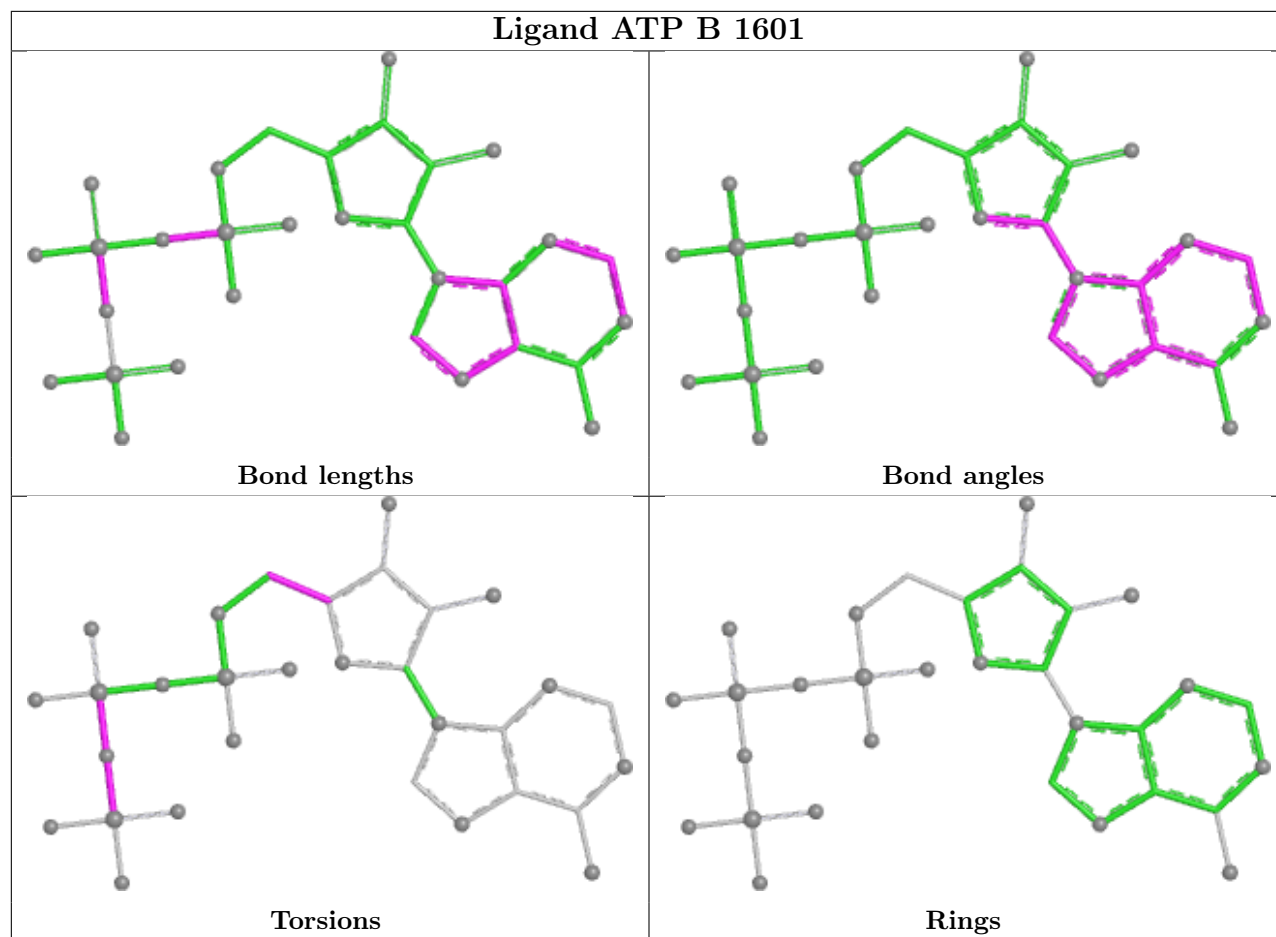
5 monomers are involved in 5 short contacts:

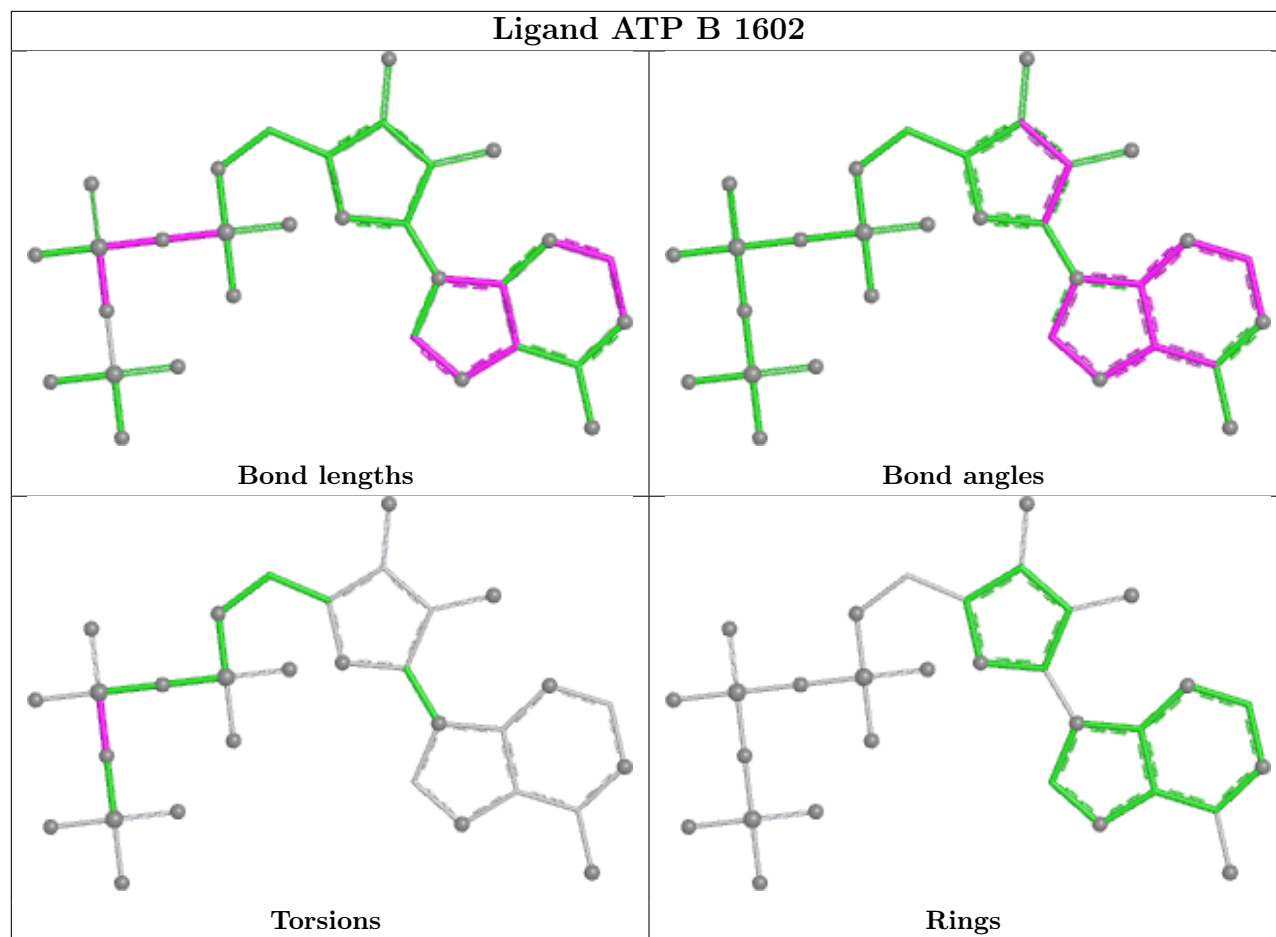
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1601	ATP	1	0
4	D	3601	ATP	1	0
2	D	3701	MLT	1	0
4	C	2602	ATP	1	0
4	A	4601	ATP	1	0

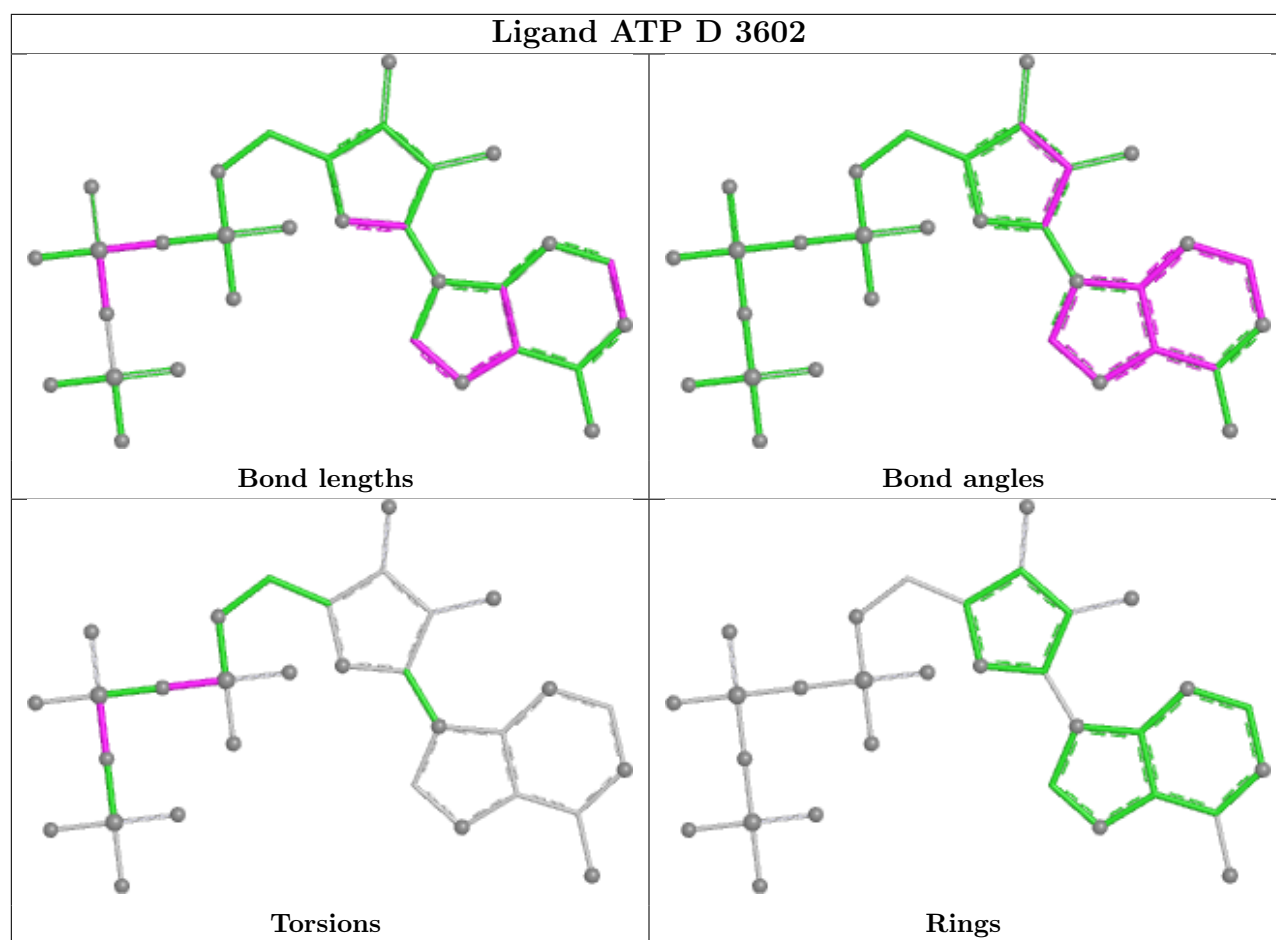
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

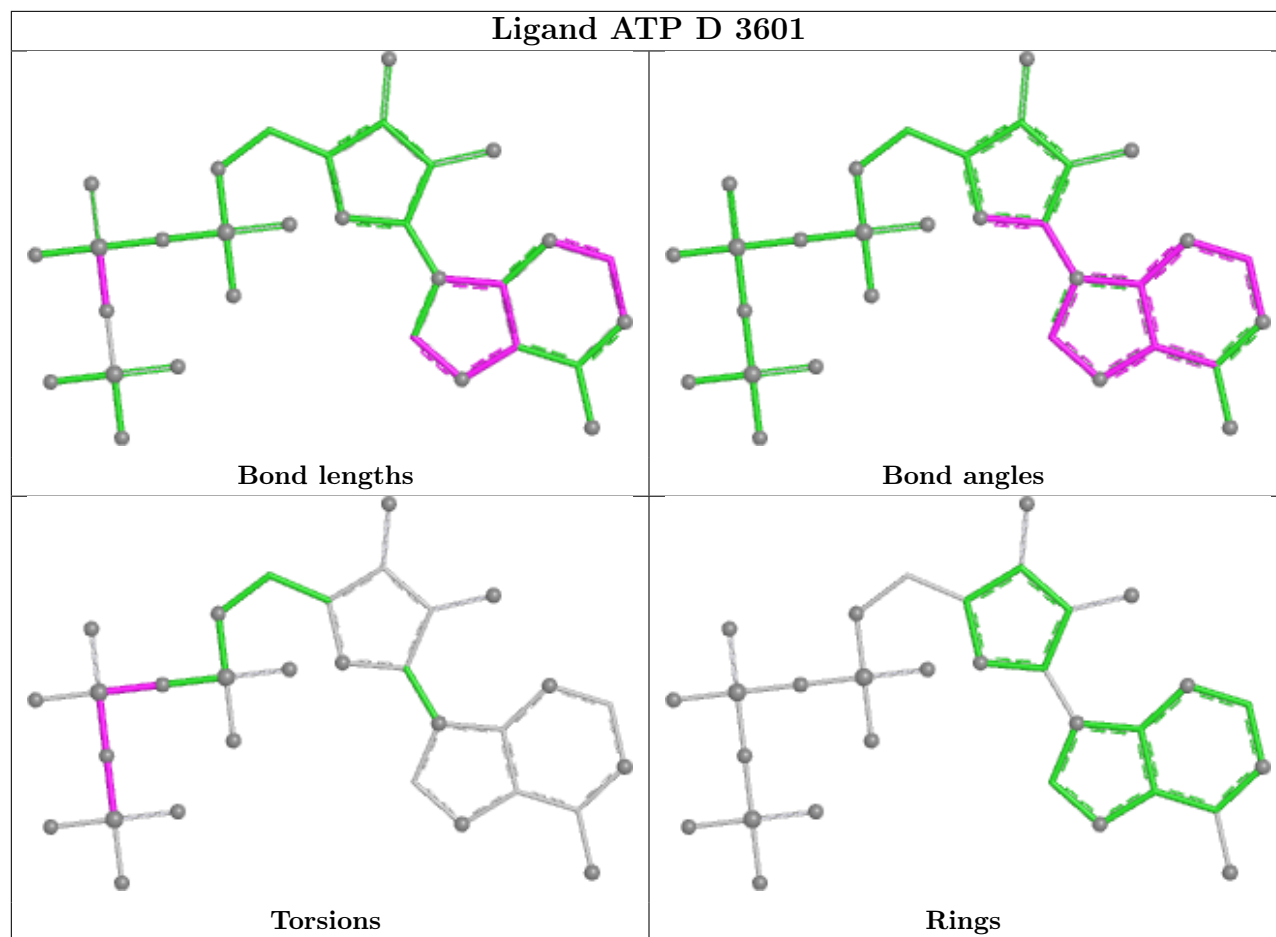


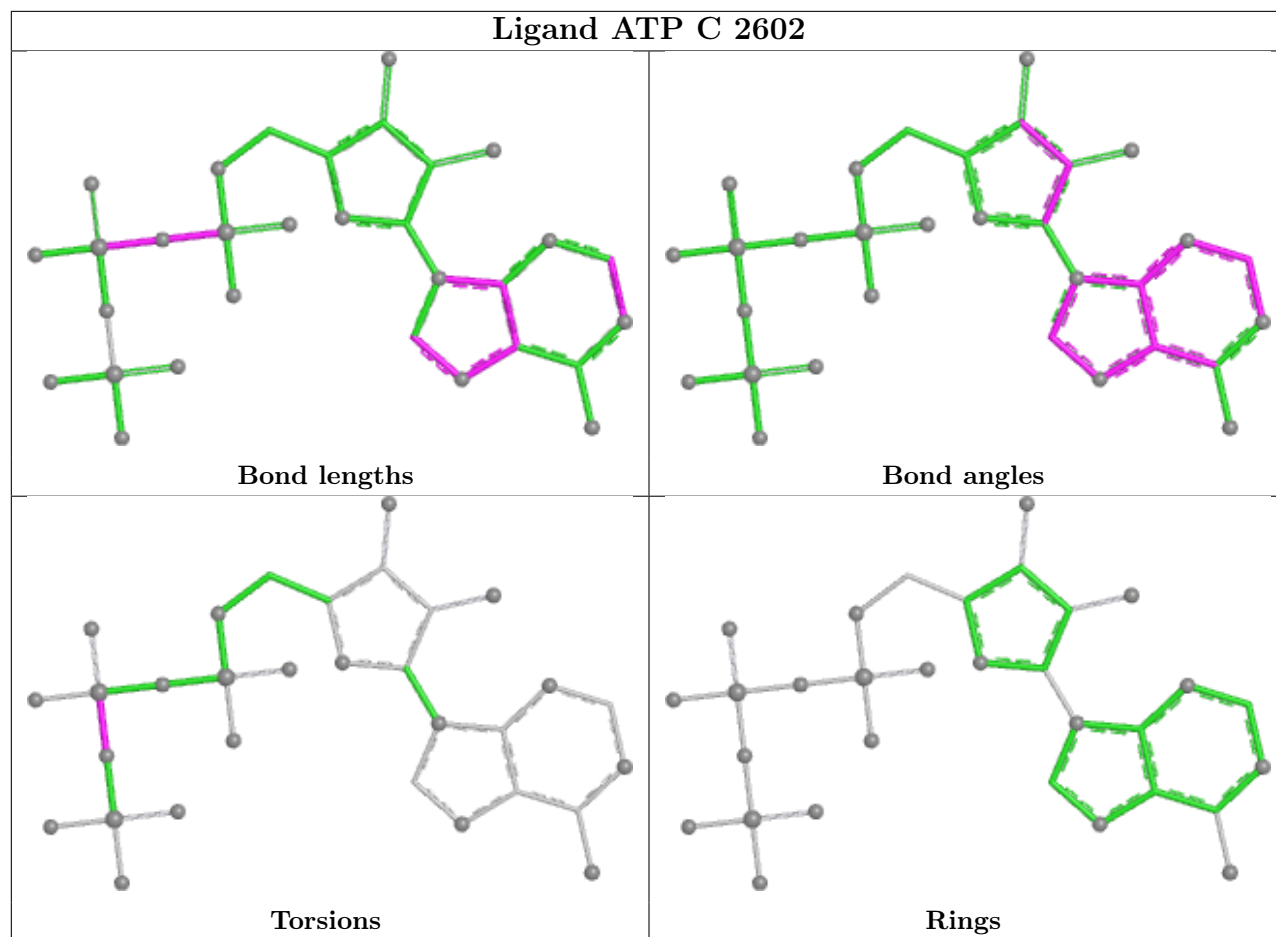


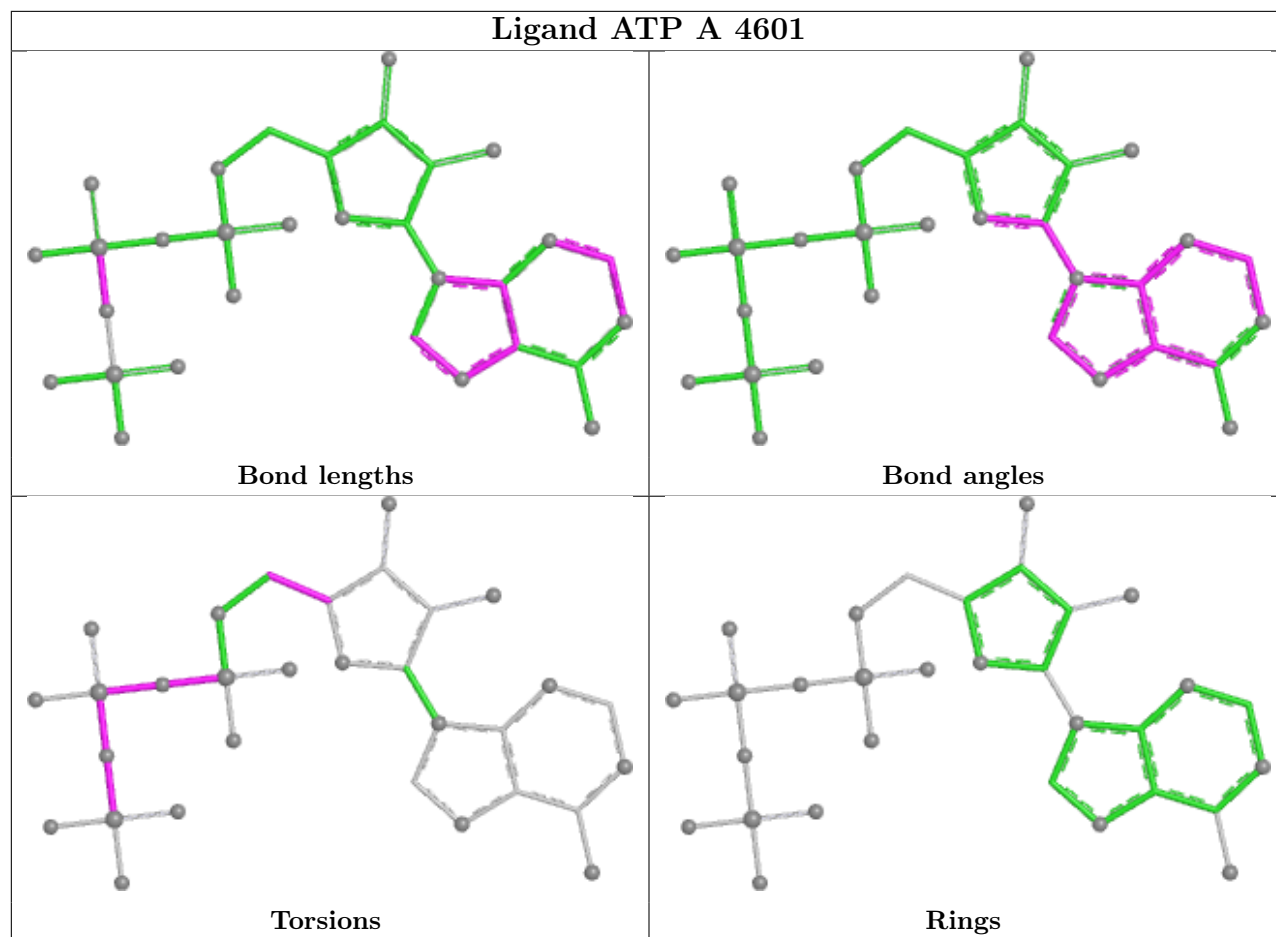












5.7 Other polymers [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	538/564 (95%)	0.12	15 (2%) 55 57	16, 27, 52, 66	0
1	B	538/564 (95%)	0.30	26 (4%) 35 37	16, 27, 53, 68	0
1	C	538/564 (95%)	0.27	25 (4%) 37 39	16, 28, 52, 60	0
1	D	538/564 (95%)	0.14	17 (3%) 50 52	15, 28, 52, 67	0
All	All	2152/2256 (95%)	0.21	83 (3%) 43 45	15, 27, 52, 68	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1543	TYR	5.4
1	B	1510	GLY	4.9
1	D	3353	GLY	4.9
1	A	508	ALA	4.7
1	D	3507	LEU	4.7
1	A	507	LEU	4.6
1	B	1507	LEU	4.4
1	B	1503	THR	4.3
1	D	3543	TYR	4.2
1	A	353	GLY	4.0
1	A	509	GLN	4.0
1	C	2335	GLN	4.0
1	C	2368	SER	4.0
1	B	1301	PRO	3.8
1	A	543	TYR	3.6
1	C	2331	GLY	3.6
1	C	2507	LEU	3.5
1	A	328	VAL	3.4
1	C	2543	TYR	3.4
1	C	2356	ALA	3.2
1	B	1120	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	3455	THR	3.0
1	B	1304	GLU	3.0
1	C	2359	ASP	2.9
1	C	2510	GLY	2.9
1	B	1508	ALA	2.9
1	B	1504	ASP	2.9
1	B	1233	ASP	2.8
1	A	336	GLU	2.8
1	B	1369	ALA	2.8
1	B	1375	ASP	2.7
1	C	2328	VAL	2.7
1	D	3369	ALA	2.7
1	D	3508	ALA	2.7
1	C	2336	GLU	2.7
1	B	1389	ILE	2.7
1	B	1303	SER	2.7
1	D	3302	ILE	2.6
1	C	2372	SER	2.6
1	A	504	ASP	2.6
1	C	2505	GLU	2.6
1	A	331	GLY	2.6
1	B	1331	GLY	2.5
1	D	3370	PRO	2.5
1	A	335	GLN	2.5
1	C	2297	VAL	2.5
1	C	2360	SER	2.4
1	C	2358	ILE	2.4
1	B	1353	GLY	2.4
1	C	2260	HIS	2.4
1	B	1371	GLU	2.4
1	C	2366	THR	2.4
1	D	3357	LYS	2.4
1	B	1372	SER	2.4
1	A	358	ILE	2.4
1	C	2375	ASP	2.3
1	C	2022	LYS	2.3
1	B	1509	GLN	2.3
1	D	3505	GLU	2.3
1	C	2330	ASN	2.3
1	B	1339	LYS	2.3
1	B	1351	VAL	2.3
1	B	1374	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	1260	HIS	2.2
1	A	22	LYS	2.2
1	C	2355	LYS	2.2
1	D	3022	LYS	2.2
1	B	1550	ALA	2.2
1	C	2085	ILE	2.2
1	A	359	ASP	2.1
1	B	1511	ARG	2.1
1	C	2248	ARG	2.1
1	C	2373	ILE	2.1
1	A	371	GLU	2.1
1	A	456	ASP	2.1
1	D	3379	ASP	2.1
1	B	1022	LYS	2.1
1	D	3408	ALA	2.1
1	D	3509	GLN	2.1
1	C	2352	LYS	2.0
1	D	3503	THR	2.0
1	D	3544	PRO	2.0
1	D	3573	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ATP	C	2601	31/31	0.85	0.14	30,32,60,61	0
4	ATP	C	2602	31/31	0.86	0.13	24,35,73,75	0
4	ATP	B	1602	31/31	0.87	0.11	24,34,71,73	0

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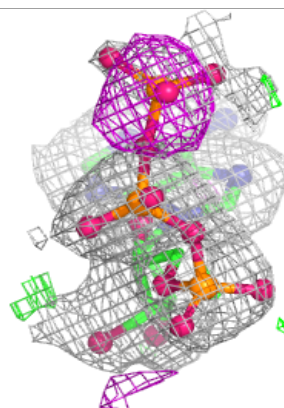
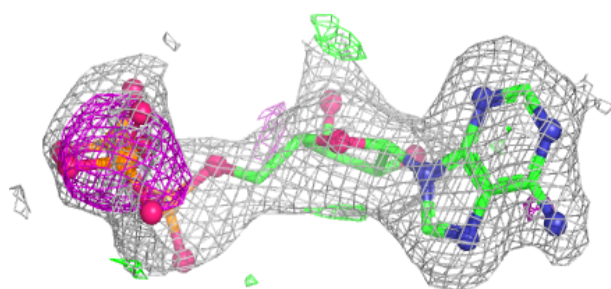
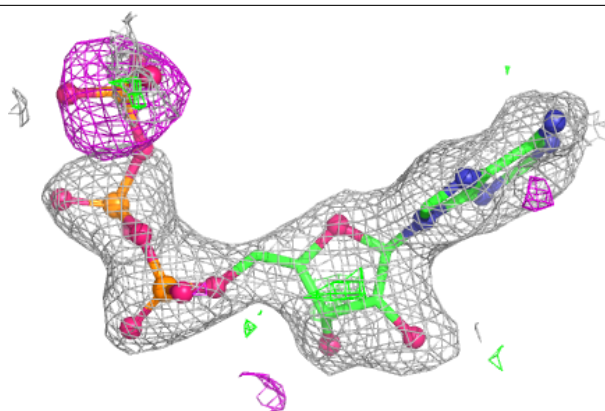
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MLT	D	3701	9/9	0.87	0.10	27,29,31,33	0
4	ATP	B	1601	31/31	0.87	0.13	28,30,59,60	0
4	ATP	A	4601	31/31	0.88	0.14	25,28,60,62	0
4	ATP	A	4602	31/31	0.88	0.13	21,35,73,74	0
4	ATP	D	3602	31/31	0.88	0.13	23,37,73,75	0
2	MLT	A	701	9/9	0.89	0.11	25,28,31,33	0
4	ATP	D	3601	31/31	0.89	0.12	27,30,59,60	0
2	MLT	C	2701	9/9	0.89	0.13	26,30,32,32	0
5	FUM	A	700	8/8	0.94	0.07	35,37,38,38	0
5	FUM	B	1700	8/8	0.94	0.07	35,39,39,40	0
5	FUM	C	2700	8/8	0.94	0.08	35,37,39,39	0
5	FUM	D	3700	8/8	0.94	0.07	35,38,38,39	0
2	MLT	B	1701	9/9	0.96	0.07	27,30,34,34	0
3	MN	C	2604	1/1	0.98	0.05	29,29,29,29	0
3	MN	B	1604	1/1	0.99	0.05	28,28,28,28	0
3	MN	D	3604	1/1	0.99	0.02	28,28,28,28	0
3	MN	A	4604	1/1	1.00	0.01	23,23,23,23	0

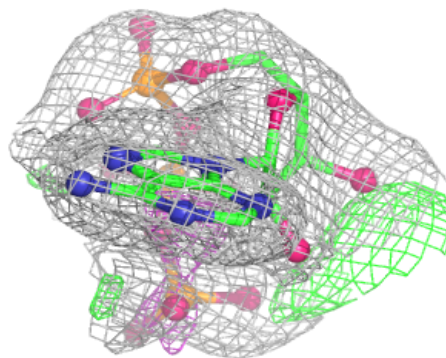
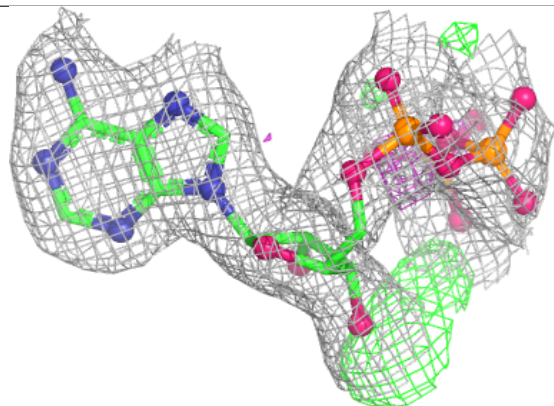
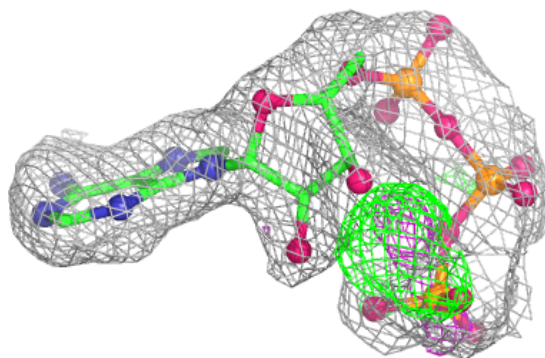
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP C 2601:

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

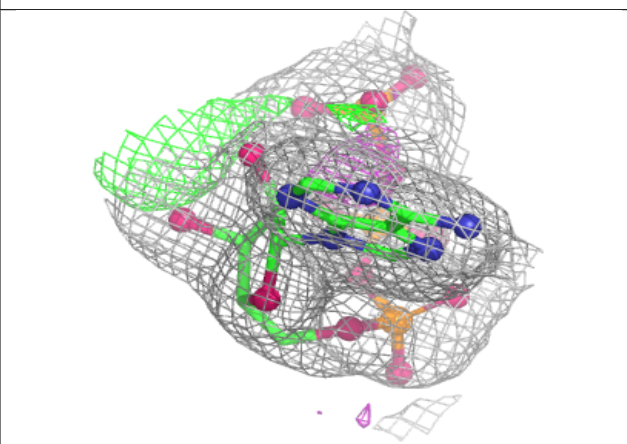
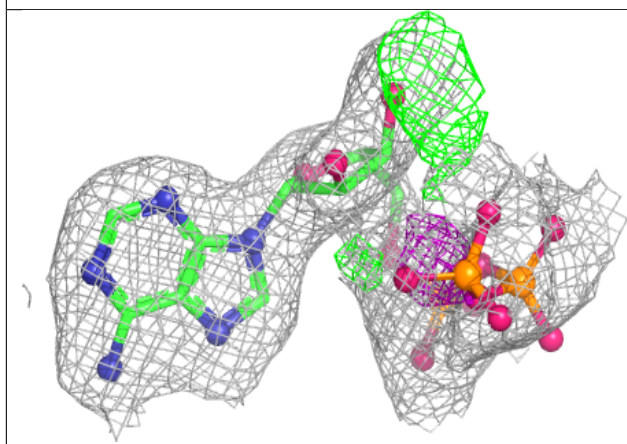
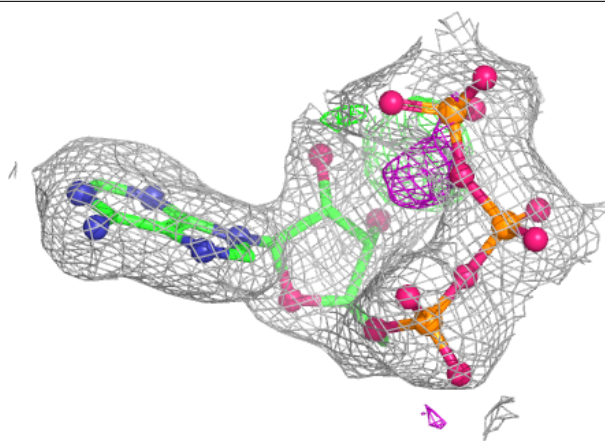
**Electron density around ATP C 2602:**

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

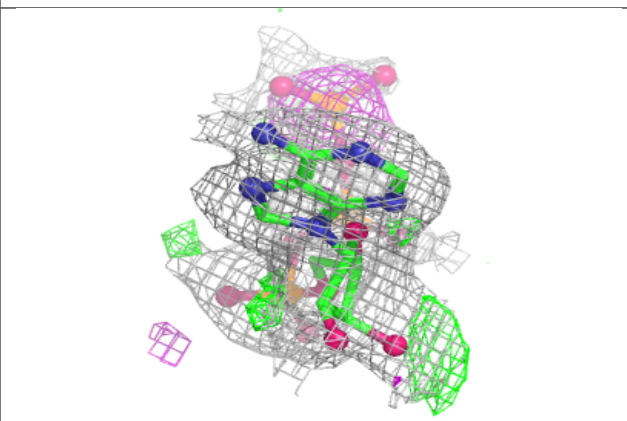
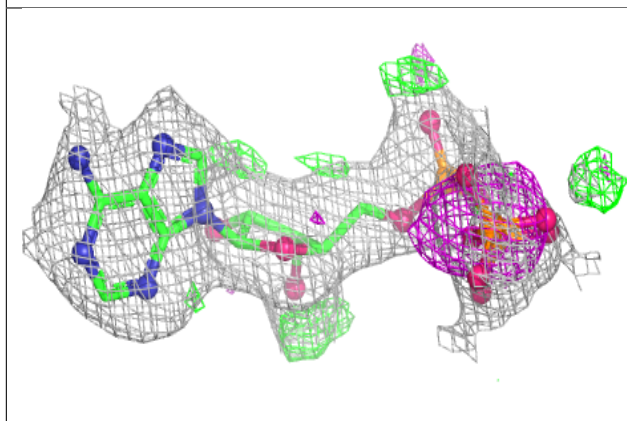
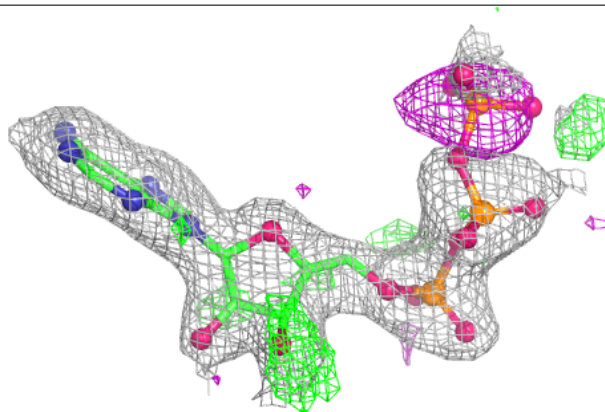


Electron density around ATP B 1602:

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

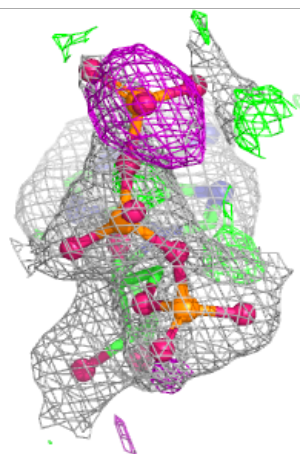
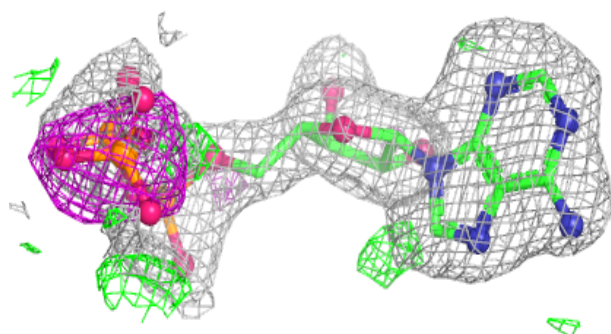
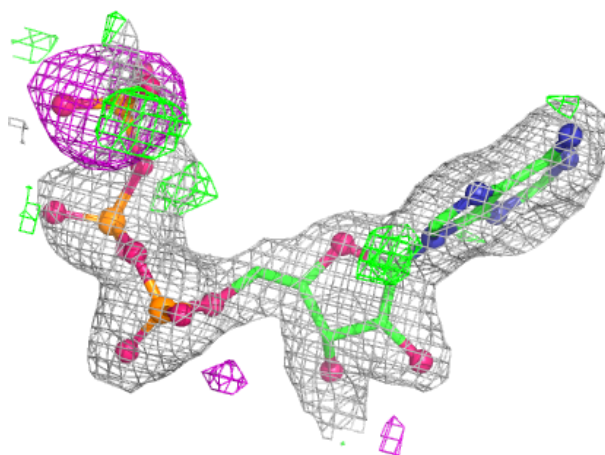
**Electron density around ATP B 1601:**

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



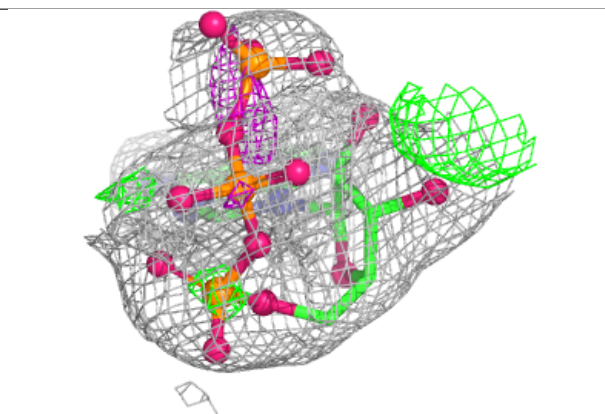
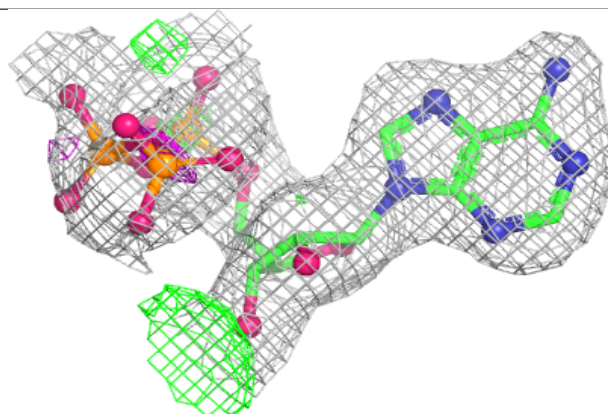
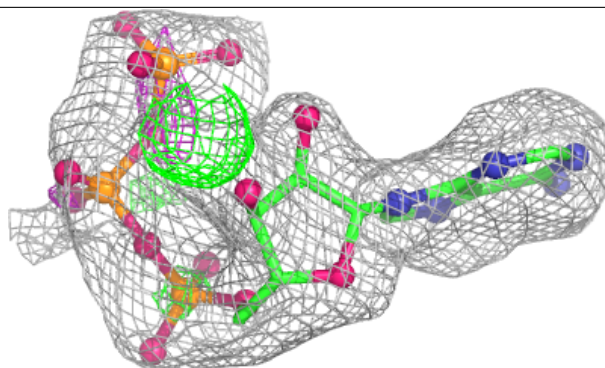
Electron density around ATP A 4601:

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

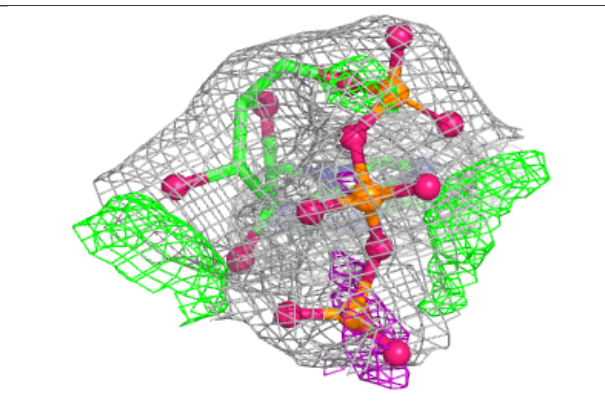
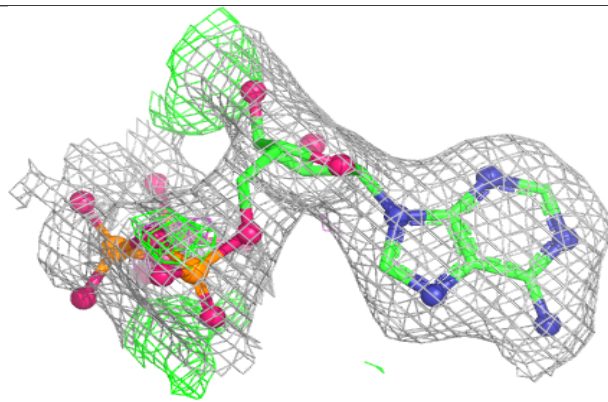
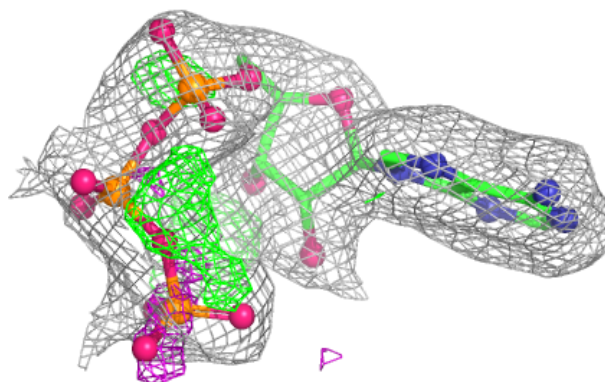


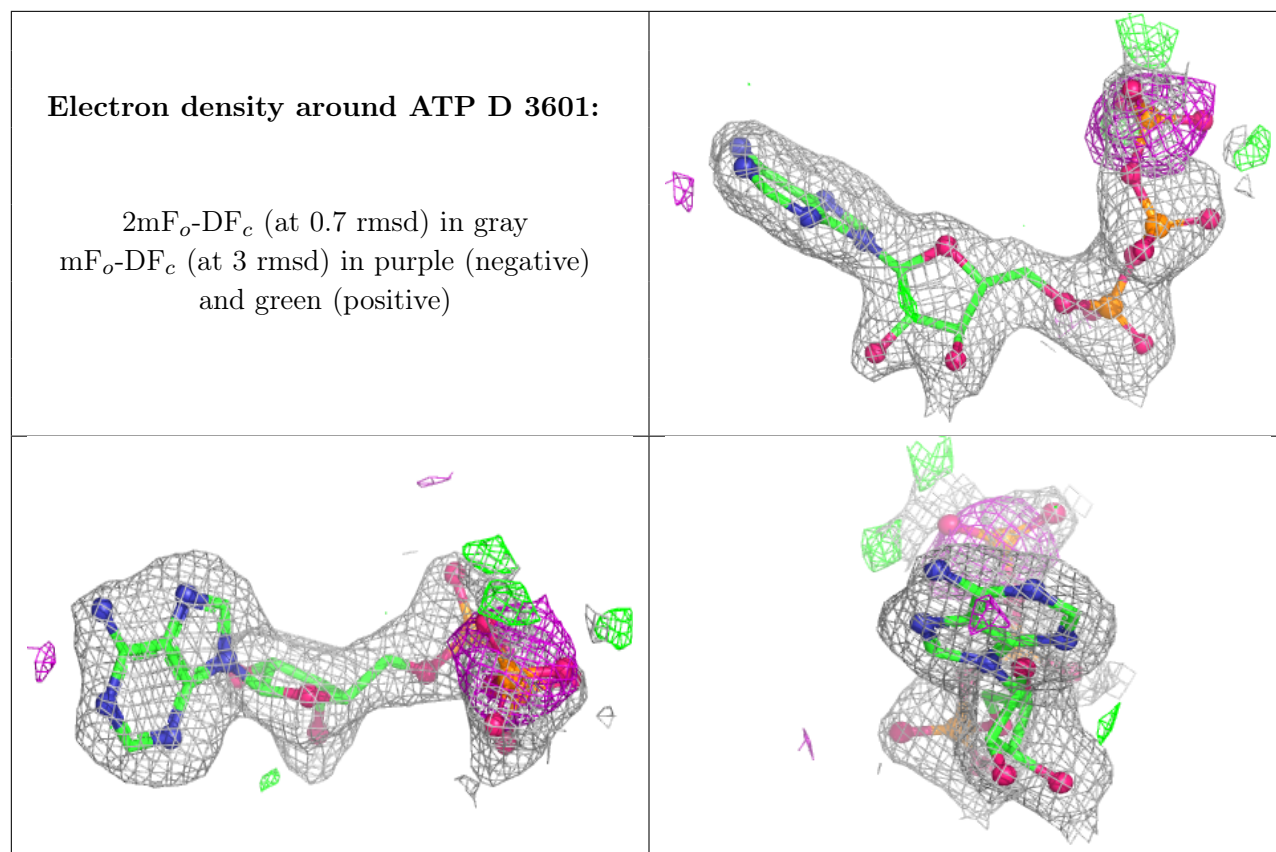
Electron density around ATP A 4602:

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

**Electron density around ATP D 3602:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.