



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 08:28 AM EDT

PDB ID : 3BJU
Title : Crystal Structure of tetrameric form of human lysyl-tRNA synthetase
Authors : Guo, M.; Yang, X.L.; Schimmel, P.
Deposited on : 2007-12-04
Resolution : 2.31 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

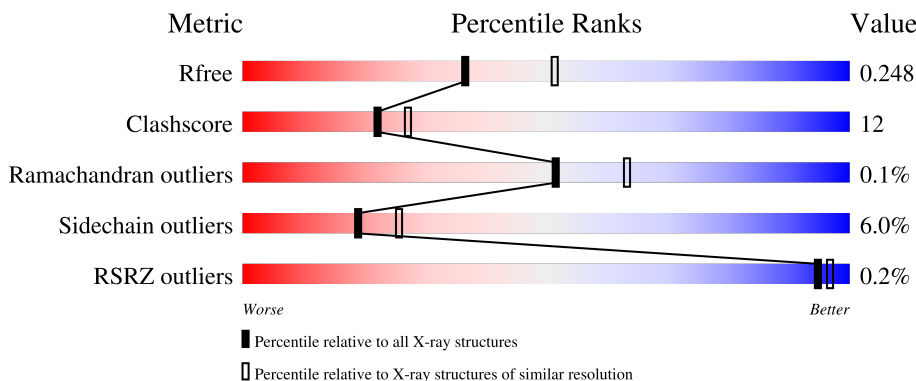
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 2.31 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}	130704	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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	521	 74% 21% . .
1	B	521	 70% 22% . 5%
1	C	521	 74% 21% . .
1	D	521	 70% 22% . .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17378 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 Lysyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	503	Total	C	N	O	S	0	1	0
			4073	2605	689	751	28			
1	B	495	Total	C	N	O	S	0	3	0
			4023	2574	681	740	28			
1	C	501	Total	C	N	O	S	0	1	0
			4058	2598	689	743	28			
1	D	499	Total	C	N	O	S	0	1	0
			4046	2589	687	742	28			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	69	MET	-	expression tag	UNP Q15046
A	582	LEU	VAL	engineered mutation	UNP Q15046
A	583	GLU	-	expression tag	UNP Q15046
A	584	HIS	-	expression tag	UNP Q15046
A	585	HIS	-	expression tag	UNP Q15046
A	586	HIS	-	expression tag	UNP Q15046
A	587	HIS	-	expression tag	UNP Q15046
A	588	HIS	-	expression tag	UNP Q15046
A	589	HIS	-	expression tag	UNP Q15046
B	69	MET	-	expression tag	UNP Q15046
B	582	LEU	VAL	engineered mutation	UNP Q15046
B	583	GLU	-	expression tag	UNP Q15046
B	584	HIS	-	expression tag	UNP Q15046
B	585	HIS	-	expression tag	UNP Q15046
B	586	HIS	-	expression tag	UNP Q15046
B	587	HIS	-	expression tag	UNP Q15046
B	588	HIS	-	expression tag	UNP Q15046
B	589	HIS	-	expression tag	UNP Q15046
C	69	MET	-	expression tag	UNP Q15046
C	582	LEU	VAL	engineered mutation	UNP Q15046
C	583	GLU	-	expression tag	UNP Q15046

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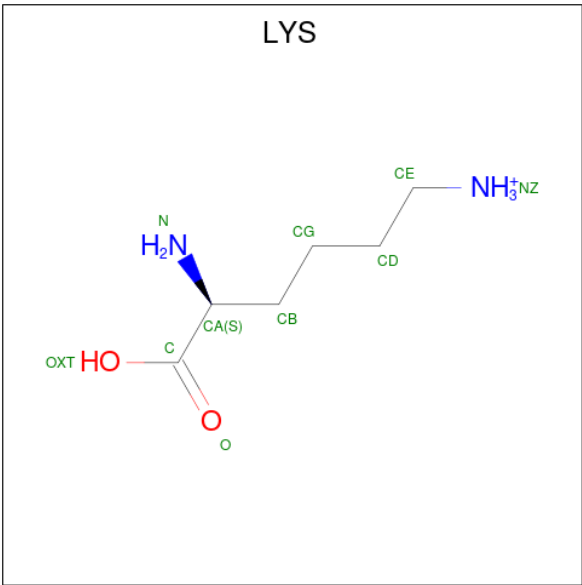
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Chain	Residue	Modelled	Actual	Comment	Reference
C	584	HIS	-	expression tag	UNP Q15046
C	585	HIS	-	expression tag	UNP Q15046
C	586	HIS	-	expression tag	UNP Q15046
C	587	HIS	-	expression tag	UNP Q15046
C	588	HIS	-	expression tag	UNP Q15046
C	589	HIS	-	expression tag	UNP Q15046
D	69	MET	-	expression tag	UNP Q15046
D	582	LEU	VAL	engineered mutation	UNP Q15046
D	583	GLU	-	expression tag	UNP Q15046
D	584	HIS	-	expression tag	UNP Q15046
D	585	HIS	-	expression tag	UNP Q15046
D	586	HIS	-	expression tag	UNP Q15046
D	587	HIS	-	expression tag	UNP Q15046
D	588	HIS	-	expression tag	UNP Q15046
D	589	HIS	-	expression tag	UNP Q15046

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

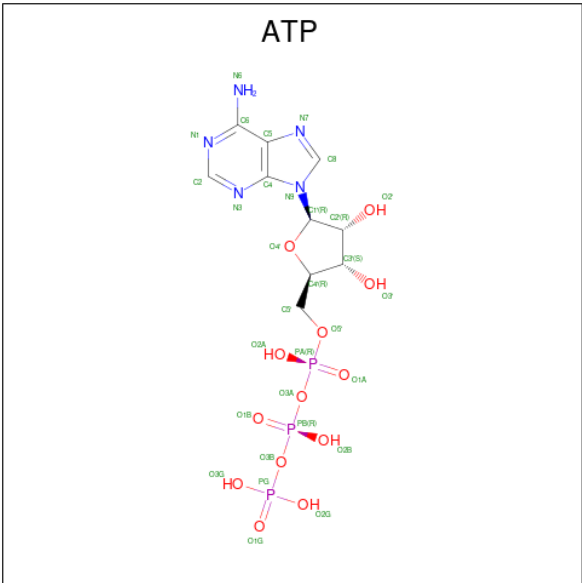
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total 3	Ca 3	0	0
2	B	3	Total 3	Ca 3	0	0
2	C	3	Total 3	Ca 3	0	0
2	D	3	Total 3	Ca 3	0	0

- Molecule 3 is LYSINE (three-letter code: LYS) (formula: C₆H₁₅N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	6	2	2		
3	B	1	Total	C	N	O	0	0
			10	6	2	2		
3	C	1	Total	C	N	O	0	0
			10	6	2	2		
3	D	1	Total	C	N	O	0	0
			10	6	2	2		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: 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	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	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

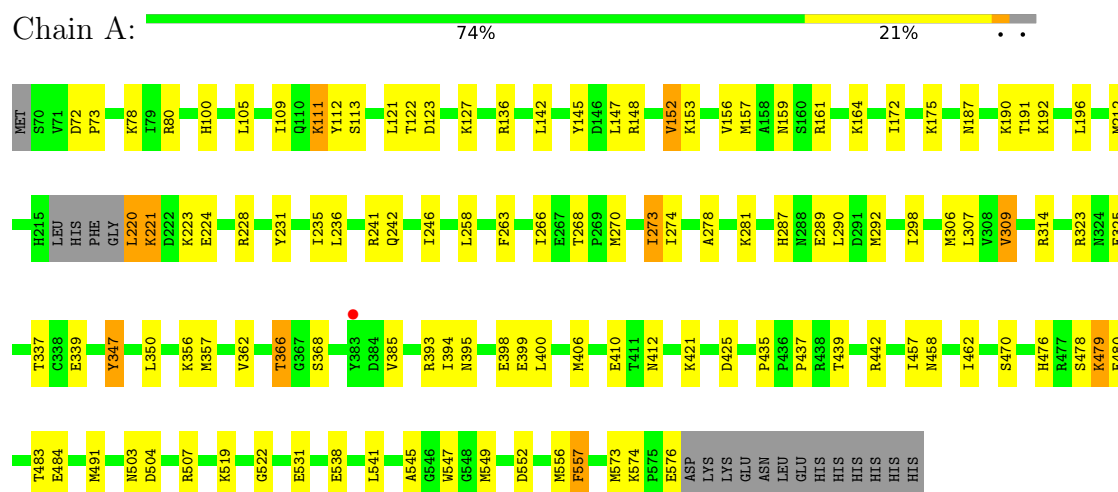
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	270	Total	O	0	0
			270	270		
5	B	245	Total	O	0	0
			245	245		
5	C	260	Total	O	0	0
			260	260		
5	D	227	Total	O	0	0
			227	227		

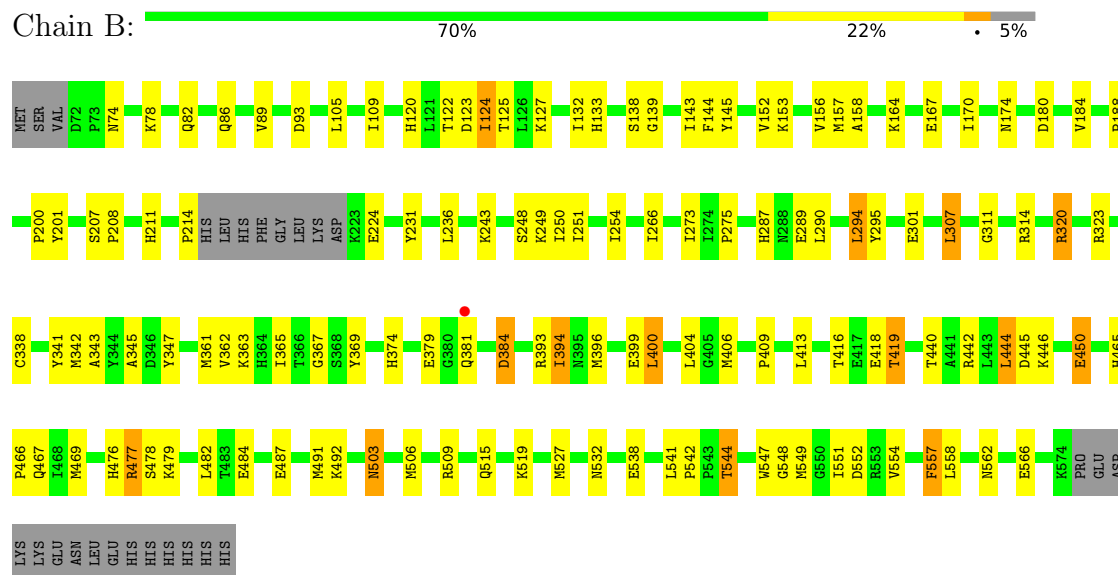
3 Residue-property plots

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: Lysyl-tRNA synthetase

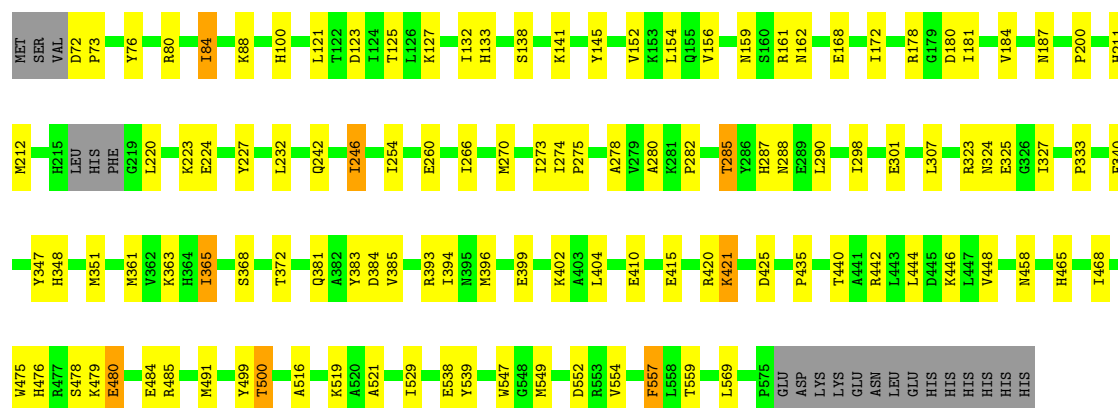


• Molecule 1: Lysyl-tRNA synthetase



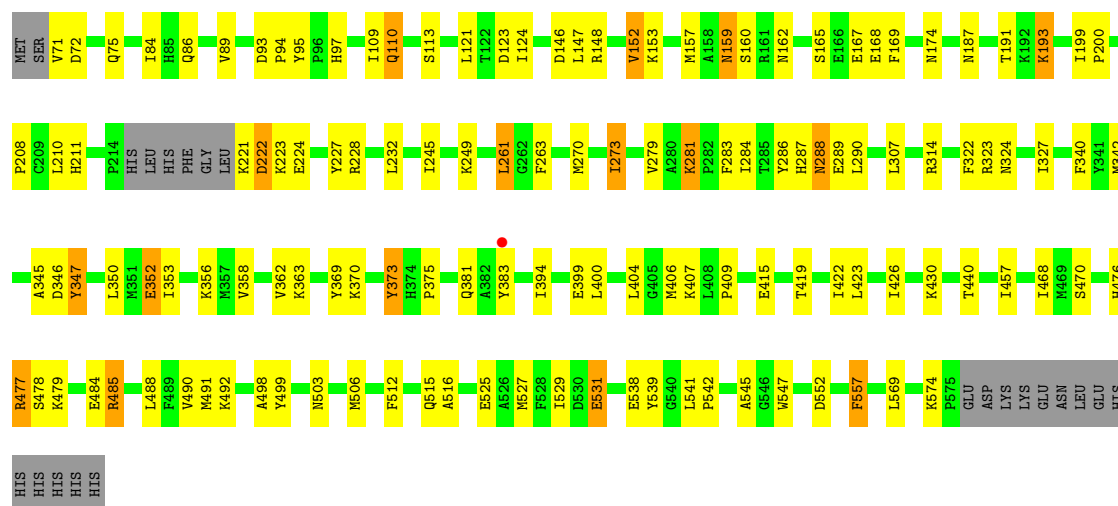
• Molecule 1: Lysyl-tRNA synthetase

Chain C:  74% 21% . .



• Molecule 1: Lysyl-tRNA synthetase

Chain D:  70% 22% . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	152.01Å 152.01Å 108.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.31 24.88 – 2.31	Depositor EDS
% Data completeness (in resolution range)	98.0 (25.00-2.31) 98.0 (24.88-2.31)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.31Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.194 , 0.252 0.192 , 0.248	Depositor DCC
R_{free} test set	5985 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	28.8	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 16.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l 0.450 for h,-h-k,-l 0.014 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17378	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.55	0/4169	0.64	0/5630
1	B	0.52	0/4122	0.62	0/5566
1	C	0.55	0/4155	0.64	0/5611
1	D	0.52	0/4143	0.64	0/5595
All	All	0.54	0/16589	0.63	0/22402

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4073	0	4060	98	0
1	B	4023	0	4016	97	0
1	C	4058	0	4053	100	0
1	D	4046	0	4037	110	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
3	A	10	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	10	0	12	0	0
3	C	10	0	12	1	0
3	D	10	0	12	0	0
4	A	31	0	12	0	0
4	B	31	0	12	0	0
4	C	31	0	12	0	0
4	D	31	0	12	0	0
5	A	270	0	0	23	0
5	B	245	0	0	18	0
5	C	260	0	0	14	0
5	D	227	0	0	18	0
All	All	17378	0	16262	382	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 12.

All (382) 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:157:MET:CE	1:D:191:THR:HG22	1.63	1.28
1:B:289:GLU:HG2	5:B:809:HOH:O	1.50	1.11
1:D:363:LYS:HD3	1:D:369:TYR:CE1	1.90	1.05
1:B:174:ASN:HB3	5:B:879:HOH:O	1.58	1.03
1:D:363:LYS:CD	1:D:369:TYR:CE1	2.43	1.02
1:D:157:MET:CE	1:D:191:THR:CG2	2.39	1.00
1:D:157:MET:HE1	1:D:191:THR:HG22	1.00	0.99
1:A:224:GLU:HG3	5:A:797:HOH:O	1.62	0.98
1:A:157:MET:CE	1:A:191:THR:HG22	1.95	0.97
1:B:542:PRO:O	1:B:544:THR:HG22	1.64	0.96
1:D:157:MET:HE1	1:D:191:THR:CG2	1.95	0.95
1:B:413:LEU:O	1:B:419:THR:HG21	1.66	0.95
1:D:531:GLU:OE2	5:D:738:HOH:O	1.85	0.95
1:C:393:ARG:HD2	5:C:780:HOH:O	1.65	0.93
1:C:484:GLU:HB2	1:C:500:THR:HG23	1.48	0.92
1:A:157:MET:HE1	1:A:191:THR:HG22	1.48	0.92
1:C:282:PRO:HB3	1:C:298:ILE:HD11	1.50	0.91
1:C:519:LYS:HE3	5:C:842:HOH:O	1.71	0.89
1:D:363:LYS:HD2	1:D:369:TYR:CD1	2.06	0.89
1:C:285:THR:HG21	1:D:283:PHE:HB3	1.59	0.85
1:C:223:LYS:HG2	1:C:227:TYR:CE1	2.12	0.85
1:D:363:LYS:HD2	1:D:369:TYR:CE1	2.12	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:476:HIS:HD2	1:D:478:SER:H	1.25	0.84
1:C:275:PRO:HB2	1:C:298:ILE:HD13	1.59	0.84
1:A:270:MET:CE	5:A:765:HOH:O	2.25	0.82
1:D:159:ASN:HD21	1:D:162:ASN:HD22	1.24	0.82
1:A:362:VAL:O	1:A:366:THR:HB	1.79	0.82
1:A:175:LYS:CE	5:A:847:HOH:O	2.28	0.81
1:C:273:ILE:HG13	1:C:274:ILE:HG13	1.61	0.81
1:B:476:HIS:HD2	1:B:478:SER:H	1.31	0.79
1:D:394:ILE:HB	1:D:399:GLU:HG3	1.65	0.78
1:D:515:GLN:HE21	1:D:527:MET:H	1.30	0.78
1:C:278:ALA:HB3	1:C:298:ILE:CG2	2.14	0.78
1:C:484:GLU:OE1	1:C:500:THR:HG21	1.84	0.77
1:A:223:LYS:HG2	5:A:792:HOH:O	1.84	0.77
1:A:394:ILE:HB	1:A:399:GLU:HG3	1.66	0.76
1:D:373:TYR:CE1	1:D:383:TYR:HD1	2.02	0.76
1:A:80:ARG:NH1	5:A:784:HOH:O	2.17	0.76
1:C:168:GLU:HG2	5:C:843:HOH:O	1.86	0.76
1:C:484:GLU:CB	1:C:500:THR:HG23	2.16	0.75
1:D:93:ASP:HB2	5:D:764:HOH:O	1.84	0.75
1:A:270:MET:HE1	5:A:765:HOH:O	1.86	0.74
1:C:161:ARG:HD2	5:C:826:HOH:O	1.87	0.74
1:D:228:ARG:NH1	1:D:574:LYS:O	2.18	0.74
1:A:159:ASN:ND2	1:A:161:ARG:HG2	2.02	0.74
1:A:268:THR:O	1:B:320:ARG:NH1	2.18	0.73
1:D:363:LYS:HD3	1:D:369:TYR:HE1	1.52	0.73
1:D:422:ILE:O	1:D:426:ILE:HG12	1.89	0.72
1:C:372:THR:HG23	5:C:859:HOH:O	1.90	0.71
1:A:287:HIS:HD2	1:A:290:LEU:H	1.36	0.71
1:C:121:LEU:O	1:C:187:ASN:ND2	2.22	0.70
1:D:415:GLU:HG2	5:D:758:HOH:O	1.90	0.70
1:C:348:HIS:HD2	1:C:351:MET:CE	2.04	0.70
1:D:370:LYS:O	5:D:727:HOH:O	2.09	0.70
1:B:394:ILE:HB	1:B:399:GLU:HG3	1.74	0.69
1:C:394:ILE:HB	1:C:399:GLU:HG3	1.74	0.69
1:A:224:GLU:HB3	5:A:823:HOH:O	1.93	0.69
1:A:412:ASN:HB3	1:A:480:GLU:HG3	1.74	0.69
1:B:515:GLN:HE21	1:B:527:MET:H	1.37	0.69
1:C:475:TRP:O	1:D:97:HIS:HE1	1.74	0.69
1:D:352:GLU:O	1:D:356:LYS:HG2	1.93	0.68
1:A:522:GLY:HA3	5:A:787:HOH:O	1.94	0.68
1:A:157:MET:HE3	1:A:191:THR:HG22	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:509:ARG:NH2	1:B:538:GLU:OE2	2.23	0.67
1:D:346:ASP:OD2	1:D:477:ARG:NH1	2.28	0.67
1:A:538:GLU:OE1	1:B:211:HIS:HE1	1.78	0.67
1:A:350:LEU:HD22	1:A:545:ALA:HB1	1.76	0.67
1:B:416:THR:OG1	1:B:419:THR:HG22	1.94	0.67
1:D:286:TYR:HE1	1:D:288:ASN:HB3	1.57	0.67
1:A:159:ASN:HD21	1:A:161:ARG:HG2	1.59	0.67
1:D:409:PRO:HG2	1:D:419:THR:HG23	1.76	0.67
1:B:138:SER:OG	1:B:139:GLY:N	2.24	0.66
1:D:71:VAL:HG22	5:D:771:HOH:O	1.94	0.66
1:D:193:LYS:HE3	5:D:756:HOH:O	1.94	0.66
1:A:476:HIS:HD2	1:A:478:SER:H	1.42	0.66
1:B:418:GLU:HG3	5:B:818:HOH:O	1.93	0.66
1:C:476:HIS:HD2	1:C:478:SER:H	1.43	0.65
1:D:109:ILE:O	1:D:113:SER:HB2	1.95	0.65
1:A:175:LYS:HE2	5:A:847:HOH:O	1.92	0.65
1:A:287:HIS:CD2	1:A:290:LEU:H	2.14	0.64
1:A:270:MET:HE2	5:A:765:HOH:O	1.92	0.64
1:D:157:MET:HE3	1:D:191:THR:CG2	2.27	0.64
1:D:286:TYR:CE1	1:D:288:ASN:HB3	2.33	0.64
1:C:84:ILE:HD11	5:C:730:HOH:O	1.98	0.64
1:A:278:ALA:HB3	1:A:298:ILE:HG22	1.79	0.63
1:D:174:ASN:HB2	5:D:833:HOH:O	1.98	0.63
1:A:145:TYR:HB2	1:A:156:VAL:HB	1.79	0.63
1:D:159:ASN:HD21	1:D:162:ASN:ND2	1.97	0.62
1:B:145:TYR:HB2	1:B:156:VAL:HB	1.79	0.62
1:C:246[B]:ILE:HG23	1:C:365:ILE:CD1	2.30	0.62
1:B:416:THR:OG1	1:B:419:THR:CG2	2.47	0.62
1:D:273:ILE:HG22	5:D:754:HOH:O	1.99	0.61
1:A:242:GLN:O	1:A:246:ILE:HG12	2.01	0.60
1:A:278:ALA:HB3	1:A:298:ILE:CG2	2.30	0.60
1:B:503:ASN:H	1:B:503:ASN:HD22	1.47	0.60
1:C:285:THR:HG23	1:D:284:ILE:O	2.00	0.60
1:B:361:MET:O	1:B:365:ILE:HG12	2.01	0.60
1:C:287:HIS:HD2	1:C:290:LEU:H	1.50	0.60
1:B:314:ARG:HD2	5:B:680:HOH:O	2.02	0.60
1:D:490:VAL:HG12	1:D:491:MET:HG3	1.84	0.60
1:D:574:LYS:HG3	5:D:717:HOH:O	2.02	0.59
1:C:521:ALA:O	5:C:829:HOH:O	2.17	0.59
1:B:133:HIS:CD2	5:B:811:HOH:O	2.55	0.59
1:A:290:LEU:HB3	1:A:292:MET:CE	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:LYS:HE2	1:C:227:TYR:OH	2.03	0.59
1:C:254:ILE:HD11	1:C:549:MET:CE	2.32	0.58
1:C:278:ALA:HB3	1:C:298:ILE:HG21	1.85	0.58
1:A:152:VAL:HG13	1:A:153:LYS:H	1.67	0.58
1:B:491:MET:O	1:B:492:LYS:HB2	2.02	0.58
1:C:159:ASN:HB3	1:C:162:ASN:HD22	1.68	0.58
1:B:124:ILE:HD11	1:B:188:PRO:HG2	1.83	0.58
1:B:413:LEU:O	1:B:419:THR:CG2	2.49	0.58
1:C:145:TYR:HB2	1:C:156:VAL:HB	1.86	0.57
1:C:396:MET:CE	1:C:448:VAL:HG21	2.34	0.57
1:A:398:GLU:CD	5:A:809:HOH:O	2.42	0.57
1:D:263:PHE:CD2	1:D:314:ARG:HB3	2.40	0.57
1:A:323:ARG:HG3	5:A:873:HOH:O	2.06	0.56
1:C:84:ILE:HD12	1:C:84:ILE:C	2.25	0.56
1:A:122:THR:HG22	1:A:122:THR:O	2.05	0.56
1:D:287:HIS:HD2	1:D:290:LEU:HD12	1.71	0.56
1:B:167:GLU:O	1:B:170:ILE:HG22	2.06	0.56
1:A:235:ILE:HG22	1:A:236:LEU:HD23	1.88	0.56
1:C:270:MET:HE1	5:C:727:HOH:O	2.05	0.56
1:C:476:HIS:CD2	1:C:478:SER:H	2.24	0.56
1:D:153:LYS:HE2	5:D:814:HOH:O	2.05	0.55
1:A:366:THR:HG22	1:A:368:SER:H	1.69	0.55
1:B:301:GLU:HG3	1:B:341:TYR:OH	2.06	0.55
1:D:270:MET:HE2	1:D:322:PHE:CE1	2.42	0.55
1:B:143:ILE:HG23	1:B:158:ALA:HB3	1.88	0.55
1:C:480:GLU:HG3	5:C:828:HOH:O	2.05	0.55
1:D:347:TYR:CD1	1:D:484:GLU:HB3	2.41	0.55
1:B:476:HIS:CD2	1:B:479:LYS:H	2.25	0.55
1:B:287:HIS:HB2	1:B:294:LEU:HD22	1.88	0.55
1:C:348:HIS:HD2	1:C:351:MET:HE1	1.72	0.55
1:B:491:MET:SD	1:B:557:PHE:HB2	2.47	0.55
1:B:519:LYS:NZ	5:B:747:HOH:O	2.30	0.55
1:A:152:VAL:CG1	1:A:153:LYS:N	2.69	0.55
1:A:425:ASP:HB2	5:A:826:HOH:O	2.06	0.55
1:A:531:GLU:HG2	5:A:767:HOH:O	2.06	0.55
1:B:109:ILE:HD12	1:B:152:VAL:HG11	1.88	0.55
1:C:246[B]:ILE:HG23	1:C:365:ILE:HD13	1.89	0.54
1:D:375:PRO:HD2	1:D:381:GLN:O	2.08	0.54
1:C:278:ALA:HB3	1:C:298:ILE:HG22	1.87	0.54
1:A:547:TRP:CZ2	1:A:549:MET:HE3	2.42	0.54
1:B:469:MET:CE	5:B:842:HOH:O	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:442:ARG:O	1:C:446:LYS:HG2	2.07	0.54
1:A:220:LEU:N	5:A:782:HOH:O	2.40	0.54
1:B:143:ILE:CG2	1:B:158:ALA:HB3	2.37	0.54
1:A:357:MET:HE1	1:A:547:TRP:CZ2	2.43	0.53
1:C:327:ILE:HG22	1:C:333:PRO:HD3	1.91	0.53
1:D:167:GLU:HG2	5:D:753:HOH:O	2.08	0.53
1:B:93:ASP:N	1:B:93:ASP:OD1	2.40	0.53
1:D:373:TYR:CE1	1:D:383:TYR:CD1	2.92	0.53
1:C:484:GLU:CB	1:C:500:THR:CG2	2.86	0.53
1:C:539:TYR:CE1	1:D:232:LEU:HD21	2.43	0.53
1:A:281:LYS:HE3	5:A:790:HOH:O	2.09	0.53
1:C:287:HIS:CD2	1:C:290:LEU:H	2.27	0.53
1:C:569:LEU:HD13	1:D:307:LEU:HD11	1.90	0.53
1:D:270:MET:HE2	1:D:322:PHE:CZ	2.43	0.53
1:C:254:ILE:HD11	1:C:549:MET:HE1	1.91	0.52
1:A:109:ILE:CD1	1:A:152:VAL:HG13	2.38	0.52
1:A:395:ASN:ND2	5:A:809:HOH:O	2.30	0.52
1:B:214:PRO:HD2	1:B:236:LEU:HD11	1.91	0.52
1:A:263:PHE:CD2	1:A:314:ARG:HB3	2.45	0.52
1:B:476:HIS:CD2	1:B:478:SER:H	2.19	0.52
1:B:93:ASP:HB2	5:B:808:HOH:O	2.10	0.52
1:C:435:PRO:O	1:C:442:ARG:NH2	2.43	0.52
1:B:289:GLU:HB3	5:B:906:HOH:O	2.10	0.52
1:C:290:LEU:HD11	1:D:327:ILE:CD1	2.40	0.52
1:C:211:HIS:HE1	1:D:538:GLU:OE1	1.91	0.52
1:A:273:ILE:HG12	1:A:274:ILE:HG13	1.92	0.52
1:B:465:HIS:H	1:B:465:HIS:CD2	2.27	0.52
1:B:519:LYS:HE2	5:B:816:HOH:O	2.10	0.51
1:A:136:ARG:NE	5:A:737:HOH:O	2.42	0.51
1:A:266:ILE:HD13	1:A:307:LEU:CD1	2.40	0.51
1:A:504:ASP:OD2	1:A:507:ARG:NH1	2.44	0.51
1:D:165:SER:HB2	1:D:168:GLU:HB2	1.91	0.51
1:B:323:ARG:HG3	5:B:814:HOH:O	2.09	0.51
1:A:224:GLU:OE1	1:A:228:ARG:NE	2.31	0.51
1:A:437:PRO:HB2	1:A:439:THR:HG23	1.93	0.51
1:B:404:LEU:HB3	1:B:406:MET:HG2	1.93	0.51
1:C:538:GLU:OE1	1:D:211:HIS:HE1	1.93	0.51
1:A:289:GLU:HG2	5:B:762:HOH:O	2.11	0.51
1:A:347:TYR:CE1	1:A:484:GLU:HB3	2.47	0.50
1:A:435:PRO:O	1:A:442:ARG:NH2	2.41	0.50
1:A:503:ASN:HB3	1:A:541:LEU:HD23	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ARG:NH2	1:A:153:LYS:HE2	2.26	0.50
1:D:281:LYS:HD2	1:D:324:ASN:HB3	1.94	0.50
1:A:157:MET:CE	1:A:191:THR:CG2	2.82	0.50
1:B:109:ILE:HD12	1:B:152:VAL:CG1	2.41	0.50
1:C:232:LEU:HD21	1:D:539:TYR:CE1	2.47	0.50
1:C:476:HIS:HD2	1:C:479:LYS:H	1.58	0.50
1:C:476:HIS:CD2	1:C:479:LYS:H	2.29	0.50
1:D:84:ILE:HD13	1:D:210:LEU:CD2	2.42	0.50
1:B:465:HIS:HE1	1:B:487:GLU:OE1	1.95	0.50
1:A:100:HIS:O	1:A:127:LYS:HD3	2.11	0.50
1:A:347:TYR:CD1	1:A:484:GLU:HB3	2.47	0.50
1:A:152:VAL:HG13	1:A:153:LYS:N	2.25	0.49
1:B:374:HIS:O	1:B:562:ASN:ND2	2.36	0.49
1:B:323:ARG:CG	5:B:814:HOH:O	2.59	0.49
1:C:223:LYS:HG2	1:C:227:TYR:HE1	1.71	0.49
1:D:261:LEU:CD2	5:D:625:HOH:O	2.60	0.49
1:D:516:ALA:HB2	1:D:529:ILE:CD1	2.41	0.49
1:D:289:GLU:HB2	5:D:741:HOH:O	2.12	0.49
1:D:340:PHE:CD1	1:D:547:TRP:CE3	3.01	0.49
1:B:442:ARG:O	1:B:446:LYS:HG2	2.12	0.49
1:C:275:PRO:HB2	1:C:298:ILE:CD1	2.38	0.49
1:C:280:ALA:HB1	1:C:323:ARG:HG2	1.95	0.49
1:C:410:GLU:HG3	5:C:819:HOH:O	2.13	0.49
1:C:348:HIS:CD2	1:C:351:MET:CE	2.92	0.49
1:A:273:ILE:HD13	5:A:799:HOH:O	2.11	0.49
1:A:547:TRP:HZ2	1:A:549:MET:HE3	1.78	0.49
1:B:243:LYS:HZ2	1:B:566:GLU:HG2	1.76	0.49
1:D:261:LEU:HD21	5:D:701:HOH:O	2.12	0.49
1:A:164:LYS:NZ	5:A:820:HOH:O	2.40	0.49
1:B:152:VAL:CG1	1:B:153:LYS:N	2.75	0.48
1:B:243:LYS:NZ	1:B:566:GLU:HG2	2.28	0.48
1:D:373:TYR:HE1	1:D:383:TYR:HD1	1.58	0.48
1:D:400:LEU:O	1:D:404:LEU:HD23	2.13	0.48
1:C:538:GLU:HG2	1:D:210:LEU:HD12	1.95	0.48
1:D:491:MET:O	1:D:492:LYS:HB2	2.12	0.48
1:D:457:ILE:N	1:D:457:ILE:HD12	2.28	0.48
1:A:241:ARG:NH2	1:B:311:GLY:O	2.43	0.48
1:A:266:ILE:HD13	1:A:307:LEU:HD12	1.95	0.48
1:B:133:HIS:CG	5:B:811:HOH:O	2.66	0.48
1:B:393:ARG:NE	5:B:851:HOH:O	2.00	0.48
1:B:409:PRO:HG2	1:B:419:THR:HB	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:GLN:O	1:C:246[A]:ILE:HG23	2.14	0.48
1:C:288:ASN:HD22	1:D:324:ASN:HD21	1.61	0.48
1:C:288:ASN:ND2	1:D:324:ASN:HD21	2.12	0.48
1:B:503:ASN:HD22	1:B:503:ASN:N	2.08	0.48
1:D:223:LYS:HB3	1:D:227:TYR:CE2	2.49	0.48
1:D:245:ILE:O	1:D:249:LYS:HG3	2.13	0.48
1:D:270:MET:CE	1:D:322:PHE:CE1	2.97	0.47
1:B:249:LYS:HB3	1:B:365:ILE:HD12	1.95	0.47
1:C:246[A]:ILE:HD11	1:C:559:THR:HG23	1.95	0.47
1:D:109:ILE:CD1	1:D:152:VAL:HG13	2.44	0.47
1:D:340:PHE:CE1	1:D:547:TRP:CE3	3.02	0.47
1:A:73:PRO:HG3	1:A:212:MET:HE2	1.95	0.47
1:A:339:GLU:HA	1:A:547:TRP:O	2.15	0.47
1:C:440:THR:O	1:C:444:LEU:HB2	2.14	0.47
1:D:279:VAL:HG12	1:D:525:GLU:HB3	1.96	0.47
1:B:477:ARG:HG3	1:B:484:GLU:OE2	2.14	0.47
1:B:123:ASP:HB3	5:B:810:HOH:O	2.13	0.47
1:D:199:ILE:HA	1:D:200:PRO:HD3	1.74	0.47
1:D:375:PRO:HG3	1:D:383:TYR:CE1	2.48	0.47
1:A:109:ILE:HD12	1:A:152:VAL:HG11	1.97	0.47
1:A:385:VAL:HG22	1:A:457:ILE:HG22	1.97	0.47
1:D:541:LEU:HD12	1:D:542:PRO:HD2	1.95	0.47
1:A:231:TYR:O	1:A:235:ILE:HG13	2.15	0.47
1:A:290:LEU:HB3	1:A:292:MET:HE3	1.96	0.47
1:A:476:HIS:CD2	1:A:478:SER:H	2.29	0.47
1:D:221:LYS:HG3	1:D:222:ASP:N	2.29	0.47
1:C:133:HIS:O	1:C:178:ARG:HD2	2.14	0.46
1:D:415:GLU:HG3	5:D:786:HOH:O	2.15	0.46
1:A:306:MET:HA	1:A:309:VAL:HG13	1.96	0.46
1:A:394:ILE:HD11	1:A:462:ILE:HG12	1.98	0.46
1:B:127:LYS:HA	1:B:184:VAL:O	2.16	0.46
1:B:250:ILE:HD13	1:B:554:VAL:HG12	1.96	0.46
1:B:243:LYS:HZ2	1:B:566:GLU:CG	2.29	0.46
1:B:467:GLN:NE2	5:B:726:HOH:O	2.46	0.46
1:C:254:ILE:CD1	1:C:549:MET:HE1	2.46	0.46
1:B:396:MET:O	1:B:400:LEU:HB2	2.17	0.45
1:C:290:LEU:HD11	1:D:327:ILE:HD11	1.97	0.45
1:D:342:MET:HG3	1:D:345:ALA:HB3	1.98	0.45
1:D:516:ALA:HB2	1:D:529:ILE:HD12	1.98	0.45
1:A:157:MET:HE3	1:A:191:THR:CG2	2.45	0.45
1:C:385:VAL:HG13	1:C:458:ASN:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:402:LYS:HE2	5:C:858:HOH:O	2.16	0.45
1:D:404:LEU:HB3	1:D:406:MET:HG2	1.98	0.45
1:B:558:LEU:HD23	1:B:558:LEU:HA	1.71	0.45
1:C:266:ILE:HD13	1:C:307:LEU:CD1	2.46	0.45
1:C:516:ALA:HA	1:C:519:LYS:HE2	1.99	0.45
1:A:357:MET:HE1	1:A:547:TRP:CH2	2.51	0.45
1:B:547:TRP:CH2	1:B:549:MET:HB2	2.52	0.45
1:C:260:GLU:O	1:C:260:GLU:HG2	2.16	0.45
1:D:160:SER:HB3	1:D:169:PHE:CD2	2.52	0.45
1:D:485:ARG:HG2	1:D:498:ALA:O	2.17	0.45
1:C:421:LYS:HB3	1:C:421:LYS:HE2	1.54	0.45
1:B:132:ILE:HD12	1:B:180:ASP:HB2	1.97	0.45
1:B:74:ASN:OD1	1:B:78:LYS:HE2	2.17	0.45
1:B:384:ASP:C	1:B:384:ASP:OD1	2.55	0.45
1:C:132:ILE:HD12	1:C:180:ASP:HB2	1.99	0.45
1:D:512:PHE:HB3	1:D:529:ILE:HG13	1.99	0.45
1:A:109:ILE:CD1	1:A:152:VAL:CG1	2.95	0.44
1:A:273:ILE:HD11	5:A:708:HOH:O	2.16	0.44
1:B:342:MET:HG3	1:B:345:ALA:HB3	1.99	0.44
1:D:95:TYR:CE2	1:D:208:PRO:HD2	2.53	0.44
1:A:113:SER:O	1:A:190:LYS:NZ	2.50	0.44
1:C:363:LYS:HD2	1:C:368:SER:HA	1.99	0.44
1:D:123:ASP:HB2	5:D:784:HOH:O	2.16	0.44
1:A:220:LEU:HD22	1:A:221:LYS:HD3	1.98	0.44
1:D:476:HIS:CD2	1:D:479:LYS:H	2.35	0.44
1:D:314:ARG:CZ	1:D:342:MET:HE3	2.47	0.44
1:B:363:LYS:HD3	1:B:369:TYR:CE1	2.53	0.44
1:C:485:ARG:HA	1:C:499:TYR:HB3	1.99	0.44
1:A:111:LYS:HD3	1:A:112:TYR:CZ	2.53	0.43
1:A:337:THR:HA	1:A:549:MET:O	2.18	0.43
1:A:385:VAL:HG13	1:A:458:ASN:HA	2.00	0.43
1:A:574:LYS:HE3	1:B:290:LEU:HD21	2.00	0.43
1:B:343:ALA:HA	1:B:544:THR:HB	2.00	0.43
1:B:444:LEU:HD11	1:B:466:PRO:HG2	1.99	0.43
1:C:325:GLU:HG3	5:C:802:HOH:O	2.17	0.43
1:C:394:ILE:HB	1:C:399:GLU:CG	2.46	0.43
1:A:109:ILE:HD12	1:A:152:VAL:CG1	2.48	0.43
1:C:184:VAL:HG13	1:C:200:PRO:HB3	1.99	0.43
1:C:325:GLU:O	1:D:287:HIS:HE1	2.01	0.43
1:D:93:ASP:HA	1:D:94:PRO:HD2	1.89	0.43
1:A:470:SER:HB2	1:A:483:THR:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:PRO:HD3	1:B:295:TYR:CD1	2.53	0.43
1:C:270:MET:CE	5:C:727:HOH:O	2.63	0.43
1:C:394:ILE:CB	1:C:399:GLU:HG3	2.46	0.43
1:C:301:GLU:OE1	3:C:601:LYS:N	2.51	0.43
1:C:554:VAL:HA	1:C:557:PHE:CE2	2.53	0.43
1:A:491:MET:SD	1:A:557:PHE:HB2	2.58	0.43
1:B:266:ILE:HD13	1:B:307:LEU:HD23	2.00	0.43
1:C:396:MET:HE3	1:C:448:VAL:HG21	1.99	0.43
1:D:358:VAL:O	1:D:362:VAL:HG23	2.19	0.43
1:A:325:GLU:O	1:B:287:HIS:HE1	2.02	0.43
1:A:519:LYS:HD3	5:A:856:HOH:O	2.18	0.43
1:B:120:HIS:CE1	1:B:122:THR:HG22	2.53	0.43
1:C:100:HIS:O	1:C:127:LYS:HD2	2.19	0.43
1:C:254:ILE:CD1	1:C:549:MET:CE	2.96	0.43
1:C:340:PHE:CE1	1:C:547:TRP:CE3	3.07	0.43
1:D:86:GLN:HA	1:D:89:VAL:HG22	2.01	0.43
1:D:503:ASN:HB3	1:D:541:LEU:HD23	2.01	0.43
1:B:207:SER:HA	1:B:208:PRO:HD2	1.91	0.43
1:A:224:GLU:O	1:A:228:ARG:HG3	2.19	0.43
1:B:156:VAL:CG1	1:B:200:PRO:HG3	2.49	0.43
1:C:425:ASP:HB2	5:C:737:HOH:O	2.19	0.43
1:C:491:MET:SD	1:C:557:PHE:HB2	2.59	0.43
1:D:270:MET:CE	1:D:322:PHE:HE1	2.32	0.43
1:B:109:ILE:CD1	1:B:152:VAL:CG1	2.97	0.42
1:B:479:LYS:HD2	1:B:482:LEU:HD12	2.00	0.42
1:C:484:GLU:HB3	1:C:500:THR:CG2	2.49	0.42
1:D:373:TYR:CZ	1:D:491:MET:HB3	2.52	0.42
1:D:485:ARG:CG	1:D:499:TYR:HB3	2.48	0.42
1:A:476:HIS:CD2	1:A:479:LYS:H	2.38	0.42
1:B:440:THR:O	1:B:444:LEU:HB2	2.18	0.42
1:B:477:ARG:HG3	1:B:477:ARG:H	1.70	0.42
1:C:181:ILE:HG21	1:D:542:PRO:HB3	2.00	0.42
1:D:110:GLN:HG2	5:D:737:HOH:O	2.19	0.42
1:D:340:PHE:CE1	1:D:547:TRP:CD2	3.08	0.42
1:A:159:ASN:ND2	1:A:161:ARG:CG	2.80	0.42
1:A:410[A]:GLU:HG3	5:A:705:HOH:O	2.18	0.42
1:C:72:ASP:HA	1:C:73:PRO:HD2	1.82	0.42
1:C:361:MET:O	1:C:365:ILE:HG23	2.19	0.42
1:C:76:TYR:HB2	1:C:212:MET:HE3	2.01	0.42
1:C:340:PHE:CD1	1:C:547:TRP:CE3	3.08	0.42
1:C:381:GLN:OE1	1:C:383:TYR:CE1	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:ASP:HB2	5:B:842:HOH:O	2.20	0.42
1:A:538:GLU:OE1	1:B:211:HIS:CE1	2.67	0.42
1:C:211:HIS:CE1	1:D:538:GLU:OE1	2.73	0.41
1:D:109:ILE:HD12	1:D:152:VAL:CG1	2.49	0.41
1:C:348:HIS:CD2	1:C:351:MET:HE1	2.54	0.41
1:D:121:LEU:O	1:D:187:ASN:HB3	2.21	0.41
1:B:450:GLU:O	1:B:450:GLU:HG3	2.19	0.41
1:A:350:LEU:HD22	1:A:545:ALA:CB	2.49	0.41
1:C:465:HIS:HB2	1:C:485:ARG:HD3	2.03	0.41
1:C:516:ALA:HB2	1:C:529:ILE:HG13	2.03	0.41
1:D:287:HIS:CD2	1:D:290:LEU:HD12	2.55	0.41
1:D:381:GLN:HB3	5:D:736:HOH:O	2.20	0.41
1:B:400:LEU:HD23	1:B:400:LEU:HA	1.90	0.41
1:B:557:PHE:C	1:B:557:PHE:CD2	2.94	0.41
1:D:350:LEU:HD11	1:D:545:ALA:HB1	2.02	0.41
1:B:338:CYS:O	1:B:548:GLY:HA2	2.21	0.41
1:C:415:GLU:HG2	1:C:468:ILE:HD12	2.03	0.41
1:D:146:ASP:OD2	1:D:148:ARG:NH2	2.48	0.41
1:D:423:LEU:HD12	1:D:440:THR:HG23	2.02	0.41
1:D:491:MET:SD	1:D:557:PHE:HB2	2.61	0.41
1:B:86:GLN:HA	1:B:89:VAL:HG22	2.03	0.40
1:B:273:ILE:HD13	1:B:294:LEU:HD12	2.02	0.40
1:D:72:ASP:HB3	1:D:75:GLN:HB2	2.03	0.40
1:A:306:MET:O	1:B:231:TYR:HB3	2.21	0.40
1:B:503:ASN:HB3	1:B:541:LEU:HD23	2.04	0.40
1:A:121:LEU:O	1:A:187:ASN:HB3	2.21	0.40
1:A:552:ASP:O	1:A:556:MET:HG3	2.21	0.40
1:B:144:PHE:CE2	1:B:157:MET:HG3	2.57	0.40
1:B:254:ILE:HD11	1:B:549:MET:CE	2.51	0.40
1:B:164:LYS:HG2	1:B:201:TYR:CZ	2.56	0.40
1:B:251:ILE:HD11	1:B:551:ILE:HG21	2.04	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	500/521 (96%)	491 (98%)	9 (2%)	0	100	100
1	B	494/521 (95%)	476 (96%)	17 (3%)	1 (0%)	47	58
1	C	498/521 (96%)	489 (98%)	9 (2%)	0	100	100
1	D	496/521 (95%)	480 (97%)	16 (3%)	0	100	100
All	All	1988/2084 (95%)	1936 (97%)	51 (3%)	1 (0%)	51	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	367	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	446/463 (96%)	419 (94%)	27 (6%)	18	25
1	B	441/463 (95%)	416 (94%)	25 (6%)	20	28
1	C	444/463 (96%)	418 (94%)	26 (6%)	19	26
1	D	443/463 (96%)	414 (94%)	29 (6%)	17	22
All	All	1774/1852 (96%)	1667 (94%)	107 (6%)	19	26

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	ASP
1	A	78	LYS
1	A	105	LEU
1	A	111	LYS
1	A	123	ASP
1	A	142	LEU
1	A	147	LEU

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Mol	Chain	Res	Type
1	A	152	VAL
1	A	172	ILE
1	A	192	LYS
1	A	196	LEU
1	A	220	LEU
1	A	221	LYS
1	A	258	LEU
1	A	273	ILE
1	A	309	VAL
1	A	347	TYR
1	A	356	LYS
1	A	366	THR
1	A	393	ARG
1	A	400	LEU
1	A	406	MET
1	A	421	LYS
1	A	479	LYS
1	A	557	PHE
1	A	573	MET
1	A	576	GLU
1	B	82	GLN
1	B	105	LEU
1	B	124	ILE
1	B	125	THR
1	B	224	GLU
1	B	248	SER
1	B	294	LEU
1	B	307	LEU
1	B	320	ARG
1	B	347	TYR
1	B	379	GLU
1	B	381	GLN
1	B	384	ASP
1	B	394	ILE
1	B	400	LEU
1	B	419	THR
1	B	444	LEU
1	B	450	GLU
1	B	477	ARG
1	B	503	ASN
1	B	506	MET
1	B	532	ASN

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Mol	Chain	Res	Type
1	B	544	THR
1	B	552	ASP
1	B	557	PHE
1	C	80	ARG
1	C	84	ILE
1	C	88	LYS
1	C	123	ASP
1	C	125	THR
1	C	138	SER
1	C	141	LYS
1	C	152	VAL
1	C	154	LEU
1	C	172	ILE
1	C	220	LEU
1	C	224	GLU
1	C	246[A]	ILE
1	C	246[B]	ILE
1	C	285	THR
1	C	324	ASN
1	C	347	TYR
1	C	365	ILE
1	C	384	ASP
1	C	404	LEU
1	C	420	ARG
1	C	421	LYS
1	C	480	GLU
1	C	500	THR
1	C	552	ASP
1	C	557	PHE
1	D	110	GLN
1	D	124	ILE
1	D	147	LEU
1	D	152	VAL
1	D	159	ASN
1	D	193	LYS
1	D	222	ASP
1	D	224	GLU
1	D	261	LEU
1	D	273	ILE
1	D	281	LYS
1	D	288	ASN
1	D	323	ARG

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Mol	Chain	Res	Type
1	D	347	TYR
1	D	352	GLU
1	D	353	ILE
1	D	373	TYR
1	D	407	LYS
1	D	430	LYS
1	D	468	ILE
1	D	470	SER
1	D	477	ARG
1	D	485	ARG
1	D	488	LEU
1	D	506	MET
1	D	531	GLU
1	D	552	ASP
1	D	557	PHE
1	D	569	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	120	HIS
1	A	155	GLN
1	A	159	ASN
1	A	187	ASN
1	A	272	ASN
1	A	287	HIS
1	A	412	ASN
1	A	476	HIS
1	B	82	GLN
1	B	85	HIS
1	B	116	GLN
1	B	133	HIS
1	B	211	HIS
1	B	293	ASN
1	B	321	GLN
1	B	465	HIS
1	B	467	GLN
1	B	476	HIS
1	B	503	ASN
1	B	515	GLN
1	C	86	GLN

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Mol	Chain	Res	Type
1	C	120	HIS
1	C	159	ASN
1	C	162	ASN
1	C	185	GLN
1	C	211	HIS
1	C	272	ASN
1	C	287	HIS
1	C	288	ASN
1	C	321	GLN
1	C	324	ASN
1	C	348	HIS
1	C	467	GLN
1	C	476	HIS
1	D	97	HIS
1	D	110	GLN
1	D	162	ASN
1	D	211	HIS
1	D	229	GLN
1	D	272	ASN
1	D	287	HIS
1	D	412	ASN
1	D	476	HIS
1	D	515	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 12 are monoatomic - leaving 8 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	603	2	26,33,33	1.06	2 (7%)	31,52,52	1.49	5 (16%)
3	LYS	D	601	-	5,9,9	0.36	0	4,10,10	0.44	0
3	LYS	C	601	-	5,9,9	0.77	0	4,10,10	0.46	0
4	ATP	C	603	2	26,33,33	1.11	2 (7%)	31,52,52	1.47	4 (12%)
3	LYS	B	601	-	5,9,9	0.33	0	4,10,10	0.45	0
4	ATP	D	603	2	26,33,33	1.03	3 (11%)	31,52,52	1.49	4 (12%)
3	LYS	A	601	-	5,9,9	0.80	0	4,10,10	0.35	0
4	ATP	B	603	2	26,33,33	1.09	2 (7%)	31,52,52	1.56	7 (22%)

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	603	2	-	4/18/38/38	0/3/3/3
3	LYS	D	601	-	-	1/5/9/9	-
3	LYS	C	601	-	-	0/5/9/9	-
4	ATP	C	603	2	-	4/18/38/38	0/3/3/3
3	LYS	B	601	-	-	1/5/9/9	-
4	ATP	D	603	2	-	3/18/38/38	0/3/3/3
3	LYS	A	601	-	-	0/5/9/9	-
4	ATP	B	603	2	-	4/18/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	603	ATP	O4'-C1'	3.26	1.45	1.41
4	D	603	ATP	O4'-C1'	2.60	1.44	1.41
4	C	603	ATP	C5-C4	2.58	1.47	1.40
4	B	603	ATP	C2-N3	2.46	1.36	1.32
4	C	603	ATP	O4'-C1'	2.38	1.44	1.41
4	B	603	ATP	C5-C4	2.32	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	603	ATP	C5-C4	2.21	1.46	1.40
4	D	603	ATP	C5-C4	2.20	1.46	1.40
4	D	603	ATP	C2-N3	2.07	1.35	1.32

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	603	ATP	N3-C2-N1	-4.57	121.54	128.68
4	A	603	ATP	N3-C2-N1	-3.50	123.21	128.68
4	B	603	ATP	N3-C2-N1	-3.46	123.28	128.68
4	C	603	ATP	N3-C2-N1	-3.27	123.56	128.68
4	B	603	ATP	C4-C5-N7	-3.08	106.19	109.40
4	A	603	ATP	C3'-C2'-C1'	2.96	105.44	100.98
4	B	603	ATP	C3'-C2'-C1'	2.83	105.23	100.98
4	C	603	ATP	C3'-C2'-C1'	2.82	105.23	100.98
4	A	603	ATP	C2-N1-C6	2.74	123.44	118.75
4	C	603	ATP	C2-N1-C6	2.64	123.27	118.75
4	D	603	ATP	C1'-N9-C4	-2.53	122.19	126.64
4	A	603	ATP	C4-C5-N7	-2.37	106.92	109.40
4	B	603	ATP	PB-O3B-PG	-2.31	124.91	132.83
4	B	603	ATP	C1'-N9-C4	-2.23	122.73	126.64
4	D	603	ATP	C2-N1-C6	2.23	122.56	118.75
4	D	603	ATP	PB-O3B-PG	-2.22	125.21	132.83
4	C	603	ATP	PB-O3B-PG	-2.10	125.61	132.83
4	B	603	ATP	C2-N1-C6	2.09	122.33	118.75
4	A	603	ATP	O2A-PA-O1A	2.08	122.54	112.24
4	B	603	ATP	O2'-C2'-C1'	-2.01	103.45	110.85

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	603	ATP	C5'-O5'-PA-O1A
4	B	603	ATP	C5'-O5'-PA-O1A
4	C	603	ATP	C5'-O5'-PA-O1A
4	D	603	ATP	C5'-O5'-PA-O1A
4	C	603	ATP	C4'-C5'-O5'-PA
4	D	603	ATP	C4'-C5'-O5'-PA
3	D	601	LYS	CG-CD-CE-NZ
4	B	603	ATP	C5'-O5'-PA-O3A
4	D	603	ATP	C5'-O5'-PA-O3A
4	A	603	ATP	C5'-O5'-PA-O2A

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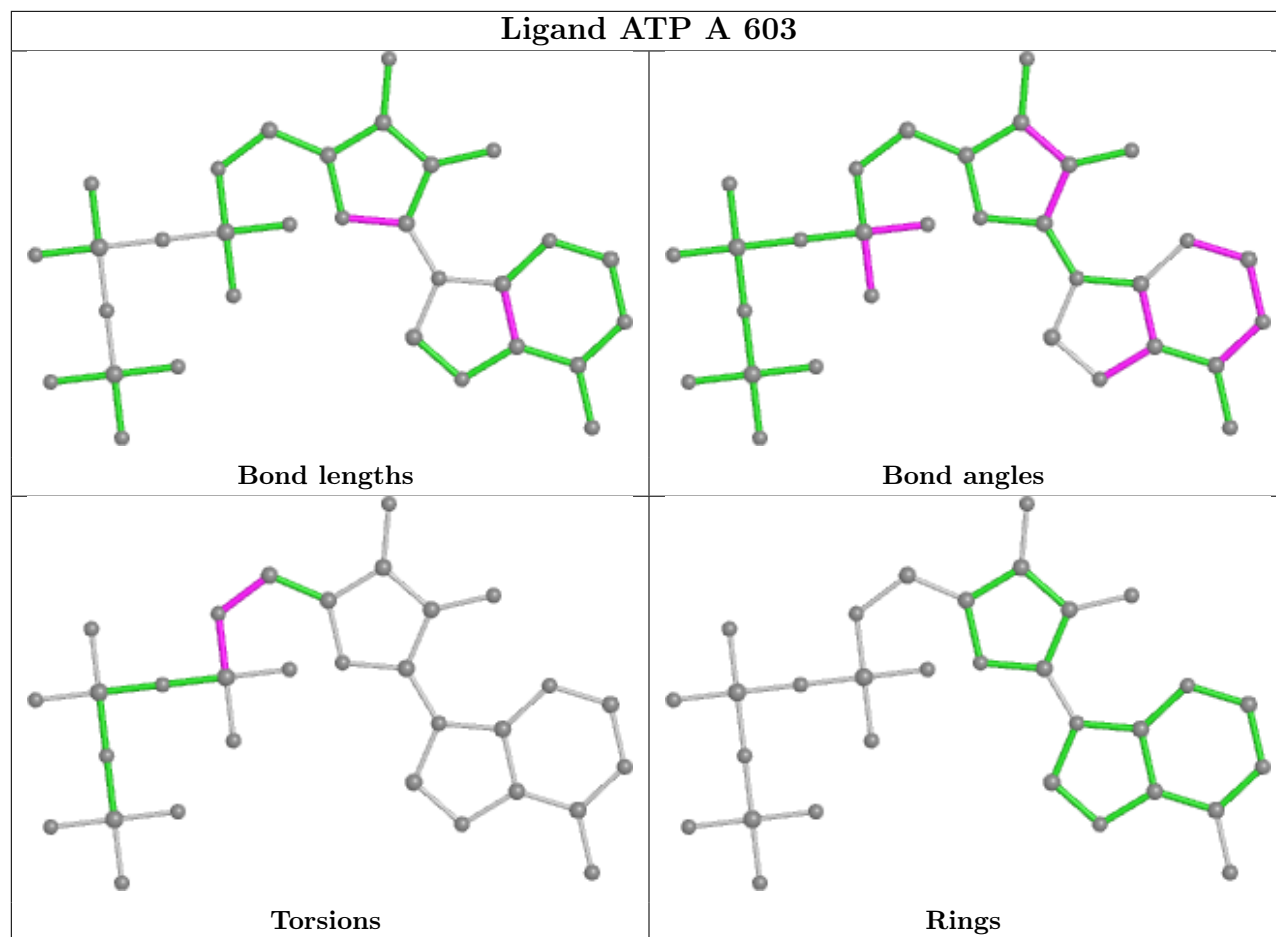
Mol	Chain	Res	Type	Atoms
4	B	603	ATP	C5'-O5'-PA-O2A
4	C	603	ATP	C5'-O5'-PA-O2A
4	A	603	ATP	C4'-C5'-O5'-PA
4	B	603	ATP	C4'-C5'-O5'-PA
4	A	603	ATP	C5'-O5'-PA-O3A
4	C	603	ATP	C5'-O5'-PA-O3A
3	B	601	LYS	CG-CD-CE-NZ

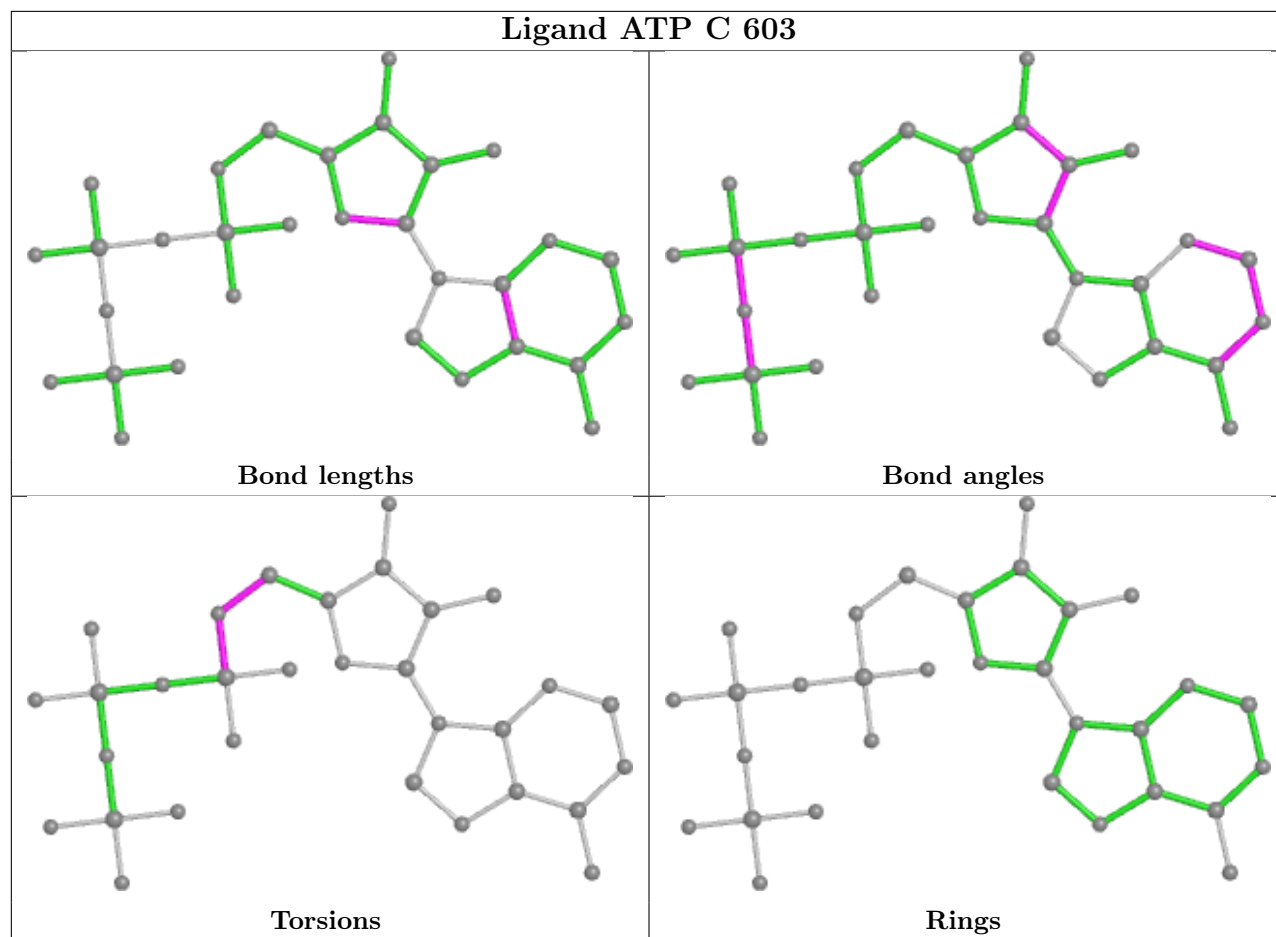
There are no ring outliers.

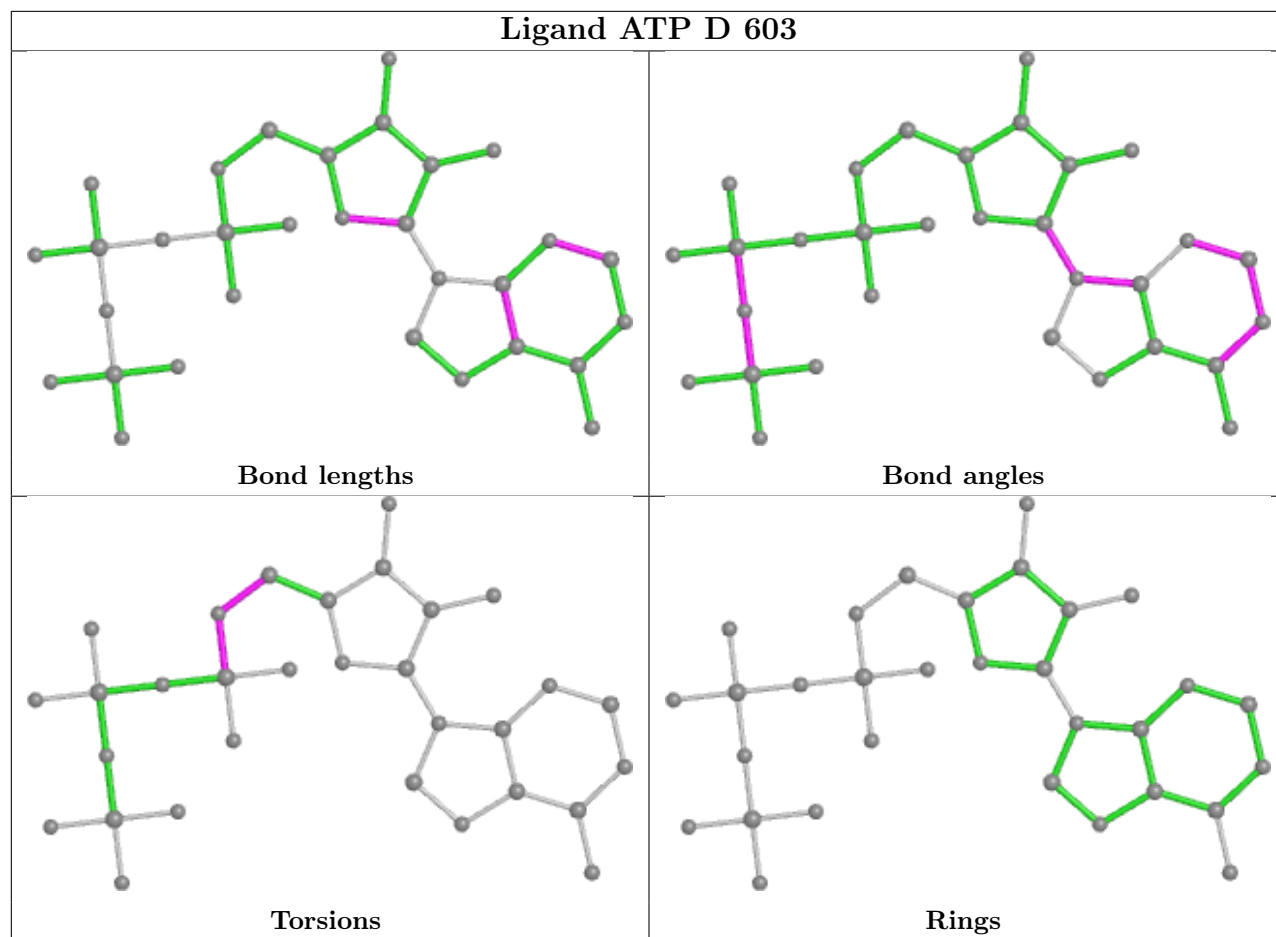
1 monomer is involved in 1 short contact:

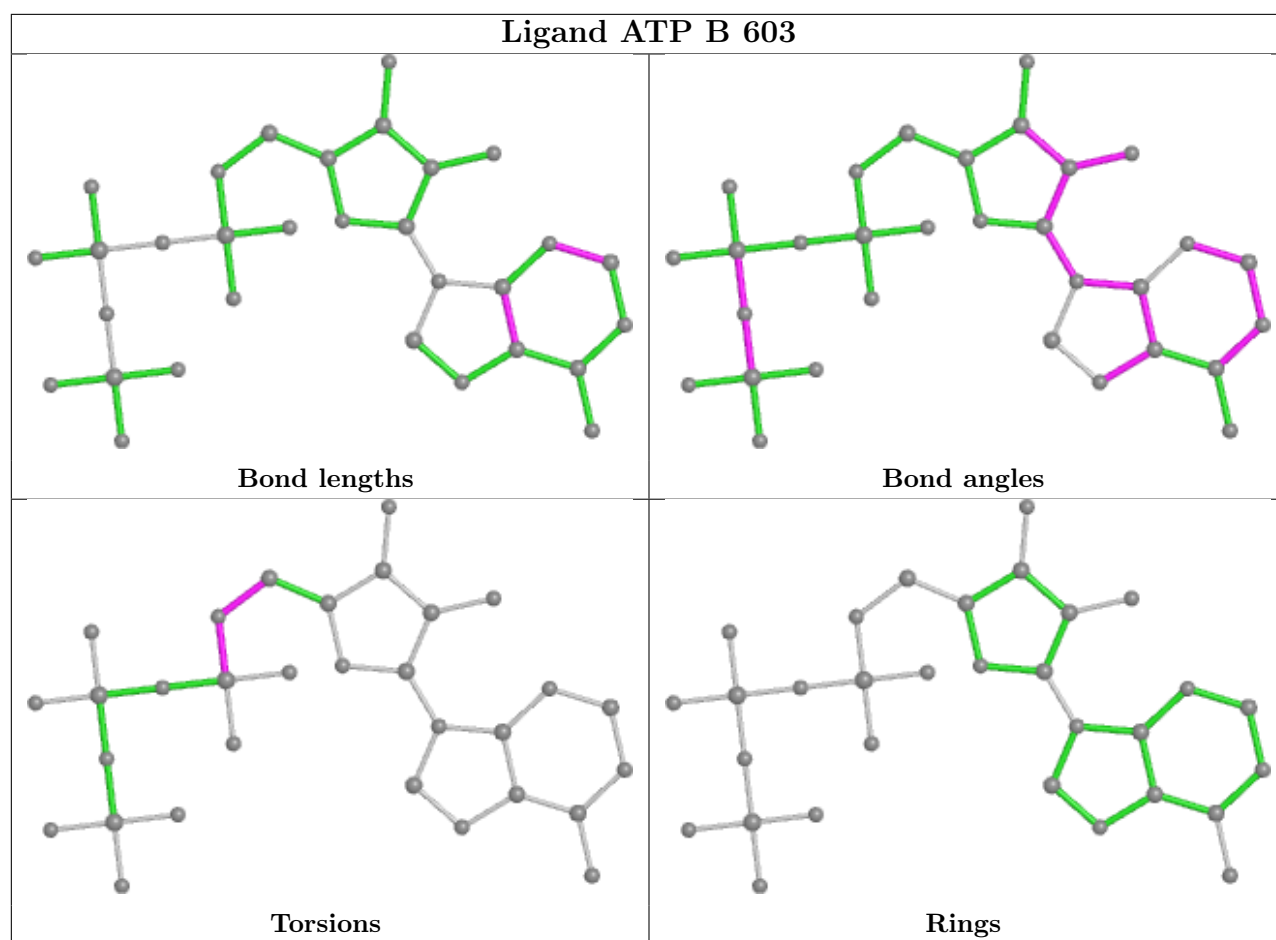
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	601	LYS	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	503/521 (96%)	-0.44	1 (0%) 95 97	14, 25, 42, 55	0
1	B	495/521 (95%)	-0.36	1 (0%) 95 97	16, 30, 47, 66	0
1	C	501/521 (96%)	-0.45	0 100 100	14, 25, 42, 53	0
1	D	499/521 (95%)	-0.33	1 (0%) 95 97	14, 30, 47, 65	0
All	All	1998/2084 (95%)	-0.40	3 (0%) 95 97	14, 27, 46, 66	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	383	TYR	2.5
1	B	381	GLN	2.3
1	A	383	TYR	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 monosaccharides in this entry.

6.4 Ligands [i](#)

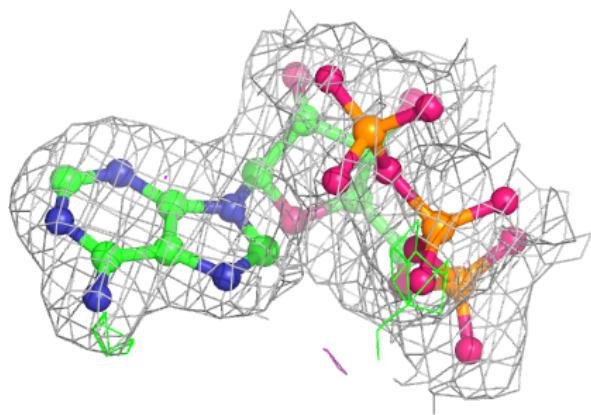
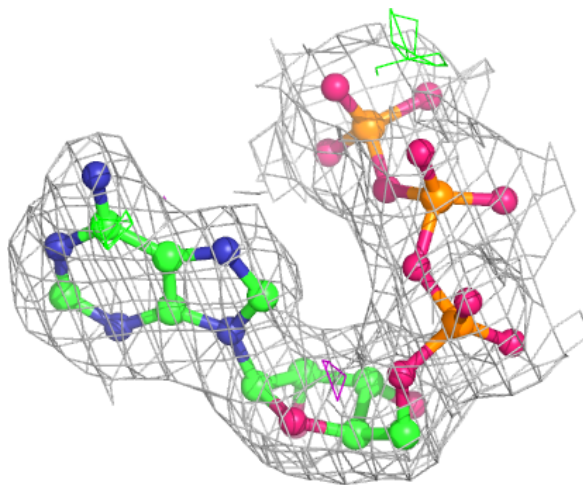
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	LYS	B	601	10/10	0.91	0.16	25,28,29,30	0
3	LYS	A	601	10/10	0.93	0.12	23,27,29,29	0
3	LYS	C	601	10/10	0.93	0.14	26,29,31,31	0
3	LYS	D	601	10/10	0.94	0.14	18,25,27,28	0
2	CA	C	607	1/1	0.96	0.13	26,26,26,26	0
2	CA	D	606	1/1	0.96	0.12	25,25,25,25	0
2	CA	C	608	1/1	0.97	0.13	23,23,23,23	0
2	CA	B	607	1/1	0.98	0.07	30,30,30,30	0
2	CA	A	607	1/1	0.98	0.13	30,30,30,30	0
4	ATP	A	603	31/31	0.98	0.11	14,16,24,25	0
4	ATP	B	603	31/31	0.98	0.10	17,21,24,24	0
2	CA	C	606	1/1	0.99	0.08	22,22,22,22	0
2	CA	D	607	1/1	0.99	0.18	28,28,28,28	0
2	CA	A	606	1/1	0.99	0.12	22,22,22,22	0
2	CA	B	608	1/1	0.99	0.08	26,26,26,26	0
4	ATP	C	603	31/31	0.99	0.09	14,18,23,23	0
4	ATP	D	603	31/31	0.99	0.11	19,21,25,26	0
2	CA	D	608	1/1	1.00	0.07	24,24,24,24	0
2	CA	B	606	1/1	1.00	0.11	22,22,22,22	0
2	CA	A	608	1/1	1.00	0.08	22,22,22,22	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.

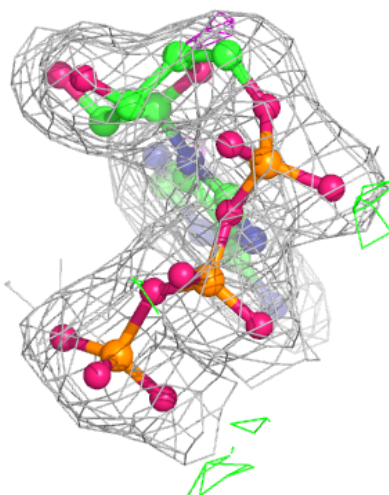
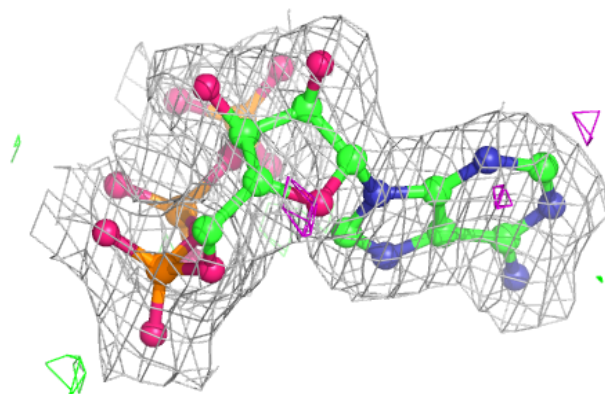
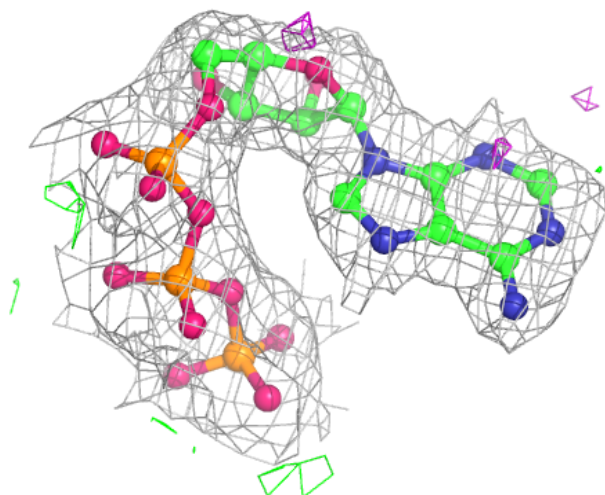
Electron density around ATP A 603:

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



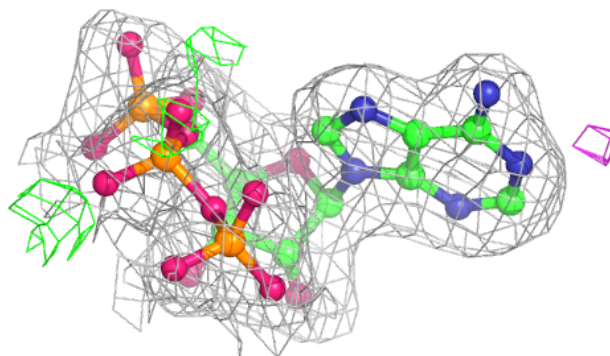
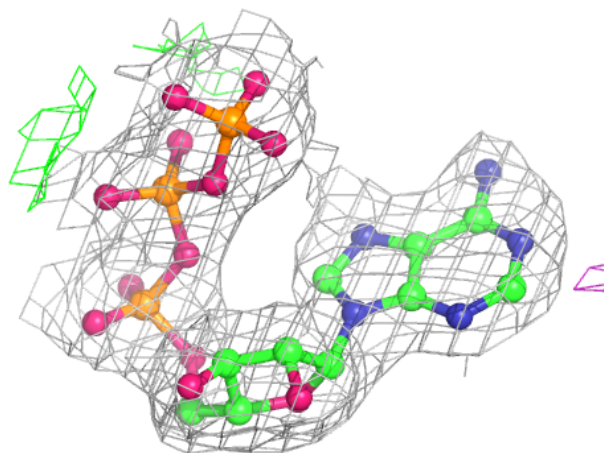
Electron density around ATP B 603:

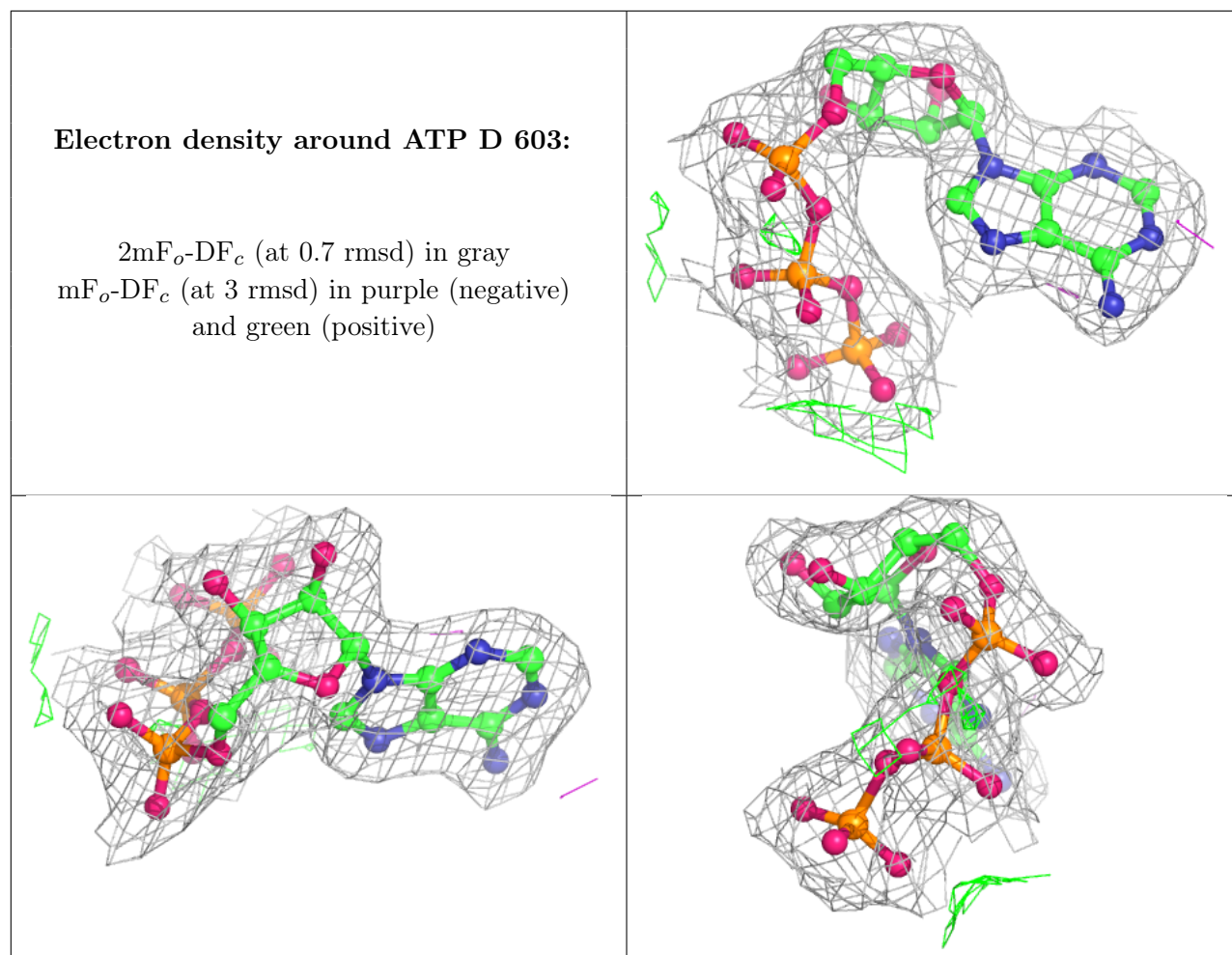
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ATP C 603:

$2mF_o-DF_c$ (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.