



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:17 AM UTC

PDB ID : 9BQ0 / pdb_00009bq0
Title : Complex structure of protein crystal of Tri17 with ATP
Authors : Zhai, R.; Zhang, W.
Deposited on : 2024-05-08
Resolution : 2.90 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

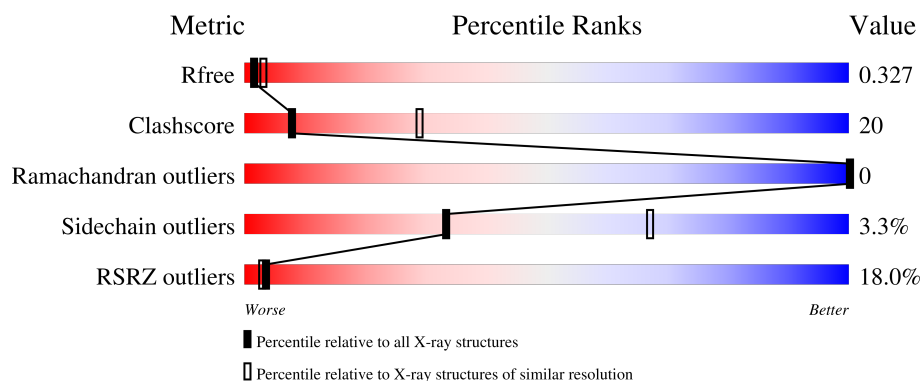
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	17% 53% 32% • 14%
1	B	564	10% 56% 27% • 15%
1	C	564	17% 51% 33% • 15%
1	D	564	18% 55% 30% • 15%

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
3	MG	C	602	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 29878 atoms, of which 14521 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 AMP-binding protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	487	Total	C	H	N	O	S	0	0	0
			7410	2385	3653	662	697	13			
1	B	479	Total	C	H	N	O	S	0	0	0
			7300	2350	3599	652	686	13			
1	C	480	Total	C	H	N	O	S	0	0	0
			7335	2361	3622	652	687	13			
1	D	482	Total	C	H	N	O	S	0	0	0
			7333	2375	3599	657	689	13			

There are 36 discrepancies between the modelled and reference sequences:

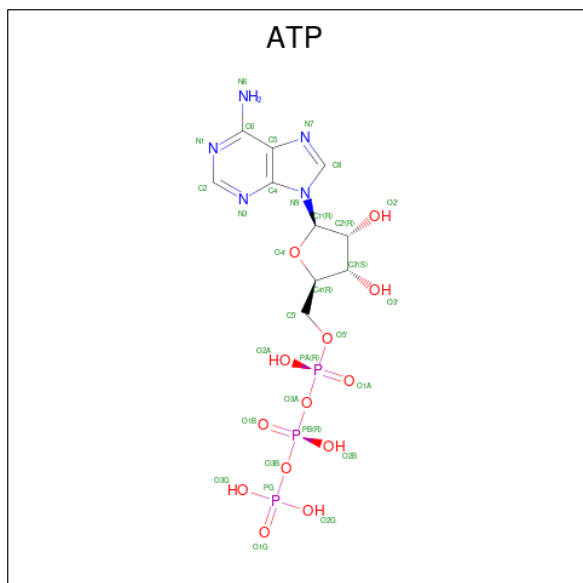
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A5H2UY12
A	557	LEU	-	expression tag	UNP A0A5H2UY12
A	558	GLU	-	expression tag	UNP A0A5H2UY12
A	559	HIS	-	expression tag	UNP A0A5H2UY12
A	560	HIS	-	expression tag	UNP A0A5H2UY12
A	561	HIS	-	expression tag	UNP A0A5H2UY12
A	562	HIS	-	expression tag	UNP A0A5H2UY12
A	563	HIS	-	expression tag	UNP A0A5H2UY12
A	564	HIS	-	expression tag	UNP A0A5H2UY12
B	1	MET	-	initiating methionine	UNP A0A5H2UY12
B	557	LEU	-	expression tag	UNP A0A5H2UY12
B	558	GLU	-	expression tag	UNP A0A5H2UY12
B	559	HIS	-	expression tag	UNP A0A5H2UY12
B	560	HIS	-	expression tag	UNP A0A5H2UY12
B	561	HIS	-	expression tag	UNP A0A5H2UY12
B	562	HIS	-	expression tag	UNP A0A5H2UY12
B	563	HIS	-	expression tag	UNP A0A5H2UY12
B	564	HIS	-	expression tag	UNP A0A5H2UY12
C	1	MET	-	initiating methionine	UNP A0A5H2UY12
C	557	LEU	-	expression tag	UNP A0A5H2UY12
C	558	GLU	-	expression tag	UNP A0A5H2UY12

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Chain	Residue	Modelled	Actual	Comment	Reference
C	559	HIS	-	expression tag	UNP A0A5H2UY12
C	560	HIS	-	expression tag	UNP A0A5H2UY12
C	561	HIS	-	expression tag	UNP A0A5H2UY12
C	562	HIS	-	expression tag	UNP A0A5H2UY12
C	563	HIS	-	expression tag	UNP A0A5H2UY12
C	564	HIS	-	expression tag	UNP A0A5H2UY12
D	1	MET	-	initiating methionine	UNP A0A5H2UY12
D	557	LEU	-	expression tag	UNP A0A5H2UY12
D	558	GLU	-	expression tag	UNP A0A5H2UY12
D	559	HIS	-	expression tag	UNP A0A5H2UY12
D	560	HIS	-	expression tag	UNP A0A5H2UY12
D	561	HIS	-	expression tag	UNP A0A5H2UY12
D	562	HIS	-	expression tag	UNP A0A5H2UY12
D	563	HIS	-	expression tag	UNP A0A5H2UY12
D	564	HIS	-	expression tag	UNP A0A5H2UY12

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 43	C 10	H 12	N 5	O 13	P 3	0	0
2	B	1	Total 43	C 10	H 12	N 5	O 13	P 3	0	0
2	C	1	Total 43	C 10	H 12	N 5	O 13	P 3	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	D	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	2	Total	Mg	0	0
			2	2		
3	C	1	Total	Mg	0	0
			1	1		
3	D	2	Total	Mg	0	0
			2	2		

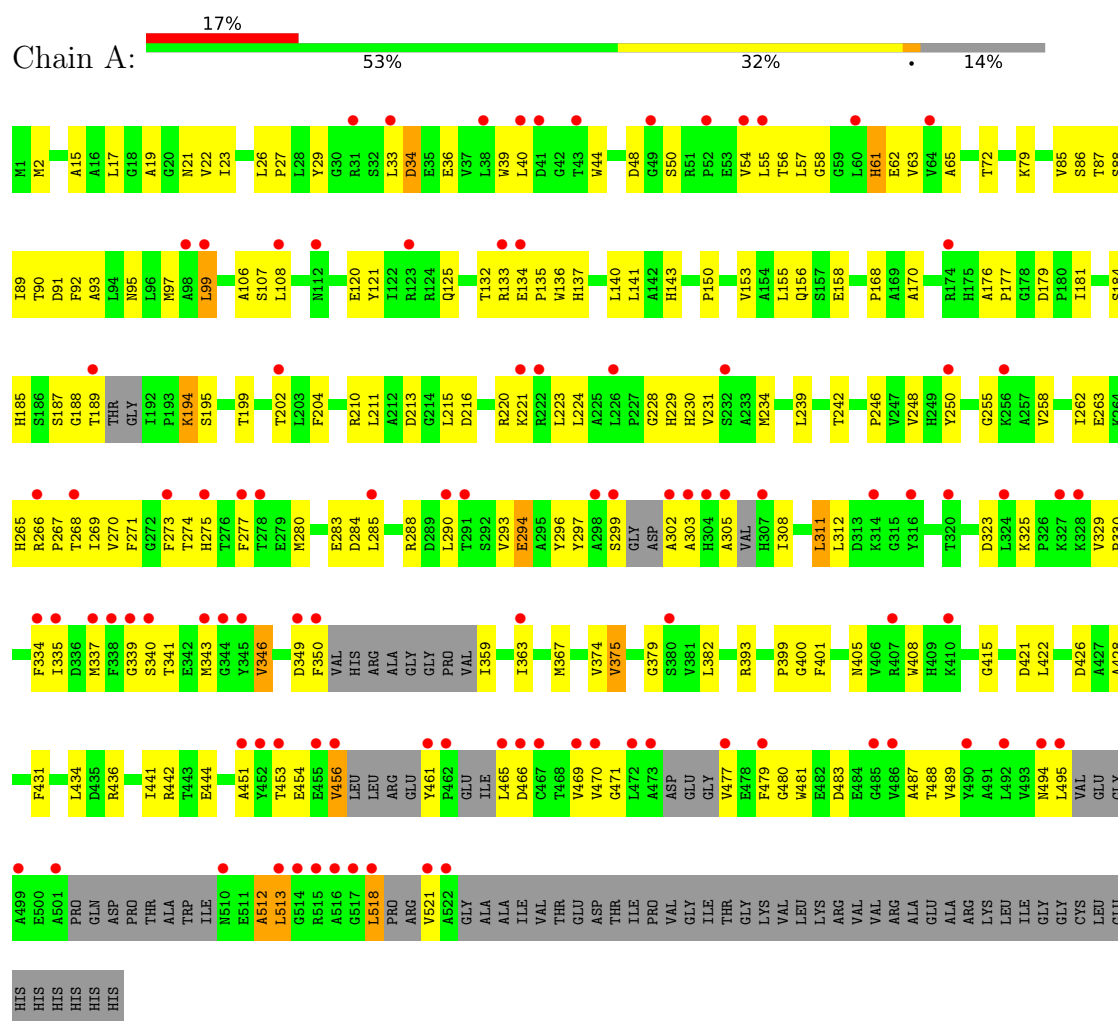
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	118	Total	O	0	0
			118	118		
4	B	74	Total	O	0	0
			74	74		
4	C	68	Total	O	0	0
			68	68		
4	D	62	Total	O	0	0
			62	62		

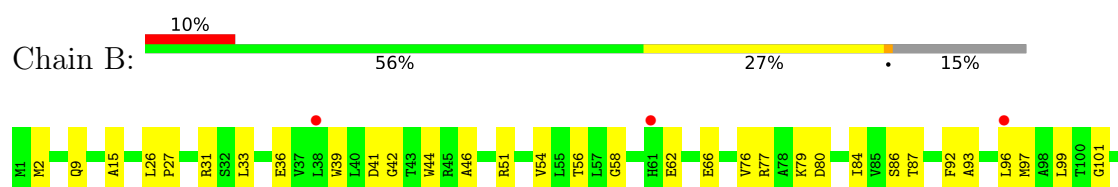
3 Residue-property plots

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.

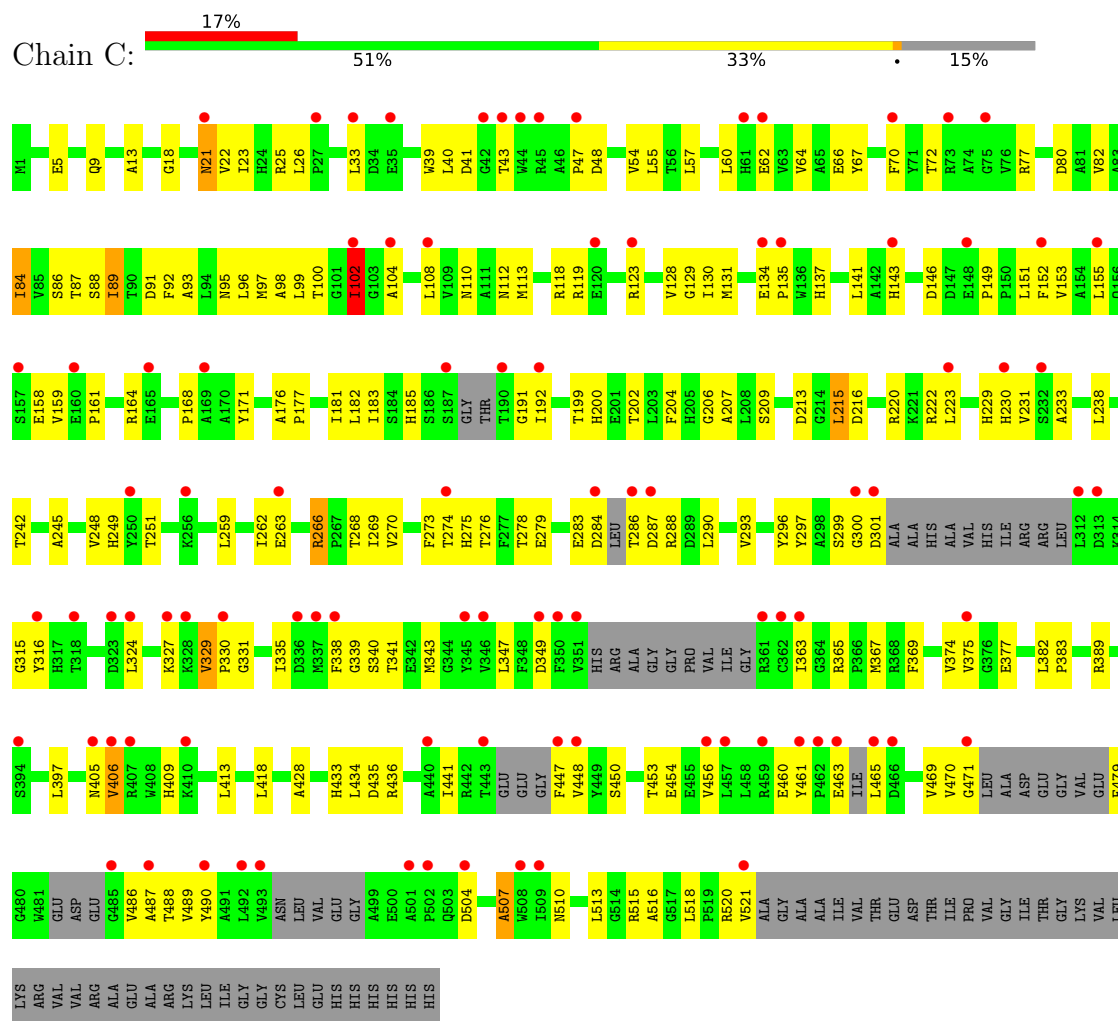
• Molecule 1: AMP-binding protein



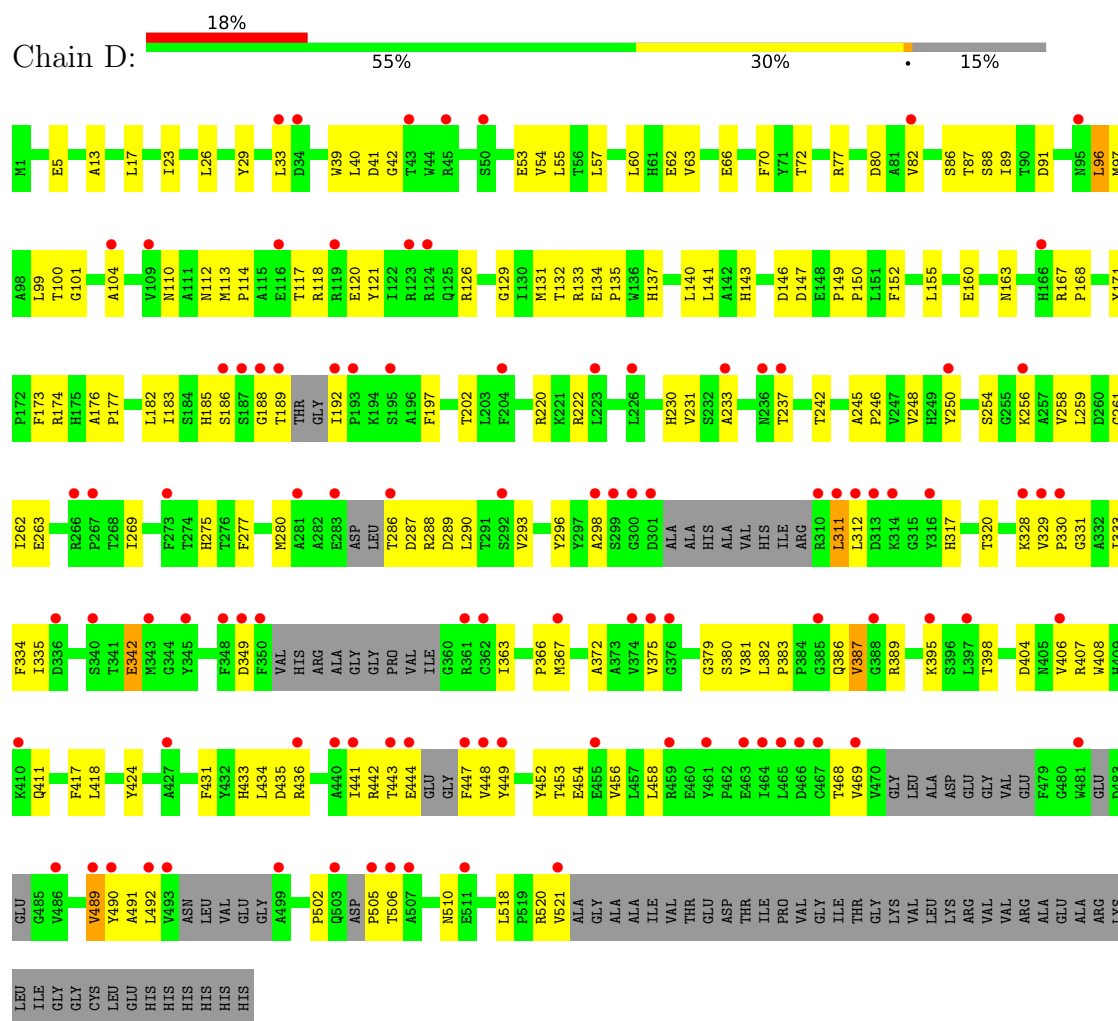
• Molecule 1: AMP-binding protein



- Molecule 1: AMP-binding protein



● Molecule 1: AMP-binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	87.09Å 152.33Å 229.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.44 – 2.90 46.44 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.44-2.90) 99.9 (46.44-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.278 , 0.330 0.278 , 0.327	Depositor DCC
R_{free} test set	3419 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	53.4	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	29878	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 60.77 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4473e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.74	1/3841 (0.0%)	1.00	2/5213 (0.0%)
1	B	0.68	0/3786	0.92	2/5142 (0.0%)
1	C	0.70	3/3801 (0.1%)	0.99	7/5165 (0.1%)
1	D	0.68	0/3821	0.95	8/5188 (0.2%)
All	All	0.70	4/15249 (0.0%)	0.97	19/20708 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	266	ARG	C-O	8.22	1.27	1.23
1	C	266	ARG	CA-C	-5.79	1.49	1.53
1	A	99	LEU	C-O	-5.71	1.17	1.24
1	C	450	SER	C-O	-5.02	1.18	1.24

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	149	PRO	N-CA-C	8.02	120.48	110.70
1	D	149	PRO	N-CA-C	7.56	119.93	110.70
1	B	405	ASN	N-CA-C	-6.54	103.99	112.23
1	D	311	LEU	N-CA-C	-6.45	105.41	113.28
1	C	507	ALA	N-CA-C	-6.40	104.22	111.07
1	D	237	THR	N-CA-C	-6.32	104.48	111.36
1	D	149	PRO	CB-CA-C	-6.18	103.39	110.92
1	A	513	LEU	N-CA-C	-6.10	103.80	111.11
1	D	63	VAL	N-CA-C	-5.76	105.11	110.53
1	B	395	LYS	N-CA-C	-5.71	106.27	113.18
1	C	436	ARG	N-CA-C	-5.62	101.39	110.32
1	D	259	LEU	N-CA-C	-5.55	105.24	112.23
1	D	331	GLY	CA-C-O	-5.38	117.56	122.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	512	ALA	N-CA-C	-5.33	105.13	111.69
1	C	102	ILE	N-CA-C	-5.29	105.83	113.07
1	C	315	GLY	CA-C-O	-5.17	116.76	121.72
1	D	436	ARG	N-CA-C	-5.08	102.23	110.32
1	C	21	ASN	N-CA-CB	5.07	119.02	111.51
1	C	450	SER	CA-C-O	-5.07	115.50	120.82

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	3757	3653	3673	168	0
1	B	3701	3599	3626	130	0
1	C	3713	3622	3630	157	0
1	D	3734	3599	3658	144	0
2	A	31	12	12	0	0
2	B	31	12	12	0	0
2	C	31	12	12	0	0
2	D	31	12	12	1	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	0	0
4	A	118	0	0	9	0
4	B	74	0	0	1	0
4	C	68	0	0	2	0
4	D	62	0	0	0	0
All	All	15357	14521	14635	588	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 20.

All (588) 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:D:280:MET:HE3	1:D:311:LEU:HD22	1.52	0.90
1:C:274:THR:HG21	1:C:301:ASP:HB2	1.54	0.89
1:C:39:TRP:HB2	1:C:248:VAL:HG22	1.54	0.87
1:C:343:MET:HA	1:C:397:LEU:HD23	1.58	0.86
1:C:39:TRP:CB	1:C:248:VAL:HG22	2.06	0.85
1:D:137:HIS:HD2	1:D:155:LEU:HG	1.40	0.84
1:C:365:ARG:HH21	1:C:428:ALA:HB1	1.43	0.84
1:A:280:MET:HE3	1:A:311:LEU:HD11	1.59	0.83
1:B:199:THR:OG1	1:B:202:THR:HG23	1.77	0.83
1:B:284:ASP:OD1	1:B:285:LEU:N	2.13	0.82
1:D:137:HIS:CD2	1:D:155:LEU:HG	2.17	0.80
1:C:21:ASN:O	1:C:25:ARG:HG2	1.82	0.79
1:B:15:ALA:HB3	1:D:13:ALA:HA	1.66	0.77
1:C:329:VAL:HG12	1:C:330:PRO:HD2	1.64	0.77
1:C:349:ASP:HB2	1:C:367:MET:HE2	1.67	0.75
1:C:89:ILE:HG23	1:C:249:HIS:ND1	2.01	0.74
1:C:329:VAL:HG12	1:C:330:PRO:CD	2.18	0.74
1:B:110:ASN:H	1:B:185:HIS:HE1	1.37	0.73
1:D:510:ASN:OD1	1:D:521:VAL:HG12	1.88	0.72
1:B:185:HIS:C	1:B:341:THR:HG21	2.15	0.71
1:A:185:HIS:C	1:A:341:THR:HG21	2.16	0.70
1:A:79:LYS:HE3	4:A:741:HOH:O	1.92	0.70
1:A:132:THR:HG21	1:A:140:LEU:HD12	1.71	0.70
1:A:199:THR:OG1	1:A:202:THR:HG23	1.92	0.69
1:B:182:LEU:CD2	1:B:231:VAL:HG23	2.22	0.69
1:C:461:TYR:O	1:C:463:GLU:HG2	1.93	0.68
1:B:283:GLU:O	1:B:285:LEU:HD12	1.93	0.68
1:B:280:MET:O	1:B:285:LEU:HD11	1.94	0.68
1:A:33:LEU:HD23	1:A:57:LEU:HD23	1.76	0.68
1:A:15:ALA:HB3	1:C:13:ALA:HA	1.76	0.68
1:C:60:LEU:HD21	1:C:97:MET:SD	2.34	0.67
1:A:121:TYR:OH	1:A:185:HIS:HB3	1.94	0.67
1:B:457:LEU:HD21	1:B:513:LEU:CD1	2.24	0.67
1:C:223:LEU:HD12	1:C:248:VAL:CG1	2.25	0.67
1:B:305:ALA:HB1	1:B:308:ILE:HG21	1.75	0.67
1:D:312:LEU:HD21	1:D:334:PHE:HB2	1.77	0.67
1:B:277:PHE:HD1	1:B:280:MET:HE2	1.61	0.66
1:A:367:MET:HE1	4:A:725:HOH:O	1.96	0.66
1:D:39:TRP:HB2	1:D:248:VAL:HG22	1.79	0.65
1:D:453:THR:O	1:D:456:VAL:HG22	1.96	0.65
1:D:387:VAL:HG22	1:D:434:LEU:HD12	1.77	0.65
1:C:339:GLY:HA2	1:C:343:MET:HE2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:SER:OG	1:C:87:THR:N	2.27	0.64
1:C:192:ILE:HD12	1:C:192:ILE:H	1.62	0.64
1:B:121:TYR:OH	1:B:185:HIS:HB3	1.97	0.64
1:C:77:ARG:O	1:C:80:ASP:HB2	1.98	0.64
1:C:89:ILE:HG13	1:C:233:ALA:HB1	1.78	0.64
1:B:491:ALA:C	1:B:492:LEU:HD23	2.22	0.64
1:D:113:MET:HE2	1:D:118:ARG:HA	1.79	0.64
1:D:120:GLU:OE1	1:D:120:GLU:HA	1.98	0.64
1:B:374:VAL:HG12	1:B:382:LEU:HD12	1.79	0.63
1:D:489:VAL:O	1:D:521:VAL:HG23	1.98	0.63
1:A:470:VAL:HG13	1:A:471:GLY:N	2.12	0.63
1:C:134:GLU:OE2	1:C:155:LEU:HD13	1.98	0.63
1:B:274:THR:HG23	1:B:305:ALA:HB2	1.81	0.63
1:C:39:TRP:HB2	1:C:248:VAL:CG2	2.28	0.63
1:C:22:VAL:HG21	1:C:238:LEU:HB3	1.81	0.62
1:C:223:LEU:HD12	1:C:248:VAL:HG12	1.80	0.62
1:C:463:GLU:CB	1:C:465:LEU:N	2.63	0.62
1:C:67:TYR:CD1	1:C:159:VAL:HG11	2.35	0.61
1:C:72:THR:HG21	1:C:168:PRO:HD3	1.82	0.61
1:B:9:GLN:OE1	1:D:174:ARG:CD	2.49	0.61
1:C:460:GLU:OE1	1:C:515:ARG:CZ	2.48	0.61
1:C:470:VAL:HG12	1:C:471:GLY:N	2.15	0.61
1:A:470:VAL:HG13	1:A:471:GLY:H	1.65	0.61
1:D:88:SER:HB3	1:D:91:ASP:HB2	1.83	0.61
1:A:210:ARG:CZ	1:A:367:MET:HE2	2.31	0.61
1:D:490:TYR:HA	1:D:521:VAL:CG2	2.31	0.61
1:A:93:ALA:O	1:A:97:MET:HE3	2.00	0.61
1:A:155:LEU:HD13	1:A:158:GLU:OE2	2.00	0.61
1:A:19:ALA:HB3	1:A:181:ILE:HD13	1.83	0.60
1:A:155:LEU:CD1	1:A:158:GLU:OE2	2.49	0.60
1:B:393:ARG:HD2	1:B:415:GLY:O	2.01	0.60
1:D:443:THR:O	1:D:444:GLU:C	2.45	0.60
1:A:285:LEU:HD22	1:A:290:LEU:HD11	1.84	0.60
1:D:77:ARG:O	1:D:80:ASP:HB2	2.00	0.60
1:A:137:HIS:NE2	1:A:141:LEU:HD11	2.16	0.60
1:C:463:GLU:HB3	1:C:465:LEU:N	2.17	0.60
1:D:382:LEU:HD13	1:D:386:GLN:HG2	1.83	0.60
1:A:405:ASN:ND2	1:B:403:ASN:H	2.00	0.60
1:C:40:LEU:HD11	1:C:55:LEU:HD12	1.83	0.60
1:A:280:MET:HE3	1:A:311:LEU:CD1	2.31	0.60
1:B:220:ARG:HD2	1:B:268:THR:HG21	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:375:VAL:HG22	1:D:379:GLY:HA2	1.84	0.60
1:B:489:VAL:C	1:B:490:TYR:HD1	2.09	0.59
1:B:113:MET:HB3	1:B:118:ARG:HG3	1.84	0.59
1:B:441:ILE:HD12	1:B:489:VAL:CG2	2.33	0.59
1:C:300:GLY:O	1:C:301:ASP:HB2	2.02	0.59
1:A:121:TYR:CZ	1:A:185:HIS:HB3	2.37	0.59
1:B:285:LEU:C	1:B:314:LYS:HE3	2.28	0.59
1:A:223:LEU:HD11	1:A:250:TYR:CD1	2.38	0.59
1:D:442:ARG:NH1	1:D:447:PHE:CZ	2.71	0.58
1:A:220:ARG:HD2	1:A:268:THR:HG21	1.84	0.58
1:B:339:GLY:HA2	1:B:343:MET:HG3	1.85	0.58
1:C:293:VAL:HG11	1:C:296:TYR:CZ	2.39	0.58
1:D:167:ARG:HD2	1:D:171:TYR:CG	2.38	0.58
1:A:480:GLY:H	1:A:483:ASP:HB2	1.69	0.58
1:C:375:VAL:HG23	1:C:389:ARG:HB2	1.85	0.58
1:B:110:ASN:H	1:B:185:HIS:CE1	2.22	0.58
1:D:375:VAL:CG2	1:D:379:GLY:HA2	2.34	0.58
1:A:337:MET:HB3	1:A:346:VAL:HG11	1.86	0.57
1:C:365:ARG:HH21	1:C:428:ALA:CB	2.14	0.57
1:B:323:ASP:OD2	1:B:325:LYS:HB2	2.04	0.57
1:D:277:PHE:HD1	1:D:280:MET:HE2	1.70	0.57
1:A:220:ARG:NH2	1:A:269:ILE:HG21	2.19	0.57
1:A:480:GLY:N	1:A:483:ASP:HB2	2.19	0.57
1:A:494:ASN:C	1:A:495:LEU:HD23	2.28	0.57
1:B:42:GLY:O	1:B:51:ARG:HD3	2.05	0.57
1:D:333:ILE:HG22	1:D:335:ILE:HG13	1.87	0.57
1:D:490:TYR:HA	1:D:521:VAL:HG23	1.87	0.57
1:A:39:TRP:HB2	1:A:248:VAL:HG22	1.86	0.57
1:C:273:PHE:O	1:C:276:THR:HG22	2.04	0.57
1:C:137:HIS:ND1	1:C:155:LEU:HG	2.20	0.57
1:A:359:ILE:HG22	1:A:359:ILE:O	2.05	0.56
1:A:202:THR:HG21	1:A:399:PRO:HD3	1.87	0.56
1:A:329:VAL:CG1	1:A:330:PRO:HD2	2.35	0.56
1:B:308:ILE:HD12	1:B:312:LEU:HD13	1.87	0.56
1:A:170:ALA:HA	4:A:747:HOH:O	2.04	0.56
1:B:223:LEU:HD11	1:B:250:TYR:CD1	2.40	0.56
1:D:280:MET:CE	1:D:311:LEU:HD22	2.32	0.56
1:A:184:SER:OG	1:A:341:THR:HG22	2.05	0.56
1:A:280:MET:O	1:A:285:LEU:HD11	2.05	0.56
1:A:302:ALA:O	1:A:303:ALA:C	2.48	0.56
1:B:110:ASN:HB2	1:B:229:HIS:CD2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:LEU:HD22	1:B:231:VAL:HG23	1.86	0.56
1:B:489:VAL:C	1:B:490:TYR:CD1	2.84	0.56
1:B:9:GLN:OE1	1:D:174:ARG:NE	2.38	0.56
1:A:305:ALA:HB1	1:A:308:ILE:CG2	2.36	0.56
1:A:213:ASP:HB2	1:A:215:LEU:HD12	1.88	0.55
1:B:185:HIS:O	1:B:341:THR:HG21	2.06	0.55
1:B:340:SER:OG	1:B:343:MET:HG2	2.07	0.55
1:D:182:LEU:C	1:D:182:LEU:HD23	2.31	0.55
1:D:118:ARG:NH1	1:D:140:LEU:HD21	2.21	0.55
1:B:513:LEU:HD23	1:B:519:PRO:O	2.07	0.55
1:C:84:ILE:HG22	1:C:92:PHE:CE1	2.42	0.55
1:A:274:THR:HB	1:A:303:ALA:HB3	1.89	0.55
1:A:374:VAL:HG12	1:A:382:LEU:HD12	1.89	0.55
1:B:93:ALA:O	1:B:97:MET:HG3	2.07	0.55
1:C:137:HIS:C	1:C:137:HIS:CD2	2.85	0.55
1:C:262:ILE:HD11	1:C:270:VAL:HG21	1.88	0.55
1:D:26:LEU:HD21	1:D:242:THR:HA	1.88	0.55
1:A:293:VAL:HG11	1:A:296:TYR:CZ	2.42	0.55
1:A:339:GLY:HA3	4:A:751:HOH:O	2.06	0.55
1:B:76:VAL:O	1:B:77:ARG:NH1	2.40	0.55
1:B:26:LEU:HD22	1:B:31:ARG:NH1	2.21	0.55
1:A:44:TRP:CH2	1:A:63:VAL:HG11	2.41	0.54
1:B:182:LEU:HD21	1:B:231:VAL:HG23	1.89	0.54
1:D:96:LEU:O	1:D:100:THR:HG23	2.07	0.54
1:D:448:VAL:HG11	1:D:489:VAL:HG21	1.90	0.54
1:A:34:ASP:O	1:A:56:THR:CG2	2.56	0.54
1:C:300:GLY:O	1:C:301:ASP:CB	2.55	0.54
1:A:33:LEU:HD22	1:A:58:GLY:HA2	1.89	0.54
1:A:422:LEU:HD21	1:A:481:TRP:CE2	2.43	0.54
1:B:227:PRO:HG2	1:B:230:HIS:CE1	2.42	0.54
1:A:195:SER:O	1:A:401:PHE:HA	2.08	0.54
1:B:441:ILE:HD12	1:B:489:VAL:HG22	1.90	0.54
1:D:342:GLU:HG3	1:D:417:PHE:CZ	2.42	0.54
1:A:329:VAL:HG13	1:A:330:PRO:HD2	1.88	0.54
1:B:312:LEU:O	1:B:331:GLY:HA2	2.07	0.54
1:C:489:VAL:HG13	1:C:521:VAL:HG23	1.89	0.54
1:B:468:THR:HG22	1:B:470:VAL:HG13	1.90	0.54
1:C:41:ASP:OD1	1:C:43:THR:HG22	2.07	0.54
1:D:113:MET:HE3	1:D:117:THR:HG22	1.89	0.53
1:D:263:GLU:OE1	1:D:288:ARG:NH1	2.38	0.53
1:D:506:THR:O	1:D:510:ASN:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:289:ASP:C	1:D:290:LEU:HD23	2.33	0.53
1:C:123:ARG:HB3	4:C:715:HOH:O	2.07	0.53
1:D:72:THR:HG21	1:D:168:PRO:HG3	1.90	0.53
1:C:26:LEU:HD21	1:C:242:THR:HA	1.91	0.53
1:C:230:HIS:CD2	1:C:231:VAL:HG22	2.43	0.53
1:D:387:VAL:O	1:D:387:VAL:HG12	2.09	0.53
1:C:375:VAL:CG2	1:C:389:ARG:HB2	2.38	0.53
1:D:33:LEU:HD23	1:D:57:LEU:HG	1.90	0.53
1:D:290:LEU:HD13	1:D:311:LEU:HD21	1.90	0.53
1:A:375:VAL:HG13	1:A:379:GLY:HA2	1.89	0.53
1:C:405:ASN:O	1:C:409:HIS:HD2	1.92	0.53
1:C:43:THR:HG21	1:C:251:THR:HG21	1.90	0.53
1:C:338:PHE:HB2	1:C:363:ILE:HG23	1.89	0.53
1:C:263:GLU:CD	4:C:705:HOH:O	2.52	0.53
1:A:349:ASP:HB2	1:A:367:MET:HE3	1.91	0.52
1:A:230:HIS:CE1	1:A:273:PHE:CZ	2.97	0.52
1:C:460:GLU:OE2	1:C:515:ARG:NH1	2.43	0.52
1:A:297:TYR:CD1	1:A:335:ILE:HD13	2.44	0.52
1:D:366:PRO:CG	1:D:372:ALA:HB3	2.39	0.52
1:C:470:VAL:HG12	1:C:471:GLY:H	1.74	0.52
1:A:79:LYS:CE	4:A:741:HOH:O	2.51	0.52
1:A:363:ILE:HD11	1:A:431:PHE:HB3	1.90	0.52
1:C:185:HIS:O	1:C:341:THR:HG21	2.10	0.52
1:C:266:ARG:HG2	1:C:266:ARG:HH11	1.75	0.52
1:D:185:HIS:HD2	1:D:186:SER:O	1.93	0.52
1:D:189:THR:HB	2:D:601:ATP:O1G	2.10	0.52
1:A:39:TRP:CD1	1:A:54:VAL:HG22	2.44	0.52
1:D:230:HIS:ND1	1:D:231:VAL:N	2.58	0.52
1:A:34:ASP:O	1:A:56:THR:HG21	2.09	0.52
1:B:392:VAL:O	1:B:393:ARG:HG3	2.10	0.52
1:B:454:GLU:HG3	1:B:469:VAL:HG23	1.92	0.52
1:A:120:GLU:OE1	1:A:120:GLU:HA	2.11	0.51
1:C:39:TRP:HB3	1:C:248:VAL:HG22	1.89	0.51
1:A:339:GLY:CA	4:A:751:HOH:O	2.58	0.51
1:B:39:TRP:CG	1:B:54:VAL:HG23	2.45	0.51
1:A:86:SER:OG	1:A:87:THR:N	2.43	0.51
1:A:263:GLU:OE2	1:A:288:ARG:HA	2.10	0.51
1:C:365:ARG:NH2	1:C:428:ALA:HB1	2.19	0.51
1:D:363:ILE:HD11	1:D:431:PHE:CB	2.41	0.51
1:D:137:HIS:CE1	1:D:141:LEU:HD11	2.46	0.51
1:D:468:THR:HB	1:D:492:LEU:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:TYR:CE2	1:C:335:ILE:HD12	2.46	0.51
1:D:277:PHE:CE2	1:D:298:ALA:HB2	2.46	0.51
1:D:293:VAL:HG11	1:D:296:TYR:CE1	2.46	0.51
1:B:181:ILE:HD11	1:B:203:LEU:HD23	1.93	0.50
1:C:137:HIS:NE2	1:C:141:LEU:HD11	2.25	0.50
1:B:434:LEU:HD13	1:C:324:LEU:HD13	1.93	0.50
1:A:39:TRP:CD1	1:A:54:VAL:CG2	2.95	0.50
1:A:280:MET:HB2	1:A:311:LEU:HD11	1.91	0.50
1:B:175:HIS:HE1	4:B:712:HOH:O	1.94	0.50
1:C:220:ARG:O	1:C:245:ALA:HB1	2.11	0.50
1:D:137:HIS:HE1	1:D:141:LEU:HD21	1.76	0.50
1:D:296:TYR:OH	1:D:311:LEU:HD23	2.11	0.50
1:B:113:MET:SD	1:B:118:ARG:HA	2.52	0.50
1:D:17:LEU:HD22	1:D:29:TYR:OH	2.12	0.50
1:A:393:ARG:HD2	1:A:415:GLY:O	2.12	0.50
1:C:155:LEU:O	1:C:158:GLU:HG3	2.11	0.50
1:C:262:ILE:CD1	1:C:270:VAL:HG21	2.41	0.50
1:A:34:ASP:HB2	4:A:744:HOH:O	2.11	0.50
1:A:434:LEU:O	1:A:451:ALA:HB3	2.11	0.50
1:B:268:THR:HG22	1:B:294:GLU:HG2	1.93	0.50
1:D:454:GLU:O	1:D:458:LEU:HD12	2.11	0.50
1:A:137:HIS:CD2	1:A:141:LEU:HD11	2.47	0.50
1:D:222:ARG:HB3	1:D:269:ILE:HD11	1.94	0.50
1:B:192:ILE:N	1:B:192:ILE:HD12	2.26	0.50
1:B:224:LEU:N	1:B:224:LEU:HD23	2.27	0.50
1:D:113:MET:HE1	1:D:121:TYR:CB	2.42	0.50
1:D:441:ILE:HD13	1:D:489:VAL:HG22	1.94	0.50
1:C:413:LEU:HB3	1:C:418:LEU:HD11	1.93	0.50
1:A:340:SER:OG	1:A:343:MET:HE3	2.11	0.49
1:D:40:LEU:HD11	1:D:55:LEU:HD12	1.94	0.49
1:A:441:ILE:HG23	1:A:479:PHE:CD2	2.47	0.49
1:D:182:LEU:HD23	1:D:183:ILE:N	2.28	0.49
1:A:137:HIS:CD2	1:A:137:HIS:C	2.91	0.49
1:D:132:THR:OG1	1:D:133:ARG:N	2.44	0.49
1:D:202:THR:HG22	1:D:395:LYS:O	2.12	0.49
1:B:33:LEU:HB3	1:B:58:GLY:HA3	1.95	0.49
1:B:491:ALA:O	1:B:492:LEU:HD23	2.12	0.49
1:D:363:ILE:HD11	1:D:431:PHE:HB3	1.94	0.49
1:D:375:VAL:CG1	1:D:389:ARG:HB2	2.42	0.49
1:D:23:ILE:HG21	1:D:97:MET:HE2	1.95	0.49
1:D:39:TRP:CD1	1:D:54:VAL:HG22	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:ARG:HH21	1:B:269:ILE:HG21	1.77	0.49
1:A:194:LYS:HD2	1:A:401:PHE:CE2	2.48	0.49
1:A:297:TYR:CE1	1:A:335:ILE:HD13	2.48	0.49
1:C:209:SER:OG	1:C:369:PHE:HB3	2.13	0.49
1:A:400:GLY:HA2	1:A:408:TRP:CD2	2.47	0.49
1:B:105:ILE:HG12	1:B:180:PRO:HB2	1.95	0.49
1:C:96:LEU:O	1:C:100:THR:HG23	2.13	0.49
1:C:129:GLY:HA3	1:C:152:PHE:CE1	2.47	0.49
1:D:258:VAL:O	1:D:262:ILE:HG13	2.12	0.49
1:C:433:HIS:CD2	1:C:435:ASP:N	2.81	0.48
1:C:40:LEU:HD11	1:C:55:LEU:CD1	2.43	0.48
1:C:128:VAL:O	1:C:151:LEU:HB2	2.13	0.48
1:C:453:THR:O	1:C:454:GLU:C	2.55	0.48
1:C:489:VAL:C	1:C:521:VAL:HG23	2.38	0.48
1:D:132:THR:HG21	1:D:140:LEU:HD12	1.95	0.48
1:A:132:THR:HG21	1:A:140:LEU:CD1	2.43	0.48
1:C:293:VAL:HG11	1:C:296:TYR:CE1	2.49	0.48
1:D:453:THR:HG22	1:D:469:VAL:HG21	1.96	0.48
1:C:510:ASN:HD21	1:C:521:VAL:HG13	1.78	0.48
1:C:405:ASN:O	1:C:409:HIS:CD2	2.66	0.48
1:D:23:ILE:CG2	1:D:97:MET:HE2	2.43	0.48
1:B:147:ASP:O	1:B:149:PRO:HD3	2.14	0.48
1:B:296:TYR:HB2	1:B:334:PHE:HD1	1.78	0.48
1:C:283:GLU:O	1:C:284:ASP:C	2.55	0.48
1:A:329:VAL:CG1	1:A:330:PRO:CD	2.92	0.48
1:B:230:HIS:CE1	1:B:273:PHE:CZ	3.02	0.48
1:C:93:ALA:O	1:C:97:MET:HG3	2.14	0.48
1:C:343:MET:HE3	1:C:347:LEU:HG	1.94	0.48
1:C:70:PHE:CG	1:C:159:VAL:HG22	2.49	0.48
1:C:84:ILE:CD1	1:C:95:ASN:HB3	2.44	0.48
1:D:398:THR:HG23	1:D:408:TRP:CH2	2.49	0.48
1:B:220:ARG:NH2	1:B:269:ILE:HG21	2.29	0.47
1:B:285:LEU:HD23	1:B:314:LYS:HD2	1.96	0.47
1:B:312:LEU:HG	1:B:332:ALA:O	2.14	0.47
1:C:375:VAL:HG22	1:C:389:ARG:O	2.14	0.47
1:A:277:PHE:HD1	1:A:280:MET:HE2	1.79	0.47
1:A:91:ASP:O	1:A:95:ASN:ND2	2.47	0.47
1:D:254:SER:O	1:D:258:VAL:HG23	2.14	0.47
1:D:293:VAL:HG11	1:D:296:TYR:CZ	2.49	0.47
1:B:223:LEU:HB3	1:B:270:VAL:HG22	1.96	0.47
1:A:23:ILE:HG13	1:A:61:HIS:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:PRO:O	1:C:161:PRO:HD3	2.14	0.47
1:C:62:GLU:O	1:C:66:GLU:HG2	2.14	0.47
1:A:223:LEU:HB3	1:A:270:VAL:HG22	1.97	0.47
1:A:359:ILE:N	4:A:704:HOH:O	2.46	0.47
1:B:41:ASP:OD2	1:B:251:THR:OG1	2.26	0.47
1:A:108:LEU:N	1:A:108:LEU:HD23	2.30	0.47
1:B:101:GLY:O	1:B:173:PHE:HB2	2.15	0.47
1:D:120:GLU:OE1	1:D:120:GLU:CA	2.63	0.47
1:D:387:VAL:HG22	1:D:434:LEU:CD1	2.43	0.47
1:D:442:ARG:NH1	1:D:447:PHE:CE1	2.83	0.47
1:A:185:HIS:HA	1:A:194:LYS:O	2.15	0.47
1:C:66:GLU:OE1	1:C:164:ARG:HB3	2.15	0.47
1:A:456:VAL:HG11	1:A:518:LEU:HD13	1.97	0.47
1:C:72:THR:OG1	1:C:168:PRO:HD3	2.15	0.47
1:C:406:VAL:HG21	1:D:126:ARG:CZ	2.45	0.47
1:A:329:VAL:HG13	1:A:330:PRO:CD	2.44	0.46
1:C:490:TYR:HA	1:C:521:VAL:CG2	2.46	0.46
1:C:513:LEU:HD12	1:C:520:ARG:HA	1.97	0.46
1:D:182:LEU:HD23	1:D:183:ILE:CA	2.45	0.46
1:A:210:ARG:NH1	1:A:367:MET:HG2	2.31	0.46
1:B:26:LEU:HD21	1:B:242:THR:HA	1.97	0.46
1:C:441:ILE:HB	1:C:448:VAL:CG2	2.46	0.46
1:D:176:ALA:O	1:D:177:PRO:C	2.57	0.46
1:B:164:ARG:O	1:B:167:ARG:NH1	2.44	0.46
1:C:516:ALA:CB	1:C:518:LEU:CD1	2.94	0.46
1:A:184:SER:HB3	1:A:231:VAL:CG1	2.46	0.46
1:A:323:ASP:OD2	1:A:325:LYS:HB2	2.15	0.46
1:A:461:TYR:CE1	1:A:512:ALA:HB2	2.50	0.46
1:B:134:GLU:N	1:B:135:PRO:CD	2.78	0.46
1:C:110:ASN:HB2	1:C:229:HIS:ND1	2.29	0.46
1:D:290:LEU:HD23	1:D:290:LEU:N	2.30	0.46
1:A:72:THR:HG21	1:A:168:PRO:HG3	1.96	0.46
1:B:223:LEU:HD12	1:B:248:VAL:CG1	2.45	0.46
1:B:461:TYR:CZ	1:B:512:ALA:HB2	2.51	0.46
1:D:23:ILE:HA	1:D:26:LEU:HD12	1.98	0.46
1:B:84:ILE:HG22	1:B:92:PHE:CD1	2.51	0.46
1:D:435:ASP:HB2	1:D:449:TYR:HB3	1.98	0.46
1:B:160:GLU:H	1:B:163:ASN:ND2	2.14	0.46
1:B:185:HIS:O	1:B:341:THR:CG2	2.64	0.46
1:C:433:HIS:HD2	1:C:435:ASP:H	1.64	0.46
1:A:26:LEU:HD21	1:A:242:THR:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:GLY:O	1:A:189:THR:HB	2.16	0.46
1:A:465:LEU:HG	1:A:495:LEU:HA	1.98	0.46
1:B:137:HIS:HB2	1:B:155:LEU:HD21	1.97	0.46
1:C:229:HIS:CD2	1:C:229:HIS:C	2.94	0.46
1:C:479:PHE:CD1	1:C:479:PHE:C	2.94	0.46
1:D:133:ARG:C	1:D:155:LEU:HD23	2.41	0.46
1:A:40:LEU:HD11	1:A:55:LEU:CD1	2.46	0.45
1:C:88:SER:HB3	1:C:91:ASP:HB2	1.97	0.45
1:C:286:THR:HG22	1:C:287:ASP:OD1	2.16	0.45
1:C:108:LEU:N	1:C:108:LEU:HD23	2.31	0.45
1:D:86:SER:OG	1:D:87:THR:N	2.49	0.45
1:A:17:LEU:HD22	1:A:29:TYR:OH	2.17	0.45
1:A:176:ALA:O	1:A:177:PRO:C	2.57	0.45
1:B:280:MET:HE3	1:B:311:LEU:HD21	1.97	0.45
1:C:131:MET:HE1	1:C:159:VAL:CG2	2.47	0.45
1:D:286:THR:HG23	1:D:287:ASP:N	2.32	0.45
1:B:133:ARG:HH11	1:B:133:ARG:HB3	1.80	0.45
1:C:510:ASN:HD21	1:C:521:VAL:CG1	2.29	0.45
1:D:502:PRO:HB2	1:D:505:PRO:N	2.31	0.45
1:A:185:HIS:O	1:A:341:THR:CG2	2.64	0.45
1:A:456:VAL:HG21	1:A:518:LEU:HD11	1.98	0.45
1:B:121:TYR:CZ	1:B:185:HIS:HB3	2.52	0.45
1:B:335:ILE:N	1:B:335:ILE:HD12	2.31	0.45
1:C:290:LEU:N	1:C:290:LEU:HD23	2.31	0.45
1:A:2:MET:SD	1:D:383:PRO:HA	2.57	0.45
1:B:335:ILE:HG22	1:B:337:MET:HG3	1.98	0.45
1:C:67:TYR:CD1	1:C:67:TYR:N	2.85	0.45
1:D:146:ASP:O	1:D:147:ASP:C	2.59	0.45
1:D:296:TYR:CZ	1:D:311:LEU:HD23	2.51	0.45
1:D:349:ASP:HB2	1:D:367:MET:HE2	1.99	0.45
1:A:89:ILE:HA	1:A:228:GLY:HA3	1.97	0.45
1:A:194:LYS:HD2	1:A:401:PHE:CZ	2.51	0.45
1:D:160:GLU:O	1:D:163:ASN:OD1	2.34	0.45
1:D:510:ASN:ND2	1:D:520:ARG:HB3	2.32	0.45
1:B:195:SER:O	1:B:401:PHE:HA	2.16	0.45
1:D:39:TRP:CZ3	1:D:246:PRO:HB3	2.52	0.45
1:B:223:LEU:HD11	1:B:250:TYR:CE1	2.52	0.45
1:B:312:LEU:HD21	1:B:334:PHE:HB2	1.98	0.45
1:C:171:TYR:CD1	1:C:171:TYR:C	2.95	0.45
1:D:250:TYR:CE2	1:D:261:GLY:HA3	2.52	0.45
1:D:366:PRO:HG2	1:D:372:ALA:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:LEU:HD12	1:A:106:ALA:HB2	1.99	0.44
1:A:269:ILE:HD11	1:A:271:PHE:HE1	1.83	0.44
1:C:67:TYR:N	1:C:67:TYR:HD1	2.15	0.44
1:C:469:VAL:CG1	1:C:489:VAL:CG2	2.95	0.44
1:D:230:HIS:CE1	1:D:231:VAL:HG22	2.52	0.44
1:D:375:VAL:HG11	1:D:418:LEU:CD2	2.47	0.44
1:A:92:PHE:CD2	1:A:228:GLY:C	2.96	0.44
1:B:389:ARG:HH11	1:B:418:LEU:HD13	1.83	0.44
1:A:220:ARG:HB3	1:A:268:THR:HB	1.99	0.44
1:B:297:TYR:CE1	1:B:335:ILE:HD13	2.52	0.44
1:B:454:GLU:OE2	1:B:468:THR:HA	2.18	0.44
1:C:60:LEU:O	1:C:64:VAL:HG23	2.17	0.44
1:C:382:LEU:HB3	1:C:383:PRO:HD2	2.00	0.44
1:A:120:GLU:HG2	4:A:770:HOH:O	2.17	0.44
1:A:210:ARG:HD3	1:A:216:ASP:OD2	2.18	0.44
1:A:273:PHE:O	1:A:274:THR:C	2.60	0.44
1:C:39:TRP:CD1	1:C:54:VAL:HG22	2.53	0.44
1:A:400:GLY:HA2	1:A:408:TRP:CE2	2.52	0.44
1:A:421:ASP:OD1	1:A:436:ARG:HG2	2.18	0.44
1:A:141:LEU:HD23	1:A:153:VAL:HB	2.00	0.44
1:A:442:ARG:NH1	1:A:483:ASP:O	2.51	0.44
1:B:327:LYS:O	1:B:329:VAL:HG13	2.18	0.44
1:C:72:THR:HG21	1:C:168:PRO:CD	2.47	0.44
1:C:220:ARG:HB3	1:C:268:THR:HB	2.00	0.44
1:C:222:ARG:HB3	1:C:269:ILE:HD11	2.00	0.44
1:D:70:PHE:CE2	1:D:131:MET:HE1	2.53	0.44
1:D:375:VAL:HG12	1:D:389:ARG:HB2	1.99	0.44
1:D:510:ASN:CG	1:D:520:ARG:HB3	2.42	0.44
1:B:44:TRP:CH2	1:B:46:ALA:HA	2.53	0.44
1:B:340:SER:H	1:B:343:MET:HG3	1.83	0.44
1:C:405:ASN:ND2	1:D:197:PHE:CE1	2.85	0.44
1:D:380:SER:O	1:D:381:VAL:C	2.59	0.44
1:D:510:ASN:OD1	1:D:521:VAL:CG1	2.63	0.44
1:A:221:LYS:HG3	1:A:246:PRO:HB2	2.00	0.44
1:A:477:VAL:HG22	1:A:479:PHE:HD1	1.83	0.44
1:B:26:LEU:HB2	1:B:27:PRO:HD3	2.00	0.44
1:A:134:GLU:OE1	1:A:134:GLU:N	2.26	0.43
1:A:135:PRO:HB2	1:A:136:TRP:CE2	2.53	0.43
1:B:374:VAL:CG1	1:B:382:LEU:HD12	2.48	0.43
1:D:113:MET:O	1:D:114:PRO:C	2.61	0.43
1:A:465:LEU:HD12	1:A:495:LEU:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:518:LEU:N	1:C:518:LEU:HD12	2.33	0.43
1:D:366:PRO:HG3	1:D:372:ALA:HB3	1.99	0.43
1:A:258:VAL:HG12	1:A:262:ILE:CD1	2.49	0.43
1:B:39:TRP:CD1	1:B:54:VAL:HG23	2.54	0.43
1:B:426:ASP:C	1:B:426:ASP:OD1	2.61	0.43
1:C:33:LEU:HD23	1:C:57:LEU:HD23	2.00	0.43
1:D:328:LYS:C	1:D:329:VAL:O	2.61	0.43
1:D:386:GLN:HE21	1:D:386:GLN:HB2	1.62	0.43
1:D:404:ASP:OD1	1:D:404:ASP:O	2.36	0.43
1:D:433:HIS:CD2	1:D:433:HIS:C	2.95	0.43
1:A:88:SER:O	1:A:89:ILE:C	2.59	0.43
1:A:202:THR:HG21	1:A:399:PRO:CD	2.48	0.43
1:A:266:ARG:N	1:A:267:PRO:CD	2.81	0.43
1:A:273:PHE:HB2	1:A:275:HIS:CE1	2.53	0.43
1:B:185:HIS:C	1:B:185:HIS:CD2	2.96	0.43
1:B:222:ARG:HB3	1:B:269:ILE:HD11	1.99	0.43
1:C:176:ALA:O	1:C:177:PRO:C	2.61	0.43
1:C:433:HIS:CD2	1:C:433:HIS:C	2.95	0.43
1:D:143:HIS:O	1:D:150:PRO:HD2	2.19	0.43
1:D:433:HIS:HD2	1:D:435:ASP:N	2.17	0.43
1:A:155:LEU:HD12	1:A:158:GLU:OE2	2.18	0.43
1:A:255:GLY:HA2	1:A:280:MET:HG2	2.01	0.43
1:A:285:LEU:HD22	1:A:290:LEU:CD1	2.47	0.43
1:A:426:ASP:OD1	1:A:428:ALA:HB3	2.18	0.43
1:A:479:PHE:CD1	1:A:487:ALA:HB2	2.54	0.43
1:B:340:SER:N	1:B:343:MET:HG3	2.33	0.43
1:D:60:LEU:HD21	1:D:97:MET:HE1	2.00	0.43
1:D:89:ILE:HG13	1:D:233:ALA:HB1	2.00	0.43
1:D:382:LEU:HB3	1:D:383:PRO:HD2	2.01	0.43
1:A:92:PHE:CE2	1:A:229:HIS:HB3	2.54	0.43
1:B:285:LEU:O	1:B:314:LYS:HE3	2.18	0.43
1:C:23:ILE:HA	1:C:26:LEU:HD12	2.00	0.43
1:C:80:ASP:O	1:C:104:ALA:HB1	2.19	0.43
1:C:274:THR:HG23	1:C:299:SER:O	2.19	0.43
1:C:504:ASP:HB3	1:C:507:ALA:HB3	2.00	0.43
1:A:26:LEU:N	1:A:27:PRO:CD	2.81	0.43
1:C:182:LEU:HD23	1:C:183:ILE:N	2.33	0.43
1:D:53:GLU:O	1:D:54:VAL:HG23	2.19	0.43
1:D:263:GLU:OE2	1:D:288:ARG:HA	2.19	0.43
1:D:490:TYR:HA	1:D:521:VAL:HG21	2.01	0.43
1:C:215:LEU:O	1:C:216:ASP:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:MET:HE1	1:D:121:TYR:HB2	2.01	0.43
1:A:184:SER:CB	1:A:231:VAL:HG13	2.49	0.42
1:A:211:LEU:HD23	1:A:211:LEU:C	2.44	0.42
1:B:259:LEU:HB3	1:B:288:ARG:CZ	2.48	0.42
1:C:134:GLU:N	1:C:135:PRO:CD	2.82	0.42
1:A:107:SER:OG	1:A:125:GLN:OE1	2.37	0.42
1:C:82:VAL:HG21	1:C:99:LEU:HD21	2.01	0.42
1:A:268:THR:HG23	1:A:294:GLU:HG3	2.00	0.42
1:B:33:LEU:O	1:B:56:THR:HB	2.19	0.42
1:C:5:GLU:OE2	1:C:9:GLN:NE2	2.51	0.42
1:C:18:GLY:HA3	1:C:200:HIS:CE1	2.53	0.42
1:D:424:TYR:HD2	1:D:434:LEU:HD11	1.84	0.42
1:D:491:ALA:O	1:D:492:LEU:HD23	2.19	0.42
1:B:388:GLY:O	1:B:422:LEU:HA	2.20	0.42
1:C:72:THR:CG2	1:C:168:PRO:HD3	2.48	0.42
1:C:98:ALA:O	1:C:102:ILE:HG23	2.19	0.42
1:C:340:SER:OG	1:C:343:MET:HG3	2.19	0.42
1:D:452:TYR:CE2	1:D:518:LEU:HD21	2.55	0.42
1:A:33:LEU:HA	1:A:57:LEU:HB3	2.01	0.42
1:B:186:SER:O	1:B:193:PRO:HB3	2.19	0.42
1:B:378:ASP:OD1	1:B:378:ASP:C	2.62	0.42
1:C:66:GLU:OE2	1:C:161:PRO:HA	2.18	0.42
1:D:250:TYR:OH	1:D:261:GLY:HA2	2.20	0.42
1:B:132:THR:HG21	1:B:140:LEU:HD12	2.02	0.42
1:D:40:LEU:HD11	1:D:55:LEU:CD1	2.49	0.42
1:A:21:ASN:O	1:A:22:VAL:C	2.61	0.42
1:A:26:LEU:HA	1:A:29:TYR:CD2	2.54	0.42
1:A:36:GLU:HB3	1:A:39:TRP:CH2	2.55	0.42
1:A:187:SER:O	1:A:188:GLY:C	2.63	0.42
1:A:305:ALA:HB1	1:A:308:ILE:HG23	2.01	0.42
1:B:77:ARG:O	1:B:80:ASP:HB2	2.20	0.42
1:C:119:ARG:HB3	1:C:123:ARG:NH1	2.34	0.42
1:A:143:HIS:O	1:A:150:PRO:HD2	2.20	0.42
1:A:210:ARG:NH1	1:A:367:MET:HE2	2.35	0.42
1:C:84:ILE:HG22	1:C:92:PHE:CD1	2.55	0.42
1:C:112:ASN:O	1:C:113:MET:C	2.62	0.42
1:C:316:TYR:HA	1:C:331:GLY:N	2.35	0.42
1:C:374:VAL:HG12	1:C:382:LEU:HD12	2.02	0.42
1:D:82:VAL:HG13	1:D:129:GLY:O	2.20	0.42
1:D:406:VAL:HG12	1:D:407:ARG:N	2.34	0.42
1:A:62:GLU:O	1:A:65:ALA:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:PHE:CE1	1:A:299:SER:HB2	2.54	0.42
1:A:453:THR:O	1:A:454:GLU:C	2.61	0.42
1:B:62:GLU:O	1:B:66:GLU:HG2	2.20	0.42
1:B:425:ARG:O	1:B:425:ARG:HG3	2.19	0.42
1:C:275:HIS:CG	1:C:276:THR:N	2.87	0.42
1:D:220:ARG:O	1:D:245:ALA:HB1	2.19	0.42
1:A:19:ALA:CB	1:A:181:ILE:CD1	2.98	0.42
1:A:296:TYR:O	1:A:335:ILE:HD12	2.20	0.42
1:B:421:ASP:HA	1:B:436:ARG:HA	2.02	0.42
1:C:206:GLY:O	1:C:207:ALA:C	2.63	0.42
1:C:278:THR:O	1:C:279:GLU:C	2.62	0.42
1:C:433:HIS:HD2	1:C:435:ASP:N	2.18	0.42
1:D:41:ASP:OD1	1:D:42:GLY:N	2.52	0.42
1:D:329:VAL:HG12	1:D:330:PRO:CD	2.50	0.42
1:D:448:VAL:O	1:D:448:VAL:HG12	2.20	0.42
1:A:33:LEU:HD23	1:A:57:LEU:CD2	2.48	0.41
1:B:96:LEU:HD12	1:B:96:LEU:O	2.20	0.41
1:B:343:MET:HA	1:B:397:LEU:HD23	2.01	0.41
1:C:18:GLY:CA	1:C:200:HIS:CE1	3.03	0.41
1:C:48:ASP:HA	1:C:161:PRO:CG	2.50	0.41
1:D:110:ASN:H	1:D:185:HIS:HE1	1.68	0.41
1:D:433:HIS:HD2	1:D:434:LEU:N	2.18	0.41
1:B:125:GLN:O	1:B:126:ARG:C	2.63	0.41
1:B:210:ARG:NH1	1:B:367:MET:SD	2.93	0.41
1:D:188:GLY:O	1:D:189:THR:C	2.62	0.41
1:A:283:GLU:O	1:A:284:ASP:C	2.63	0.41
1:B:400:GLY:HA2	1:B:408:TRP:CE2	2.54	0.41
1:C:259:LEU:HB3	1:C:288:ARG:CZ	2.50	0.41
1:A:39:TRP:C	1:A:40:LEU:HD23	2.45	0.41
1:D:5:GLU:O	1:D:5:GLU:HG3	2.20	0.41
1:C:123:ARG:HG2	1:C:146:ASP:OD2	2.21	0.41
1:C:191:GLY:O	1:C:192:ILE:C	2.63	0.41
1:C:199:THR:OG1	1:C:202:THR:HG23	2.19	0.41
1:C:470:VAL:CG1	1:C:471:GLY:N	2.81	0.41
1:D:312:LEU:HD11	1:D:334:PHE:HB2	2.02	0.41
1:A:359:ILE:CD1	1:D:320:THR:O	2.68	0.41
1:B:36:GLU:OE1	1:B:39:TRP:CZ2	2.73	0.41
1:B:374:VAL:HG12	1:B:382:LEU:HB2	2.03	0.41
1:C:433:HIS:CD2	1:C:434:LEU:N	2.89	0.41
1:A:19:ALA:HB3	1:A:181:ILE:CD1	2.48	0.41
1:A:184:SER:OG	1:A:341:THR:CG2	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:PHE:CD2	1:A:479:PHE:O	2.73	0.41
1:A:513:LEU:CD1	1:A:521:VAL:HG13	2.51	0.41
1:C:130:ILE:HD12	1:C:153:VAL:HG22	2.01	0.41
1:C:433:HIS:HD2	1:C:434:LEU:N	2.17	0.41
1:D:317:HIS:CD2	1:D:317:HIS:C	2.97	0.41
1:A:221:LYS:HE2	1:A:265:HIS:HB3	2.02	0.41
1:A:285:LEU:CD2	1:A:290:LEU:HD11	2.48	0.41
1:B:188:GLY:O	1:B:189:THR:CB	2.68	0.41
1:B:277:PHE:CD1	1:B:280:MET:HE2	2.46	0.41
1:B:280:MET:HE3	1:B:311:LEU:CD2	2.51	0.41
1:C:89:ILE:HG23	1:C:249:HIS:CG	2.54	0.41
1:C:479:PHE:CD2	1:C:487:ALA:HB2	2.56	0.41
1:D:441:ILE:HD13	1:D:489:VAL:CG2	2.51	0.41
1:A:224:LEU:CD2	1:A:271:PHE:CD1	3.04	0.41
1:A:466:ASP:H	1:A:494:ASN:HB2	1.86	0.41
1:A:470:VAL:CG1	1:A:471:GLY:N	2.80	0.41
1:B:2:MET:SD	1:C:383:PRO:HA	2.60	0.41
1:B:119:ARG:O	1:B:119:ARG:HG3	2.20	0.41
1:B:223:LEU:C	1:B:224:LEU:HD23	2.46	0.41
1:B:461:TYR:HB3	1:B:463:GLU:CD	2.46	0.41
1:C:113:MET:SD	1:C:118:ARG:HA	2.61	0.41
1:C:489:VAL:O	1:C:521:VAL:HG23	2.21	0.41
1:D:152:PHE:CD1	1:D:152:PHE:C	2.99	0.41
1:A:92:PHE:HB2	1:A:234:MET:HE3	2.02	0.41
1:A:495:LEU:HD23	1:A:495:LEU:N	2.35	0.41
1:B:203:LEU:HD11	1:B:235:SER:HB3	2.03	0.41
1:A:91:ASP:CG	1:A:156:GLN:HE22	2.28	0.40
1:A:335:ILE:HA	1:A:350:PHE:CZ	2.55	0.40
1:A:454:GLU:HG3	1:A:469:VAL:HG23	2.04	0.40
1:A:513:LEU:HD22	1:A:518:LEU:HD22	2.02	0.40
1:B:86:SER:OG	1:B:87:THR:N	2.53	0.40
1:B:107:SER:HA	1:B:183:ILE:HB	2.03	0.40
1:B:457:LEU:HD21	1:B:513:LEU:HD13	1.99	0.40
1:C:513:LEU:CD1	1:C:520:ARG:HA	2.52	0.40
1:D:99:LEU:HD22	1:D:104:ALA:HB3	2.03	0.40
1:D:112:ASN:O	1:D:113:MET:C	2.63	0.40
1:D:375:VAL:HG12	1:D:389:ARG:O	2.20	0.40
1:A:176:ALA:HB3	1:A:179:ASP:CG	2.46	0.40
1:A:312:LEU:HD11	1:A:334:PHE:HB2	2.03	0.40
1:C:377:GLU:OE2	1:C:389:ARG:NE	2.54	0.40
1:D:404:ASP:OD1	1:D:404:ASP:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:GLY:HA2	1:A:489:VAL:HA	2.02	0.40
1:B:194:LYS:HD2	1:B:401:PHE:CE2	2.56	0.40
1:B:280:MET:HB2	1:B:311:LEU:HD11	2.02	0.40
1:B:426:ASP:OD1	1:B:428:ALA:N	2.51	0.40
1:C:273:PHE:O	1:C:274:THR:C	2.63	0.40
1:D:101:GLY:O	1:D:173:PHE:HB2	2.21	0.40
1:A:239:LEU:O	1:A:239:LEU:HD12	2.22	0.40
1:C:123:ARG:HG3	1:C:143:HIS:CE1	2.56	0.40
1:D:134:GLU:N	1:D:135:PRO:CD	2.84	0.40
1:A:335:ILE:HD12	1:A:335:ILE:N	2.37	0.40
1:B:99:LEU:CD1	1:B:106:ALA:HB2	2.52	0.40
1:C:84:ILE:HD11	1:C:95:ASN:HB3	2.03	0.40
1:D:82:VAL:HG21	1:D:99:LEU:HD21	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	465/564 (82%)	443 (95%)	22 (5%)	0	100	100
1	B	461/564 (82%)	447 (97%)	14 (3%)	0	100	100
1	C	460/564 (82%)	442 (96%)	18 (4%)	0	100	100
1	D	461/564 (82%)	436 (95%)	25 (5%)	0	100	100
All	All	1847/2256 (82%)	1768 (96%)	79 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	387/447 (87%)	370 (96%)	17 (4%)	25	59
1	B	383/447 (86%)	373 (97%)	10 (3%)	40	73
1	C	385/447 (86%)	371 (96%)	14 (4%)	31	65
1	D	387/447 (87%)	377 (97%)	10 (3%)	40	73
All	All	1542/1788 (86%)	1491 (97%)	51 (3%)	33	67

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ASP
1	A	48	ASP
1	A	50	SER
1	A	61	HIS
1	A	85	VAL
1	A	90	THR
1	A	133	ARG
1	A	194	LYS
1	A	204	PHE
1	A	294	GLU
1	A	311	LEU
1	A	346	VAL
1	A	375	VAL
1	A	444	GLU
1	A	456	VAL
1	A	488	THR
1	A	518	LEU
1	B	79	LYS
1	B	189	THR
1	B	202	THR
1	B	204	PHE
1	B	269	ILE
1	B	278	THR
1	B	327	LYS

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Mol	Chain	Res	Type
1	B	329	VAL
1	B	489	VAL
1	B	495	LEU
1	C	84	ILE
1	C	89	ILE
1	C	102	ILE
1	C	181	ILE
1	C	204	PHE
1	C	213	ASP
1	C	215	LEU
1	C	327	LYS
1	C	329	VAL
1	C	406	VAL
1	C	447	PHE
1	C	456	VAL
1	C	486	VAL
1	C	488	THR
1	D	62	GLU
1	D	66	GLU
1	D	96	LEU
1	D	192	ILE
1	D	256	LYS
1	D	275	HIS
1	D	342	GLU
1	D	387	VAL
1	D	411	GLN
1	D	489	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	137	HIS
1	A	156	GLN
1	A	163	ASN
1	A	230	HIS
1	A	405	ASN
1	A	409	HIS
1	B	24	HIS
1	B	185	HIS
1	B	198	HIS
1	B	229	HIS

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Mol	Chain	Res	Type
1	B	230	HIS
1	B	433	HIS
1	C	21	ASN
1	C	166	HIS
1	C	200	HIS
1	C	230	HIS
1	C	317	HIS
1	C	409	HIS
1	D	9	GLN
1	D	137	HIS
1	D	163	ASN
1	D	166	HIS
1	D	185	HIS
1	D	205	HIS
1	D	265	HIS
1	D	317	HIS
1	D	386	GLN
1	D	433	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 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	$\# Z > 2$
2	ATP	A	601	3	32,33,33	0.59	0	48,52,52	0.63	0
2	ATP	C	601	3	32,33,33	0.62	0	48,52,52	0.63	0
2	ATP	D	601	3	32,33,33	0.55	0	48,52,52	0.61	0
2	ATP	B	601	3	32,33,33	0.57	0	48,52,52	0.63	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
2	ATP	A	601	3	-	7/22/38/38	0/3/3/3
2	ATP	C	601	3	-	8/22/38/38	0/3/3/3
2	ATP	D	601	3	-	6/22/38/38	0/3/3/3
2	ATP	B	601	3	-	8/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	ATP	C5'-O5'-PA-O1A
2	A	601	ATP	C5'-O5'-PA-O2A
2	A	601	ATP	C5'-O5'-PA-O3A
2	B	601	ATP	C5'-O5'-PA-O1A
2	B	601	ATP	C5'-O5'-PA-O2A
2	B	601	ATP	C5'-O5'-PA-O3A
2	C	601	ATP	PB-O3A-PA-O5'
2	C	601	ATP	C5'-O5'-PA-O1A
2	C	601	ATP	C5'-O5'-PA-O2A
2	C	601	ATP	C5'-O5'-PA-O3A
2	D	601	ATP	C5'-O5'-PA-O2A
2	B	601	ATP	O4'-C4'-C5'-O5'
2	C	601	ATP	O4'-C4'-C5'-O5'
2	B	601	ATP	C3'-C4'-C5'-O5'
2	C	601	ATP	C3'-C4'-C5'-O5'

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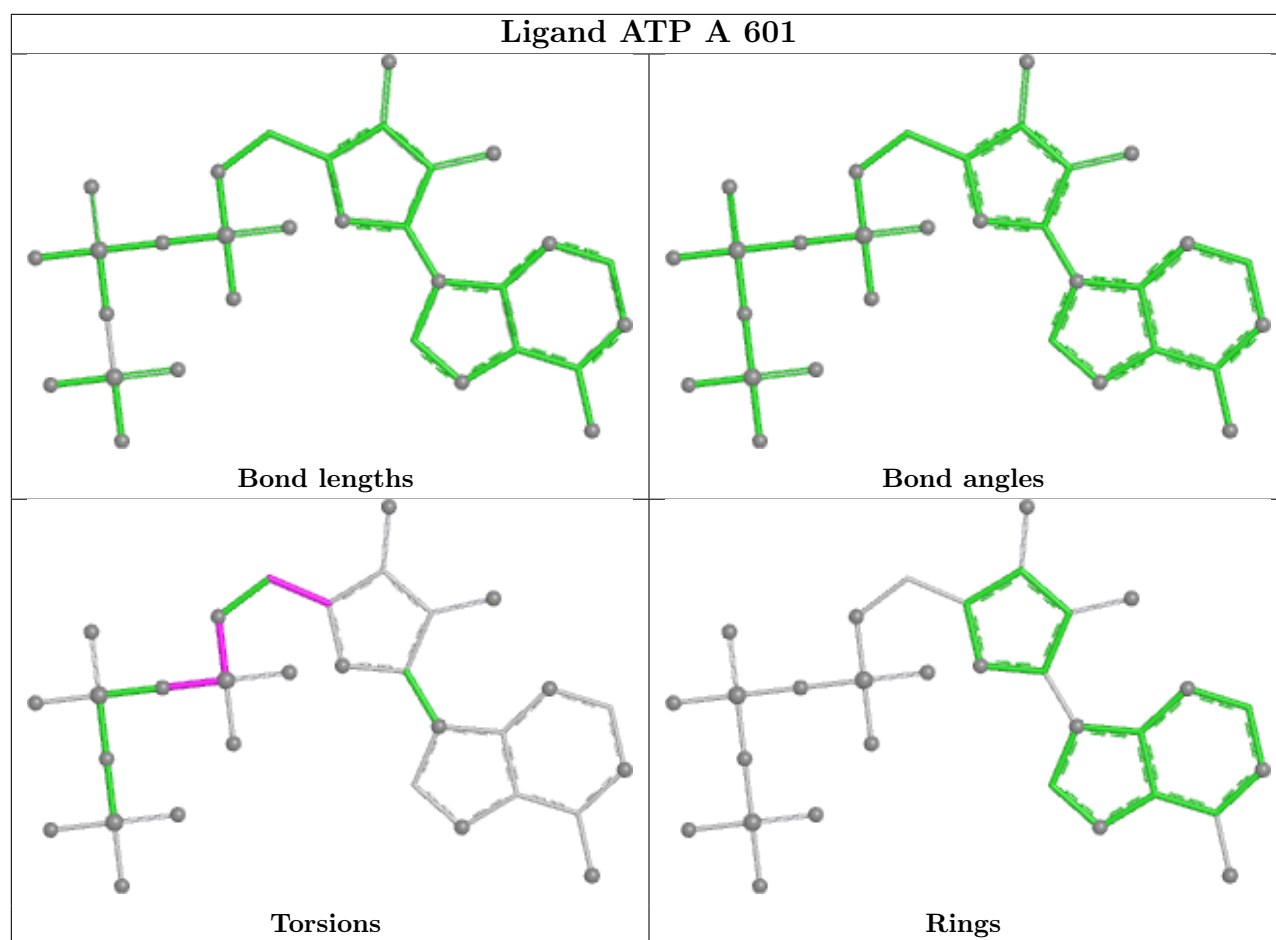
Mol	Chain	Res	Type	Atoms
2	A	601	ATP	C3'-C4'-C5'-O5'
2	A	601	ATP	PB-O3A-PA-O1A
2	A	601	ATP	PB-O3A-PA-O5'
2	B	601	ATP	PB-O3A-PA-O5'
2	D	601	ATP	PB-O3A-PA-O5'
2	D	601	ATP	C5'-O5'-PA-O1A
2	D	601	ATP	C5'-O5'-PA-O3A
2	C	601	ATP	C4'-C5'-O5'-PA
2	C	601	ATP	PB-O3B-PG-O3G
2	B	601	ATP	PG-O3B-PB-O2B
2	D	601	ATP	PA-O3A-PB-O1B
2	D	601	ATP	PA-O3A-PB-O2B
2	A	601	ATP	O4'-C4'-C5'-O5'
2	B	601	ATP	PB-O3A-PA-O2A

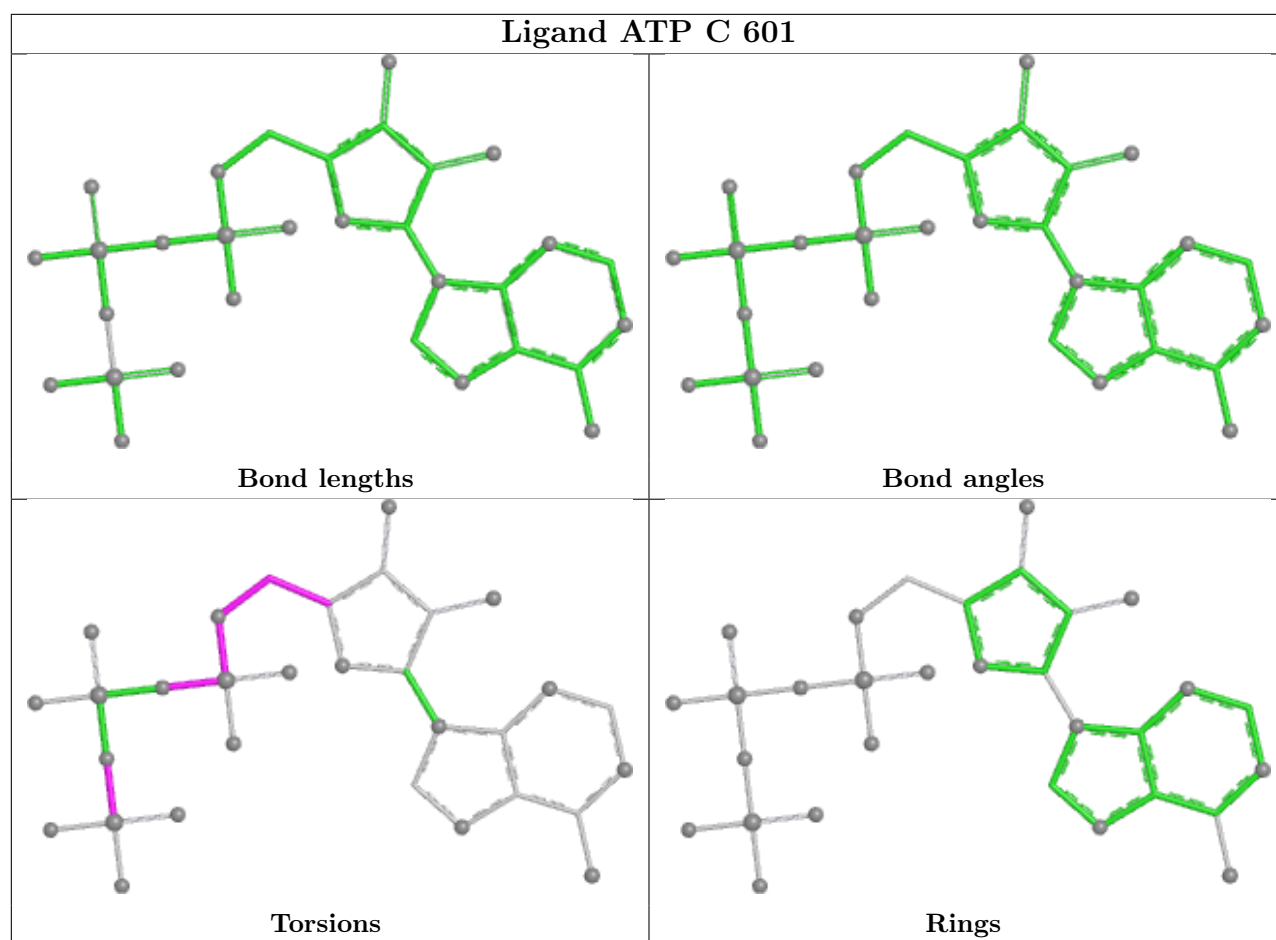
There are no ring outliers.

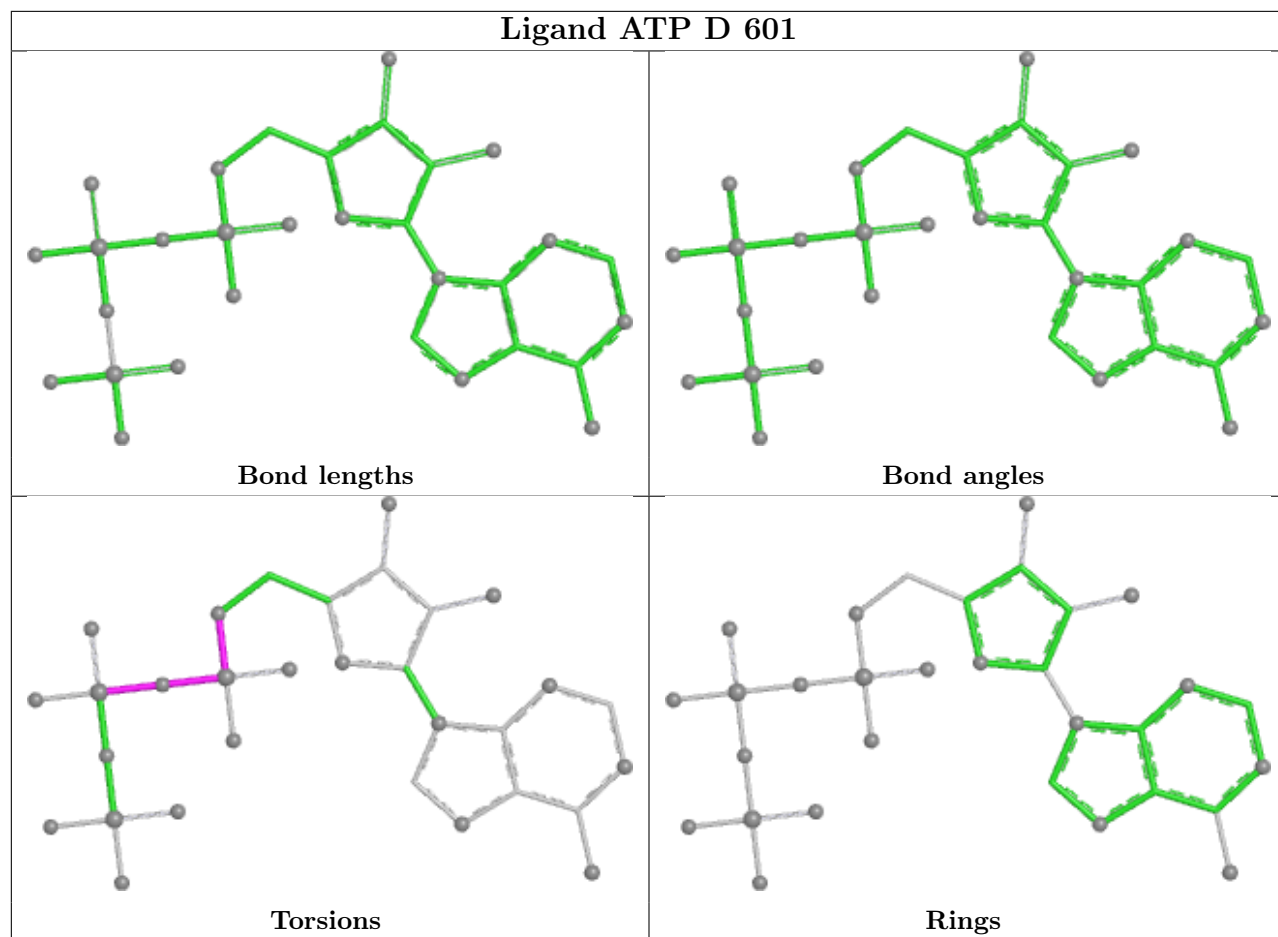
1 monomer is involved in 1 short contact:

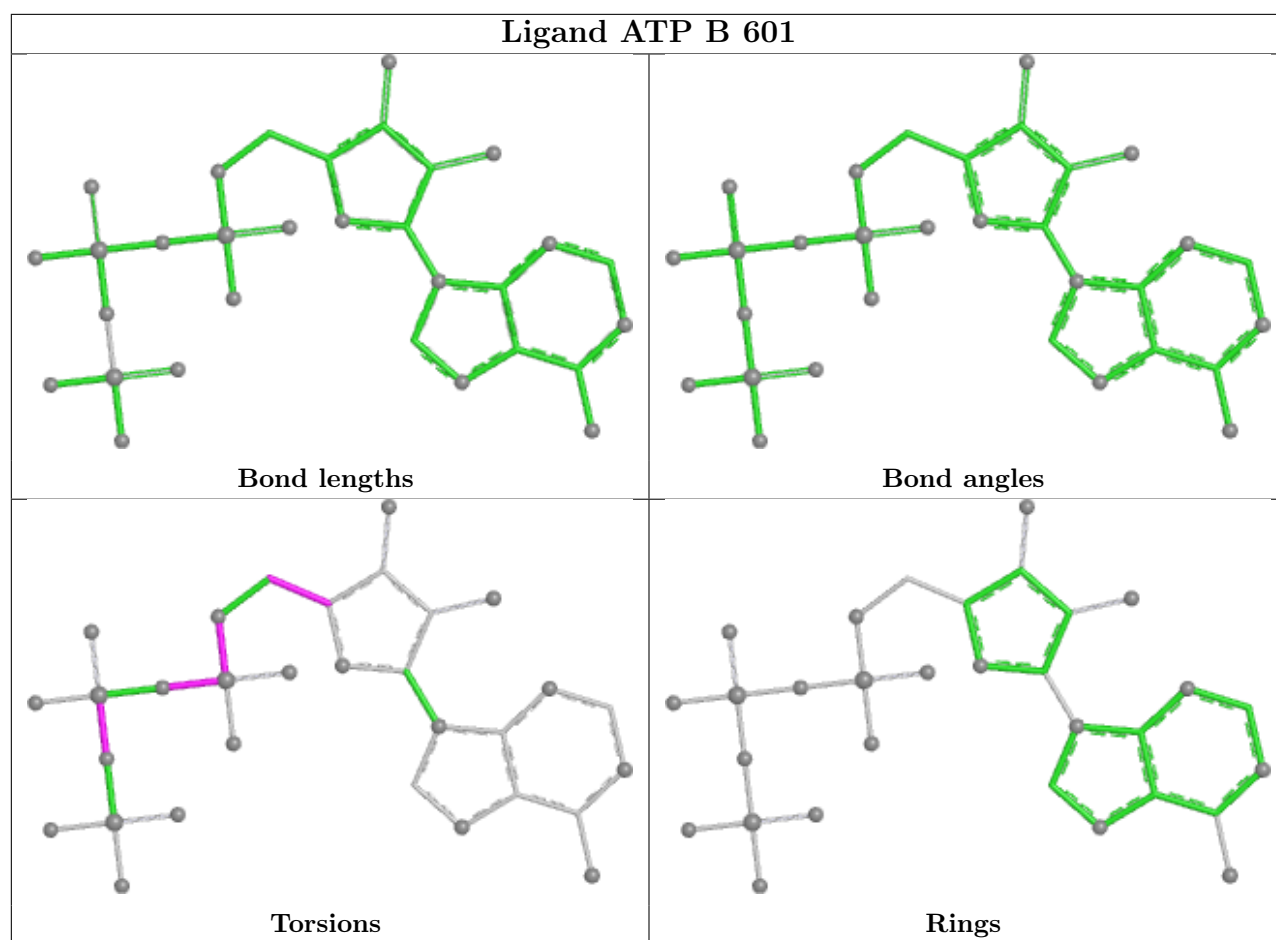
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	ATP	1	0

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.









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	487/564 (86%)	1.20	98 (20%) 3 2	28, 53, 101, 124	0
1	B	479/564 (84%)	0.76	57 (11%) 9 7	27, 50, 95, 116	0
1	C	480/564 (85%)	1.19	94 (19%) 3 2	28, 64, 94, 113	0
1	D	482/564 (85%)	1.26	99 (20%) 2 2	27, 64, 96, 118	0
All	All	1928/2256 (85%)	1.10	348 (18%) 3 3	27, 57, 96, 124	0

All (348) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	350	PHE	10.0
1	A	455	GLU	9.0
1	A	299	SER	7.2
1	A	41	ASP	7.1
1	A	302	ALA	7.0
1	B	301	ASP	6.8
1	D	301	ASP	6.7
1	C	465	LEU	6.6
1	A	350	PHE	6.2
1	A	518	LEU	6.1
1	D	310	ARG	6.1
1	D	447	PHE	6.0
1	A	304	HIS	5.4
1	B	302	ALA	5.4
1	A	305	ALA	5.2
1	A	522	ALA	5.2
1	D	375	VAL	5.2
1	C	493	VAL	5.2
1	A	521	VAL	5.1
1	C	301	ASP	5.1
1	C	447	PHE	5.0

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Mol	Chain	Res	Type	RSRZ
1	C	463	GLU	5.0
1	D	45	ARG	4.9
1	A	303	ALA	4.9
1	D	188	GLY	4.9
1	C	21	ASN	4.8
1	B	344	GLY	4.7
1	A	456	VAL	4.7
1	C	62	GLU	4.6
1	A	516	ALA	4.6
1	A	290	LEU	4.5
1	D	467	CYS	4.5
1	D	350	PHE	4.5
1	A	328	LYS	4.4
1	B	516	ALA	4.4
1	B	458	LEU	4.4
1	B	308	ILE	4.3
1	A	298	ALA	4.2
1	C	457	LEU	4.2
1	A	232	SER	4.2
1	B	456	VAL	4.2
1	D	443	THR	4.2
1	B	305	ALA	4.2
1	A	38	LEU	4.1
1	B	303	ALA	4.1
1	D	189	THR	4.1
1	A	55	LEU	4.1
1	A	473	ALA	4.1
1	B	442	ARG	4.1
1	D	397	LEU	4.1
1	B	519	PRO	4.0
1	B	298	ALA	4.0
1	D	300	GLY	4.0
1	B	480	GLY	4.0
1	A	465	LEU	4.0
1	D	312	LEU	4.0
1	B	467	CYS	4.0
1	A	343	MET	4.0
1	D	505	PRO	4.0
1	C	300	GLY	4.0
1	D	388	GLY	3.9
1	A	273	PHE	3.9
1	D	109	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	495	LEU	3.9
1	B	448	VAL	3.8
1	A	513	LEU	3.8
1	C	45	ARG	3.8
1	D	374	VAL	3.7
1	C	443	THR	3.7
1	A	54	VAL	3.7
1	C	492	LEU	3.7
1	D	349	ASP	3.7
1	A	490	TYR	3.6
1	D	195	SER	3.6
1	D	481	TRP	3.6
1	B	189	THR	3.6
1	B	457	LEU	3.6
1	C	471	GLY	3.6
1	D	465	LEU	3.6
1	A	285	LEU	3.5
1	C	490	TYR	3.5
1	C	134	GLU	3.5
1	D	311	LEU	3.5
1	B	328	LYS	3.5
1	A	501	ALA	3.5
1	C	351	VAL	3.5
1	D	466	ASP	3.5
1	C	361	ARG	3.5
1	C	284	ASP	3.4
1	A	453	THR	3.4
1	D	490	TYR	3.4
1	B	495	LEU	3.4
1	D	493	VAL	3.4
1	C	405	ASN	3.4
1	A	314	LYS	3.4
1	A	278	THR	3.4
1	C	502	PRO	3.4
1	D	367	MET	3.4
1	C	338	PHE	3.4
1	B	485	GLY	3.3
1	C	190	THR	3.3
1	C	324	LEU	3.3
1	A	338	PHE	3.3
1	D	187	SER	3.3
1	C	312	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	133	ARG	3.2
1	D	266	ARG	3.2
1	B	443	THR	3.2
1	B	471	GLY	3.2
1	D	506	THR	3.2
1	C	263	GLU	3.2
1	A	461	TYR	3.2
1	A	462	PRO	3.2
1	B	518	LEU	3.2
1	A	174	ARG	3.2
1	D	256	LYS	3.2
1	D	286	THR	3.2
1	A	337	MET	3.2
1	D	204	PHE	3.2
1	D	362	CYS	3.1
1	C	394	SER	3.1
1	C	169	ALA	3.1
1	C	501	ALA	3.1
1	A	307	HIS	3.1
1	B	188	GLY	3.1
1	D	33	LEU	3.1
1	D	233	ALA	3.1
1	C	123	ARG	3.1
1	D	250	TYR	3.1
1	B	304	HIS	3.1
1	D	336	ASP	3.1
1	D	503	GLN	3.1
1	D	511	GLU	3.1
1	D	123	ARG	3.1
1	A	345	TYR	3.1
1	D	236	ASN	3.1
1	A	517	GLY	3.1
1	D	104	ALA	3.0
1	B	461	TYR	3.0
1	A	344	GLY	3.0
1	A	266	ARG	3.0
1	A	380	SER	3.0
1	D	361	ARG	3.0
1	D	444	GLU	3.0
1	D	299	SER	3.0
1	B	463	GLU	3.0
1	C	337	MET	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	102	ILE	3.0
1	C	407	ARG	3.0
1	A	472	LEU	3.0
1	D	95	ASN	2.9
1	D	489	VAL	2.9
1	A	515	ARG	2.9
1	A	256	LYS	2.9
1	A	479	PHE	2.9
1	D	521	VAL	2.9
1	D	119	ARG	2.9
1	A	466	ASP	2.9
1	C	466	ASP	2.9
1	D	376	GLY	2.9
1	D	316	TYR	2.9
1	C	349	ASP	2.9
1	D	448	VAL	2.9
1	D	486	VAL	2.9
1	D	492	LEU	2.9
1	A	339	GLY	2.8
1	A	52	PRO	2.8
1	D	461	TYR	2.8
1	C	521	VAL	2.8
1	B	349	ASP	2.8
1	C	61	HIS	2.8
1	D	328	LYS	2.8
1	C	350	PHE	2.8
1	D	43	THR	2.8
1	C	256	LYS	2.8
1	D	385	GLY	2.8
1	A	334	PHE	2.8
1	C	250	TYR	2.8
1	A	123	ARG	2.7
1	A	469	VAL	2.7
1	C	316	TYR	2.7
1	D	410	LYS	2.7
1	A	407	ARG	2.7
1	D	124	ARG	2.7
1	D	166	HIS	2.7
1	D	330	PRO	2.7
1	B	510	ASN	2.7
1	C	75	GLY	2.7
1	C	459	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	292	SER	2.7
1	D	436	ARG	2.7
1	B	345	TYR	2.6
1	A	43	THR	2.6
1	A	291	THR	2.6
1	B	395	LYS	2.6
1	A	221	LYS	2.6
1	A	324	LEU	2.6
1	A	477	VAL	2.6
1	B	285	LEU	2.6
1	C	152	PHE	2.6
1	D	459	ARG	2.6
1	C	327	LYS	2.6
1	A	134	GLU	2.6
1	D	463	GLU	2.6
1	D	193	PRO	2.6
1	C	509	ILE	2.6
1	C	120	GLU	2.6
1	C	104	ALA	2.6
1	C	508	TRP	2.5
1	B	360	GLY	2.5
1	A	316	TYR	2.5
1	C	448	VAL	2.5
1	D	329	VAL	2.5
1	D	34	ASP	2.5
1	D	314	LYS	2.5
1	B	486	VAL	2.5
1	C	192	ILE	2.5
1	C	287	ASP	2.5
1	C	313	ASP	2.5
1	C	328	LYS	2.5
1	D	340	SER	2.5
1	C	148	GLU	2.5
1	D	455	GLU	2.5
1	D	281	ALA	2.5
1	C	27	PRO	2.5
1	A	49	GLY	2.5
1	B	125	GLN	2.5
1	A	189	THR	2.5
1	C	223	LEU	2.4
1	D	313	ASP	2.4
1	C	330	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	64	VAL	2.4
1	A	340	SER	2.4
1	C	232	SER	2.4
1	D	499	ALA	2.4
1	D	237	THR	2.4
1	C	375	VAL	2.4
1	B	455	GLU	2.4
1	C	155	LEU	2.4
1	D	267	PRO	2.4
1	D	469	VAL	2.4
1	C	410	LYS	2.4
1	A	277	PHE	2.4
1	C	487	ALA	2.4
1	A	250	TYR	2.4
1	C	345	TYR	2.4
1	D	464	ILE	2.4
1	C	462	PRO	2.4
1	A	349	ASP	2.4
1	D	440	ALA	2.4
1	D	50	SER	2.4
1	D	345	TYR	2.4
1	C	135	PRO	2.4
1	A	470	VAL	2.3
1	D	273	PHE	2.3
1	A	499	ALA	2.3
1	A	33	LEU	2.3
1	A	226	LEU	2.3
1	A	268	THR	2.3
1	C	143	HIS	2.3
1	D	441	ILE	2.3
1	C	485	GLY	2.3
1	C	504	ASP	2.3
1	B	380	SER	2.3
1	B	449	TYR	2.3
1	A	222	ARG	2.3
1	C	346	VAL	2.3
1	A	485	GLY	2.3
1	C	440	ALA	2.3
1	A	275	HIS	2.3
1	B	275	HIS	2.3
1	D	192	ILE	2.3
1	A	202	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	318	THR	2.3
1	B	272	GLY	2.3
1	D	406	VAL	2.3
1	C	70	PHE	2.2
1	B	196	ALA	2.2
1	A	108	LEU	2.2
1	A	327	LYS	2.2
1	D	395	LYS	2.2
1	C	363	ILE	2.2
1	C	406	VAL	2.2
1	D	186	SER	2.2
1	D	427	ALA	2.2
1	A	410	LYS	2.2
1	A	494	ASN	2.2
1	A	31	ARG	2.2
1	A	467	CYS	2.2
1	B	358	VAL	2.2
1	B	489	VAL	2.2
1	A	40	LEU	2.2
1	A	363	ILE	2.2
1	A	320	THR	2.2
1	C	286	THR	2.2
1	C	187	SER	2.2
1	D	298	ALA	2.2
1	C	73	ARG	2.2
1	B	61	HIS	2.2
1	C	323	ASP	2.2
1	C	43	THR	2.2
1	B	376	GLY	2.2
1	C	461	TYR	2.2
1	A	99	LEU	2.2
1	A	492	LEU	2.2
1	D	223	LEU	2.2
1	C	165	GLU	2.2
1	A	335	ILE	2.1
1	A	510	ASN	2.1
1	B	343	MET	2.1
1	C	336	ASP	2.1
1	A	98	ALA	2.1
1	C	42	GLY	2.1
1	C	274	THR	2.1
1	B	38	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	155	LEU	2.1
1	D	348	PHE	2.1
1	B	107	SER	2.1
1	C	157	SER	2.1
1	C	362	CYS	2.1
1	C	230	HIS	2.1
1	D	343	MET	2.1
1	A	60	LEU	2.1
1	B	96	LEU	2.1
1	C	44	TRP	2.1
1	A	451	ALA	2.1
1	A	452	TYR	2.1
1	C	160	GLU	2.1
1	D	116	GLU	2.1
1	B	182	LEU	2.1
1	B	422	LEU	2.1
1	D	226	LEU	2.1
1	A	514	GLY	2.1
1	B	517	GLY	2.1
1	B	363	ILE	2.1
1	A	112	ASN	2.0
1	C	33	LEU	2.0
1	B	487	ALA	2.0
1	A	486	VAL	2.0
1	D	82	VAL	2.0
1	C	47	PRO	2.0
1	C	108	LEU	2.0
1	B	273	PHE	2.0
1	D	507	ALA	2.0
1	C	35	GLU	2.0
1	D	283	GLU	2.0
1	D	449	TYR	2.0
1	C	456	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

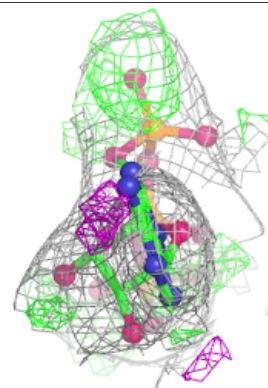
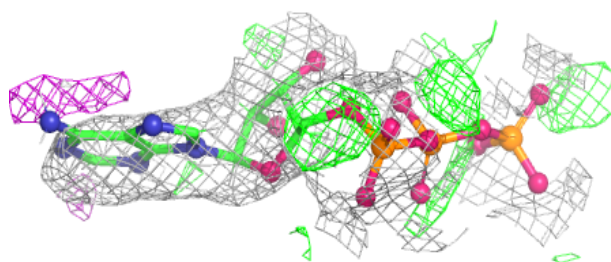
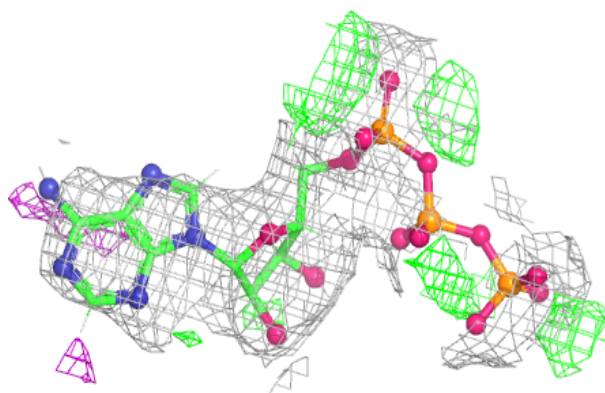
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	D	603	1/1	0.36	0.17	30,30,30,30	0
3	MG	C	602	1/1	0.46	0.47	85,85,85,85	0
2	ATP	C	601	31/31	0.71	0.21	53,86,103,124	0
2	ATP	D	601	31/31	0.79	0.17	57,74,102,114	0
3	MG	B	602	1/1	0.86	0.36	50,50,50,50	0
2	ATP	B	601	31/31	0.87	0.14	45,64,81,83	0
2	ATP	A	601	31/31	0.87	0.14	45,70,90,109	0
3	MG	B	603	1/1	0.88	0.10	30,30,30,30	0
3	MG	D	602	1/1	0.90	0.39	50,50,50,50	0
3	MG	A	602	1/1	0.90	0.27	48,48,48,48	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.

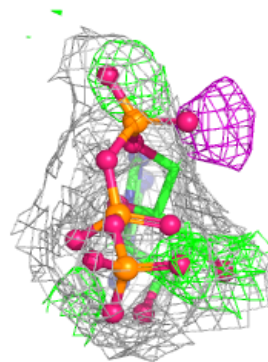
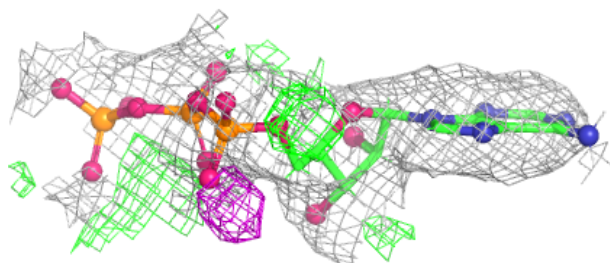
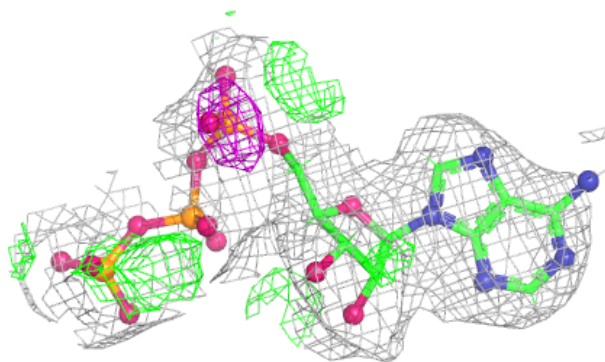
Electron density around ATP C 601:

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

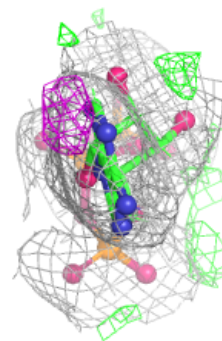
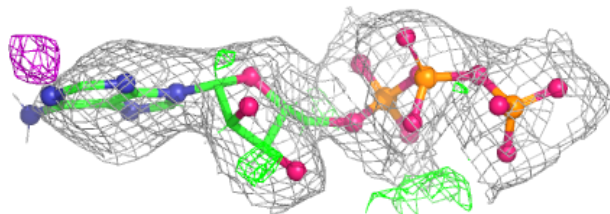
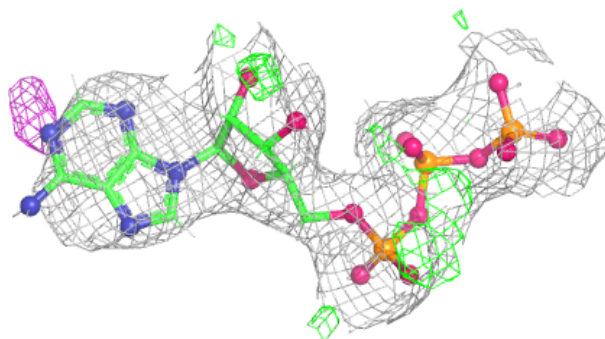


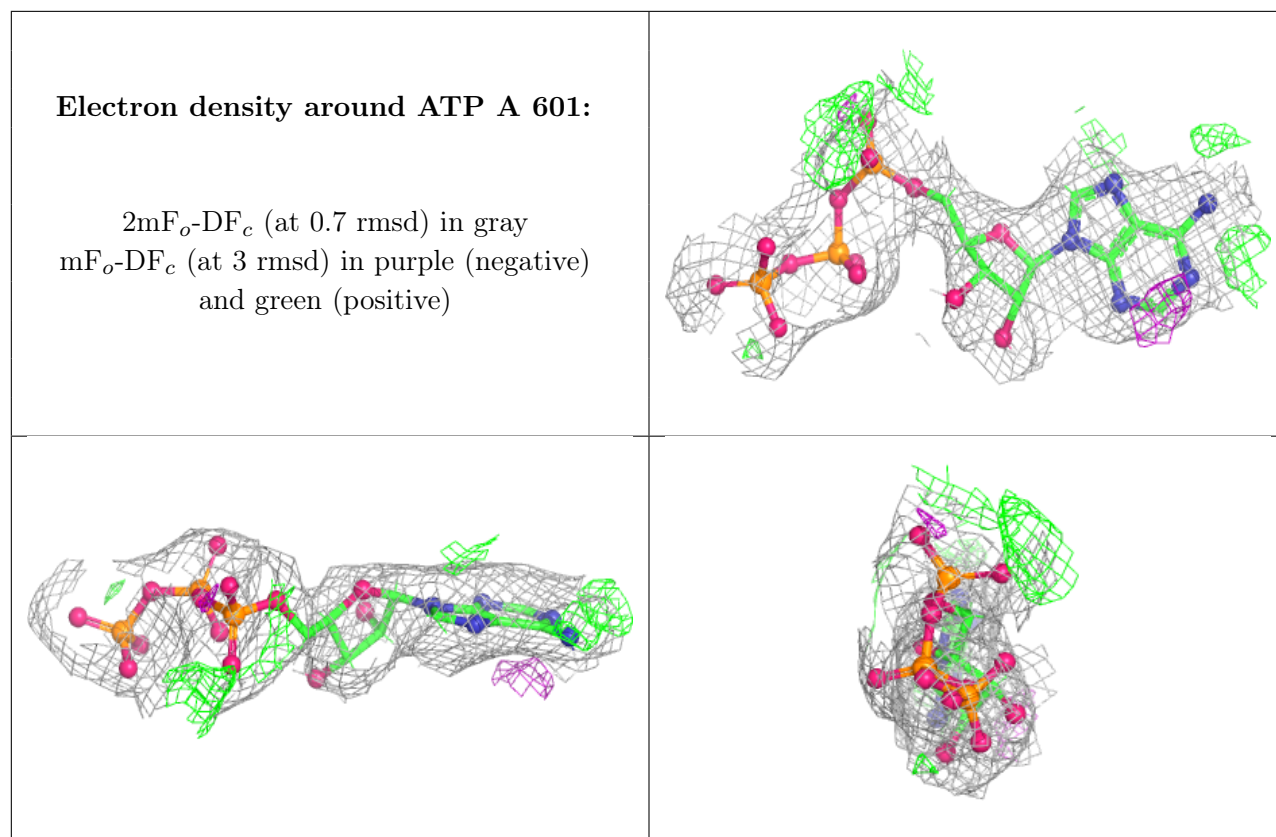
Electron density around ATP D 601:

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

**Electron density around ATP B 601:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.