W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2024 – 11:53 AM EST

PDB ID	:	3LCB
Title	:	The crystal structure of isocitrate dehydrogenase kinase/phosphatase in complex with its substrate, isocitrate dehydrogenase, from Escherichia coli.
Authors	:	Zheng, J.; Jia, Z.
Deposited on	:	2010-01-10
Resolution	:	2.90 Å(reported)

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

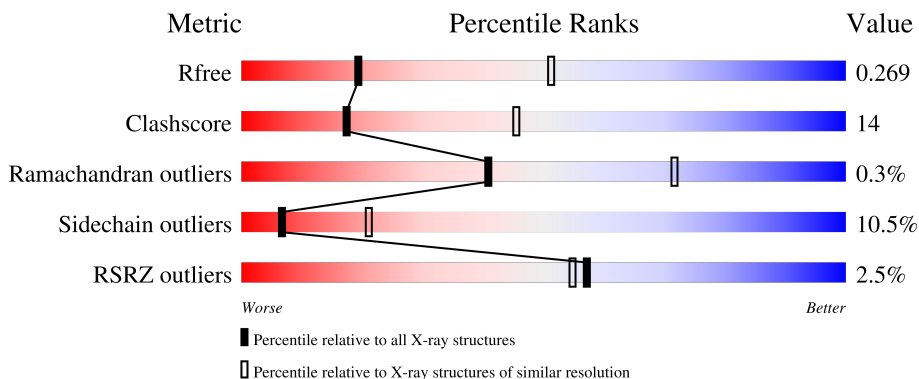|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	Percentile Ranks	Value
Rfree		0.269
Clashscore		14
Ramachandran outliers		0.3%
Sidechain outliers		10.5%
RSRZ outliers		2.5%

Worse .... *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 <=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	578	3% / 68% 22% 5% •
1	B	578	3% / 64% 28% 6% •
2	C	416	% / 81% 17% •
2	D	416	2% / 78% 18% •

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
4	ATP	B	1761	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 15771 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 Isocitrate dehydrogenase kinase/phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	554	Total	C	N	O	S	0	0	0
			4578	2947	799	811	21			
1	B	561	Total	C	N	O	S	0	0	0
			4652	2993	815	823	21			

- Molecule 2 is a protein called Isocitrate dehydrogenase [NADP].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	415	Total	C	N	O	S	0	0	0
			3205	2040	539	608	18			
2	D	415	Total	C	N	O	S	0	0	0
			3205	2040	539	608	18			

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).
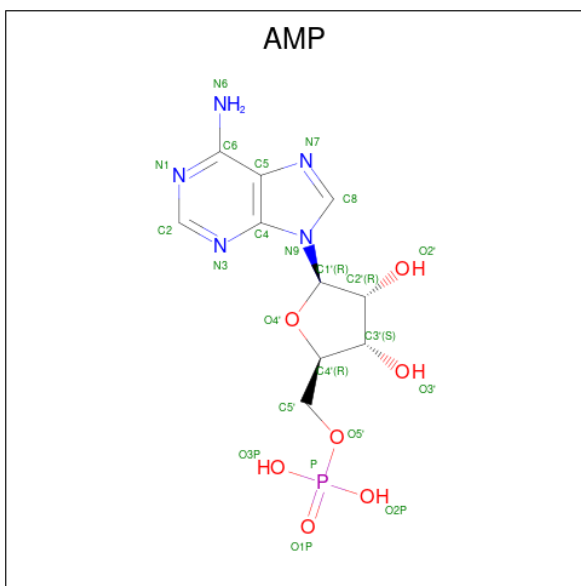
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	B	1	Total 23	C 10	N 5	O 7	P 1	0	0

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).
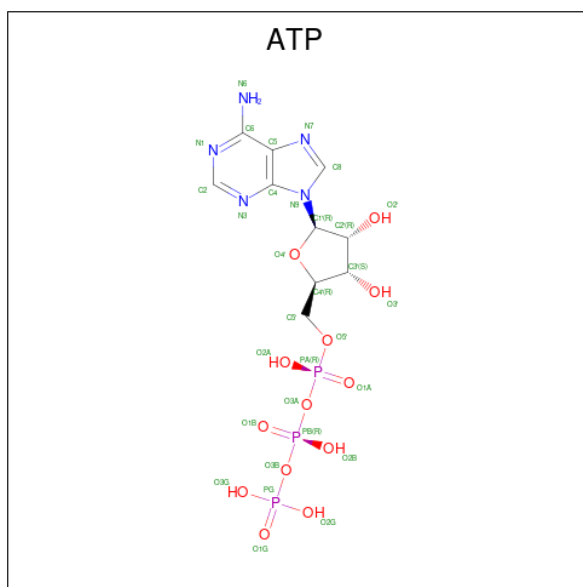
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
4	B	1	Total 31	C 10	N 5	O 13	P 3	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Mg 1	0	0
5	B	1	Total 1	Mg 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	5	Total 5	O 5	0	0
6	C	5	Total 5	O 5	0	0
6	D	8	Total 8	O 8	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second g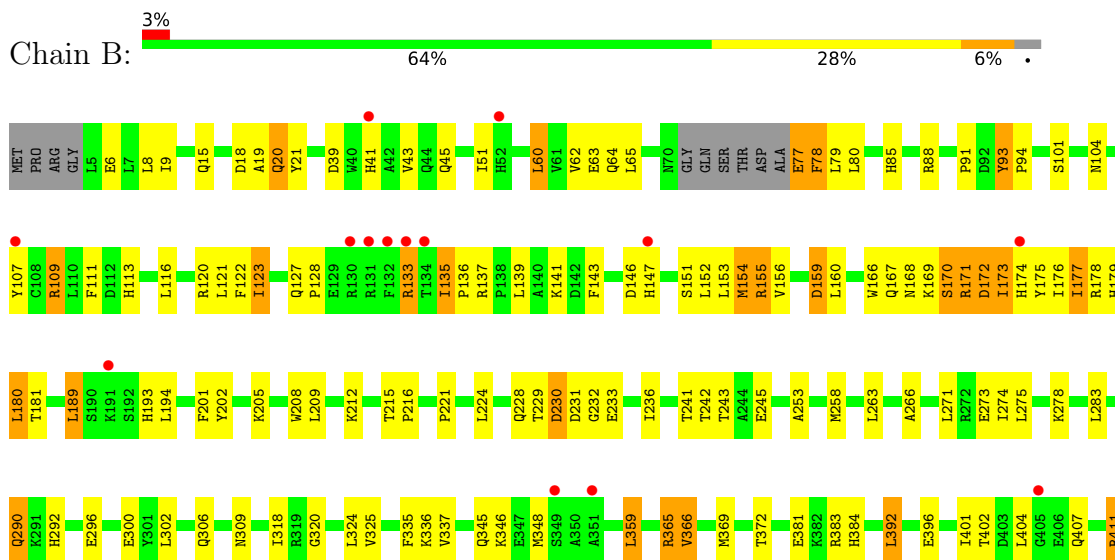raphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a 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: Isocitrate dehydrogenase kinase/phosphatase

• Molecule 1: Isocitrate dehydrogenase kinase/phosphatase

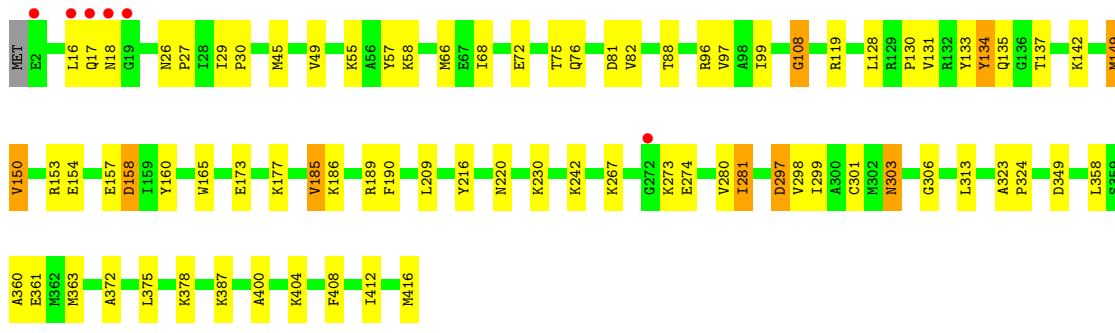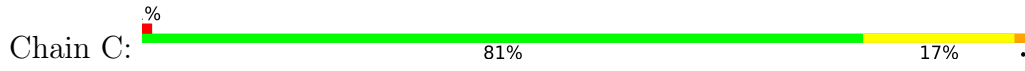H412 L413 R417 V420 P421 L422 N423 I424 W425 L426 E427 Q428 V429 E430 G431 Q432 R435 D436 A437 I438 E439 E440 Y441 G442 I445 I453 G456 D457 M458 L459 F460 K461 N462 V465 T466 R467 H468 Y474 I479 V485 R488 D489 R494 D498 W505

V508 S509 H520 W521 L522 D525 I528 L531 E534 M535 H536 A537 D538 D543 Q549 H556 D559 R565 R566 Q567 R568 F569 S570 V571 ARG TYR GLY MET LEU PHE

• Molecule 2: Isocitrate dehydrogenase [NADP]

Chain C:

%

81% 17% •

MET E2 L16 Q17 N18 G19 N26 P27 I28 I29 P30 M45 V49 K55 A56 Y57 K58 M66 E67 I68 E72 T75 Q76 D81 V82 T88 R96 V97 A98 I99 G108 R119 L128 R129 P130 V131 R132 Y133 Y134 Q135 G136 T137 K142 M149

V150 R153 E154 E157 D158 I159 Y160 W165 E173 K177 V185 K186 R189 F190 L209 Y216 N220 K230 K242 K267 G272 K273 E274 V280 I281 D297 V298 I299 A300 C301 M302 N303 G306 L313 A323 P324 D349 L358 S359

A360 E361 M362 M363 A372 L375 K378 K387 A400 K404 F408 I412 M416

• Molecule 2: Isocitrate dehydrogenase [NADP]

Chain D:

2%

78% 18% •

MET E2 S3 K4 V5 V6 A9 Q10 G11 K12 K13 L16 Q17 N18 N26 P30 I37 E54 K58 G59 E60 M66 E67 I68 E72 T75 Q76 V77 Y78 W83 E87 T88 L91 E94 Y95 R96 V97 K100 T105 P106 I111 R112 S113

L114 N115 V116 A117 Q120 E121 I126 R129 Y133 S139 P144 I159 S169 A170 D171 K174 V175 I176 K177 F178 L179 R180 E181 E182 K199 E203 K207 R211 K230 M234 E238 K242 E256 D259 G260 G261 P262 W263 K267 N268

P269 Y296 D297 V298 N327 E331 E336 V351 I357 A360 E361 M362 R365 T370 M380 I384 N385 T388 E394 R395 L403 G409 I412 M416

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	196.80Å 196.80Å 156.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.90 29.78 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.2 (30.00-2.90) 99.3 (29.78-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.72 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.190 , 0.222 0.233 , 0.269	Depositor DCC
R_{free} test set	3809 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	74.7	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 34.5	EDS
L-test for twinning[2]	$< |L| > = 0.55$, $< L^2 > = 0.40$	Xtriage
Estimated twinning fraction	0.000 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.698 for H, K, L 0.302 for K, H, -L	Depositor
Outliers	1 of 75577 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	15771	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, AMP

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	0.48	1/4702 (0.0%)	0.58	2/6371 (0.0%)
1	B	0.49	0/4779	0.61	2/6477 (0.0%)
2	C	0.58	2/3266 (0.1%)	0.62	3/4417 (0.1%)
2	D	0.47	1/3266 (0.0%)	0.54	0/4417
All	All	0.51	4/16013 (0.0%)	0.59	7/21682 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	298	VAL	CB-CG1	-5.40	1.41	1.52
2	C	134	TYR	CD1-CE1	-5.38	1.31	1.39
1	A	560	VAL	CB-CG1	-5.03	1.42	1.52
2	D	296	TYR	CD1-CE1	-5.01	1.31	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	150	VAL	N-CA-C	-7.57	90.56	111.00
1	B	232	GLY	N-CA-C	7.54	131.96	113.10
1	A	189	LEU	CA-CB-CG	6.78	130.89	115.30
1	B	230	ASP	N-CA-C	-6.25	94.14	111.00
2	C	149	MET	N-CA-C	-6.12	94.49	111.00
2	C	185	VAL	N-CA-C	5.72	126.44	111.00
1	A	89	LEU	CA-CB-CG	5.63	128.26	115.30

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	4578	0	4486	138	0
1	B	4652	0	4564	193	0
2	C	3205	0	3228	49	0
2	D	3205	0	3228	59	0
3	A	23	0	12	0	0
3	B	23	0	12	2	0
4	A	31	0	12	6	0
4	B	31	0	12	12	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	3	0	0	0	0
6	B	5	0	0	0	0
6	C	5	0	0	0	0
6	D	8	0	0	1	0
All	All	15771	0	15554	431	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (431) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:LEU:C	1:B:155:ARG:HE	1.49	1.16
1:A:411:ARG:HG3	1:A:411:ARG:HH11	1.08	1.11
2:D:106:PRO:HB3	2:D:111:ILE:HD11	1.20	1.11
1:B:171:ARG:HG2	1:B:171:ARG:HH11	1.04	1.09
1:B:230:ASP:O	1:B:231:ASP:HB2	1.53	1.09
1:A:120:ARG:NH1	1:A:120:ARG:H	1.51	1.07
1:B:153:LEU:N	1:B:155:ARG:HH21	1.55	1.04
1:B:154:MET:HB2	1:B:155:ARG:NH1	1.72	1.02
1:B:133:ARG:H	1:B:133:ARG:HD3	1.24	1.02
2:D:106:PRO:HB3	2:D:111:ILE:CD1	1.92	0.99
1:B:365:ARG:HG2	1:B:365:ARG:HH21	1.27	0.97
1:B:571:VAL:HG22	1:B:571:VAL:O	1.62	0.97
2:D:2:GLU:HG2	2:D:3:SER:H	1.28	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:LEU:H	1:B:155:ARG:NH2	1.64	0.95
1:A:456:GLY:HA3	1:A:478:GLU:HB2	1.47	0.95
1:A:117:THR:OG1	1:A:120:ARG:CZ	2.16	0.92
1:A:137:ARG:HG3	1:A:137:ARG:HH11	1.31	0.92
1:B:171:ARG:HG2	1:B:171:ARG:NH1	1.71	0.90
1:B:172:ASP:O	1:B:176:ILE:HD13	1.72	0.89
1:A:118:PRO:C	1:A:120:ARG:HH12	1.77	0.88
1:A:117:THR:O	1:A:120:ARG:NH1	2.07	0.87
1:B:180:LEU:HD13	1:B:189:LEU:CD1	2.05	0.87
1:B:508:VAL:HG21	2:C:108:GLY:HA3	1.54	0.86
1:A:126:SER:O	1:A:127:GLN:HB2	1.73	0.86
1:A:117:THR:C	1:A:120:ARG:NH1	2.28	0.85
1:B:107:TYR:CD2	1:B:121:LEU:HD23	2.12	0.85
1:B:153:LEU:N	1:B:155:ARG:NH2	2.22	0.85
1:B:173:ILE:O	1:B:177:ILE:HG12	1.77	0.84
2:D:175:VAL:O	2:D:179:LEU:HD12	1.78	0.84
1:A:467:ARG:H	1:A:467:ARG:HE	1.26	0.83
1:B:154:MET:H	1:B:155:ARG:CZ	1.93	0.81
1:B:153:LEU:H	1:B:155:ARG:HH21	0.83	0.81
1:B:171:ARG:HH11	1:B:171:ARG:CG	1.87	0.81
1:B:453:ILE:HG23	1:B:479:ILE:HD11	1.60	0.81
1:B:85:HIS:HD2	1:B:88:ARG:NH2	1.79	0.81
1:B:365:ARG:HG3	1:B:369:MET:HB2	1.63	0.81
2:D:113:SER:HB3	2:D:116:VAL:CG1	2.11	0.80
1:A:119:GLU:N	1:A:120:ARG:HH12	1.78	0.80
1:B:173:ILE:O	1:B:177:ILE:CD1	2.29	0.80
1:B:143:PHE:HB3	1:B:152:LEU:HD11	1.62	0.80
1:B:104:ASN:HD21	1:B:122:PHE:H	1.26	0.80
1:A:475:ASP:OD1	4:A:1760:ATP:O1A	2.00	0.80
1:B:525:ASP:HA	2:C:76:GLN:HE22	1.45	0.80
1:B:169:LYS:O	1:B:173:ILE:CD1	2.30	0.79
1:B:172:ASP:O	1:B:176:ILE:CD1	2.30	0.79
1:B:180:LEU:HD13	1:B:189:LEU:HD11	1.64	0.79
1:B:152:LEU:C	1:B:155:ARG:NE	2.33	0.79
1:B:173:ILE:O	1:B:177:ILE:CG1	2.30	0.79
1:A:342:PHE:N	1:A:342:PHE:HD1	1.80	0.78
1:A:411:ARG:HH11	1:A:411:ARG:CG	1.95	0.78
1:B:173:ILE:O	1:B:177:ILE:HD11	1.83	0.78
2:D:106:PRO:CB	2:D:111:ILE:HD11	2.10	0.78
1:B:135:ILE:HD12	1:B:136:PRO:HD2	1.66	0.78
1:A:467:ARG:H	1:A:467:ARG:NE	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:ARG:HD3	1:B:155:ARG:N	1.99	0.78
1:B:169:LYS:O	1:B:173:ILE:HD11	1.84	0.77
1:A:411:ARG:HG3	1:A:411:ARG:NH1	1.88	0.77
1:B:152:LEU:CA	1:B:155:ARG:HE	1.97	0.77
1:A:560:VAL:O	1:A:560:VAL:HG13	1.85	0.77
2:D:2:GLU:CG	2:D:3:SER:H	1.98	0.77
2:D:66:MET:SD	6:D:421:HOH:O	2.41	0.77
1:B:155:ARG:H	1:B:155:ARG:CD	1.98	0.76
1:A:342:PHE:N	1:A:342:PHE:CD1	2.50	0.76
1:B:170:SER:HA	1:B:173:ILE:HG13	1.68	0.76
1:B:168:ASN:HB3	1:B:171:ARG:HB3	1.68	0.75
1:A:117:THR:OG1	1:A:120:ARG:NE	2.19	0.75
1:B:242:THR:HG22	1:B:245:GLU:H	1.51	0.75
1:A:104:ASN:HD21	1:A:122:PHE:H	1.34	0.74
1:A:120:ARG:H	1:A:120:ARG:HH11	1.35	0.74
1:B:365:ARG:HH21	1:B:365:ARG:CG	1.98	0.73
1:B:571:VAL:O	1:B:571:VAL:CG2	2.37	0.73
1:A:119:GLU:N	1:A:120:ARG:NH1	2.36	0.73
1:A:167:GLN:HG2	1:A:233:GLU:HG2	1.70	0.73
2:D:106:PRO:HB3	2:D:111:ILE:CG1	2.20	0.72
1:A:119:GLU:H	1:A:120:ARG:HH22	1.36	0.72
1:B:127:GLN:HG3	1:B:128:PRO:HD2	1.70	0.72
1:B:101:SER:OG	1:B:292:HIS:HD2	1.72	0.72
1:A:171:ARG:HD2	1:A:175:TYR:HE2	1.54	0.72
1:A:119:GLU:H	1:A:120:ARG:NH2	1.88	0.71
2:D:116:VAL:O	2:D:120:GLN:HG2	1.88	0.71
1:A:171:ARG:HD2	1:A:175:TYR:CE2	2.26	0.71
2:D:171:ASP:O	2:D:175:VAL:HG23	1.90	0.71
1:B:85:HIS:CD2	1:B:88:ARG:NH2	2.59	0.70
1:A:417:ARG:HE	1:A:467:ARG:HH12	1.36	0.70
1:A:117:THR:OG1	1:A:120:ARG:NH2	2.23	0.70
1:A:442:GLY:HA3	1:A:536:HIS:CE1	2.28	0.69
2:C:157:GLU:O	2:C:158:ASP:HB2	1.92	0.69
1:A:439:GLU:O	1:A:443:ASN:ND2	2.26	0.69
1:A:167:GLN:HG2	1:A:233:GLU:CG	2.23	0.68
1:B:525:ASP:HB3	1:B:528:ILE:HG12	1.75	0.68
1:B:152:LEU:N	1:B:155:ARG:CZ	2.56	0.68
1:B:77:GLU:HG2	1:B:78:PHE:N	2.08	0.68
1:B:221:PRO:O	1:B:241:THR:HA	1.94	0.67
2:C:72:GLU:O	2:C:75:THR:HB	1.94	0.67
1:B:170:SER:HA	1:B:173:ILE:CG1	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:LEU:O	1:A:9:ILE:HG12	1.95	0.67
1:A:242:THR:HB	1:A:245:GLU:HG3	1.77	0.67
1:B:85:HIS:HD2	1:B:88:ARG:HH21	1.42	0.67
1:A:167:GLN:H	1:A:233:GLU:CD	1.98	0.67
1:A:320:GLY:HA2	4:A:1760:ATP:O1B	1.94	0.67
1:B:155:ARG:N	1:B:155:ARG:CD	2.58	0.67
4:B:1761:ATP:O2A	4:B:1761:ATP:O2B	2.13	0.67
1:A:441:TYR:OH	1:A:458:MET:HB3	1.95	0.66
1:B:365:ARG:HG2	1:B:365:ARG:NH2	2.05	0.66
2:C:273:LYS:HG3	2:C:274:GLU:N	2.10	0.66
2:C:16:LEU:HB3	2:C:96:ARG:HH21	1.61	0.66
2:D:117:ALA:O	2:D:121:GLU:HB2	1.95	0.66
1:A:166:TRP:HA	1:A:233:GLU:OE1	1.95	0.66
1:B:325:VAL:HG11	4:B:1761:ATP:O4'	1.95	0.65
1:B:520:HIS:CD2	2:C:72:GLU:OE2	2.49	0.65
1:A:167:GLN:CG	1:A:233:GLU:HG2	2.27	0.65
1:B:151:SER:HA	1:B:155:ARG:NH1	2.13	0.64
1:B:320:GLY:HA2	4:B:1761:ATP:O2A	1.97	0.64
1:A:120:ARG:NH1	1:A:120:ARG:N	2.34	0.64
2:C:149:MET:HA	2:C:297:ASP:O	1.98	0.64
1:B:152:LEU:CA	1:B:155:ARG:NE	2.60	0.64
1:A:490:ILE:HG22	1:A:516:GLU:OE2	1.97	0.63
1:A:137:ARG:HG3	1:A:137:ARG:NH1	2.07	0.63
1:B:253:ALA:O	1:B:365:ARG:HB3	1.98	0.63
1:B:171:ARG:NH1	1:B:171:ARG:CG	2.50	0.63
1:B:152:LEU:N	1:B:155:ARG:NH2	2.48	0.62
1:B:177:ILE:HA	1:B:180:LEU:HG	1.81	0.62
1:B:79:LEU:HD11	1:B:111:PHE:CZ	2.34	0.62
1:B:113:HIS:HE1	3:B:1604:AMP:O2P	1.83	0.62
1:A:50:ARG:NH2	1:A:288:GLY:HA3	2.14	0.62
1:B:366:VAL:HG12	1:B:366:VAL:O	2.00	0.62
1:A:525:ASP:HB3	1:A:528:ILE:HG12	1.82	0.61
2:C:30:PRO:HD2	2:C:97:VAL:O	2.01	0.61
1:B:104:ASN:HD21	1:B:122:PHE:N	1.98	0.61
1:A:417:ARG:HE	1:A:467:ARG:NH1	1.97	0.61
1:A:141:LYS:HE3	1:A:143:PHE:CZ	2.36	0.60
1:A:439:GLU:HG2	1:A:443:ASN:HD21	1.66	0.60
1:A:490:ILE:HG22	1:A:516:GLU:CD	2.21	0.60
1:A:429:VAL:HG13	1:A:433:GLN:HB2	1.83	0.60
1:B:169:LYS:O	1:B:173:ILE:HG12	2.02	0.60
1:B:18:ASP:OD2	1:B:93:TYR:OH	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:LYS:HE2	1:B:273:GLU:HB3	1.84	0.60
1:B:494:ARG:HD2	1:B:505:TRP:NE1	2.15	0.60
1:B:154:MET:HB2	1:B:155:ARG:HH11	1.64	0.60
2:D:2:GLU:HG2	2:D:3:SER:N	2.10	0.60
1:B:168:ASN:O	1:B:172:ASP:OD1	2.18	0.60
1:A:50:ARG:HH22	1:A:288:GLY:HA3	1.66	0.59
1:A:169:LYS:H	1:A:169:LYS:HD2	1.66	0.59
2:D:234:MET:HG3	2:D:238:GLU:HG3	1.84	0.59
2:D:203:GLU:HG3	2:D:207:LYS:HE3	1.83	0.59
1:B:176:ILE:HD12	1:B:176:ILE:N	2.17	0.59
2:C:153:ARG:HE	2:C:303:ASN:HD22	1.49	0.59
2:C:324:PRO:HG3	2:C:358:LEU:HB3	1.85	0.59
1:A:274:ILE:HG22	1:A:275:LEU:H	1.66	0.59
1:B:154:MET:N	1:B:155:ARG:CZ	2.65	0.59
2:D:10:GLN:CD	2:D:10:GLN:H	2.05	0.58
1:A:168:ASN:CG	1:A:171:ARG:HB2	2.23	0.58
1:A:101:SER:OG	1:A:292:HIS:HD2	1.86	0.58
1:A:425:TRP:HZ3	1:A:437:ALA:HB2	1.68	0.58
1:B:101:SER:OG	1:B:292:HIS:CD2	2.55	0.58
1:B:153:LEU:N	1:B:155:ARG:HE	1.98	0.58
2:C:378:LYS:NZ	2:C:416:MET:O	2.37	0.58
1:A:475:ASP:OD2	4:A:1760:ATP:O3B	2.21	0.58
1:B:152:LEU:N	1:B:155:ARG:NE	2.52	0.57
2:D:2:GLU:CG	2:D:3:SER:N	2.67	0.57
1:A:212:LYS:HG2	1:A:274:ILE:HD11	1.85	0.57
1:B:39:ASP:O	1:B:43:VAL:HG23	2.04	0.57
1:B:18:ASP:CG	1:B:93:TYR:OH	2.43	0.57
2:C:230:LYS:HD2	2:C:281:ILE:HG22	1.87	0.57
1:A:167:GLN:HG2	1:A:233:GLU:CB	2.35	0.57
2:D:5:VAL:HG12	2:D:67:GLU:O	2.05	0.57
1:B:169:LYS:O	1:B:173:ILE:CG1	2.53	0.56
1:B:224:LEU:HD22	1:B:236:ILE:HG21	1.87	0.56
2:D:100:LYS:HE3	2:D:336:GLU:HB3	1.87	0.56
1:B:109:ARG:HH11	1:B:109:ARG:CG	2.18	0.56
1:A:19:ALA:HA	1:B:18:ASP:HB3	1.87	0.56
1:A:166:TRP:HB2	1:A:169:LYS:HE3	1.88	0.56
1:B:325:VAL:HG11	4:B:1761:ATP:C1'	2.36	0.56
2:D:113:SER:HB3	2:D:116:VAL:HG12	1.88	0.56
1:A:457:ASP:HB3	1:A:462:ASN:ND2	2.21	0.56
1:B:121:LEU:CD1	1:B:123:ILE:HG22	2.36	0.56
1:A:167:GLN:HG2	1:A:233:GLU:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:HIS:CD2	1:B:88:ARG:HH21	2.20	0.55
1:B:151:SER:C	1:B:155:ARG:CZ	2.75	0.55
1:A:328:LEU:HB2	1:A:331:PHE:HB2	1.88	0.55
1:B:169:LYS:C	1:B:173:ILE:HD11	2.26	0.55
1:A:378:PHE:CB	1:A:413:LEU:HD11	2.37	0.55
1:A:180:LEU:O	1:A:184:LEU:HD23	2.07	0.55
1:B:111:PHE:HE2	1:B:120:ARG:HH21	1.55	0.55
4:B:1761:ATP:H8	4:B:1761:ATP:H5'2	1.71	0.55
1:B:79:LEU:HD11	1:B:111:PHE:HZ	1.71	0.55
1:B:425:TRP:HZ3	1:B:437:ALA:HB2	1.71	0.55
1:A:560:VAL:O	1:A:560:VAL:CG1	2.54	0.54
2:C:157:GLU:O	2:C:158:ASP:CB	2.55	0.54
1:A:153:LEU:O	1:A:157:ILE:HG12	2.07	0.54
2:D:388:THR:HB	2:D:403:LEU:HD11	1.89	0.54
1:B:457:ASP:HB3	1:B:462:ASN:HD22	1.72	0.54
1:B:520:HIS:NE2	2:C:72:GLU:OE2	2.40	0.53
1:A:467:ARG:H	1:A:467:ARG:CD	2.21	0.53
1:B:494:ARG:HD3	1:B:498:ASP:OD2	2.08	0.53
1:B:79:LEU:CD1	1:B:111:PHE:HZ	2.22	0.53
2:C:153:ARG:HE	2:C:303:ASN:ND2	2.06	0.53
1:A:9:ILE:HG23	1:A:65:LEU:HD22	1.90	0.53
1:B:153:LEU:N	1:B:155:ARG:CZ	2.72	0.53
2:C:57:TYR:HE2	2:C:372:ALA:HB2	1.74	0.53
1:A:490:ILE:HD12	1:A:506:TYR:OH	2.07	0.53
2:D:30:PRO:HD2	2:D:97:VAL:O	2.09	0.53
1:B:159:ASP:OD2	1:B:159:ASP:N	2.30	0.52
1:A:429:VAL:HG13	1:A:433:GLN:CB	2.39	0.52
1:A:475:ASP:OD1	4:A:1760:ATP:PA	2.67	0.52
1:B:153:LEU:N	1:B:155:ARG:NE	2.56	0.52
2:C:30:PRO:HA	2:C:66:MET:O	2.09	0.52
1:A:457:ASP:HB3	1:A:462:ASN:HD22	1.73	0.52
1:B:121:LEU:HD11	1:B:123:ILE:HG22	1.91	0.52
1:B:177:ILE:HG22	1:B:180:LEU:HD11	1.90	0.52
1:B:172:ASP:OD1	1:B:172:ASP:N	2.42	0.52
1:B:296:GLU:O	1:B:300:GLU:HG3	2.10	0.52
2:C:301:CYS:SG	2:C:306:GLY:HA2	2.50	0.52
1:B:166:TRP:CB	1:B:169:LYS:HG3	2.40	0.52
1:B:441:TYR:O	1:B:445:ILE:HG12	2.10	0.52
2:D:68:ILE:HD12	2:D:88:THR:HG23	1.91	0.51
1:B:156:VAL:HA	1:B:159:ASP:OD1	2.11	0.51
2:D:207:LYS:O	2:D:211:ARG:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:LEU:HD13	1:B:189:LEU:HD12	1.91	0.51
2:C:68:ILE:HD12	2:C:88:THR:HG23	1.91	0.51
2:D:159:ILE:HD11	2:D:199:LYS:HB2	1.93	0.51
2:D:5:VAL:HG21	2:D:91:LEU:HD11	1.93	0.51
2:C:149:MET:HE2	2:C:299:ILE:HG13	1.92	0.51
1:A:215:THR:HG22	1:A:217:SER:H	1.75	0.51
1:A:21:TYR:OH	1:A:264:PRO:HG3	2.11	0.50
1:B:143:PHE:O	1:B:193:HIS:HB2	2.11	0.50
1:B:209:LEU:HB3	1:B:224:LEU:HB2	1.93	0.50
1:B:543:ASP:N	1:B:543:ASP:OD1	2.45	0.50
2:C:189:ARG:HG3	2:C:190:PHE:CD2	2.47	0.50
1:A:170:SER:O	1:A:174:HIS:HB2	2.12	0.50
1:A:29:SER:HB2	1:B:137:ARG:HD2	1.93	0.50
1:A:104:ASN:ND2	1:A:122:PHE:H	2.05	0.50
1:B:230:ASP:O	1:B:231:ASP:CB	2.30	0.50
1:A:425:TRP:CZ3	1:A:437:ALA:HB2	2.47	0.50
2:C:216:TYR:O	2:C:220:ASN:ND2	2.41	0.50
1:A:153:LEU:HD13	1:A:176:ILE:HG13	1.94	0.50
2:D:267:LYS:H	2:D:267:LYS:HD3	1.76	0.50
1:B:221:PRO:HA	1:B:274:ILE:HD12	1.95	0.49
1:B:366:VAL:O	1:B:366:VAL:CG1	2.60	0.49
1:B:60:LEU:O	1:B:64:GLN:HG3	2.12	0.49
2:D:267:LYS:H	2:D:267:LYS:CD	2.26	0.49
1:B:228:GLN:HA	1:B:233:GLU:O	2.12	0.49
1:A:333:ARG:HH22	1:A:373:GLN:NE2	2.10	0.49
1:A:462:ASN:HB3	1:A:475:ASP:HB2	1.95	0.49
1:B:177:ILE:O	1:B:180:LEU:HD12	2.13	0.49
1:A:456:GLY:HA3	1:A:478:GLU:CB	2.32	0.48
1:B:62:VAL:HG21	1:B:109:ARG:HB3	1.95	0.48
1:A:54:TYR:CD1	1:A:291:LYS:HG3	2.48	0.48
1:A:167:GLN:N	1:A:233:GLU:OE1	2.47	0.48
1:B:461:LYS:HE3	4:B:1761:ATP:O1G	2.13	0.48
2:C:49:VAL:HG21	2:C:360:ALA:HB1	1.96	0.48
1:A:118:PRO:CA	1:A:120:ARG:HH12	2.25	0.48
1:A:514:PHE:O	1:A:517:GLU:HG2	2.13	0.48
2:C:134:TYR:O	2:C:137:THR:OG1	2.29	0.48
1:B:170:SER:C	1:B:173:ILE:HG12	2.34	0.48
2:C:185:VAL:O	2:C:186:LYS:HB2	2.13	0.48
1:B:275:LEU:HB3	1:B:278:LYS:HG3	1.96	0.48
1:A:172:ASP:O	1:A:176:ILE:HG12	2.14	0.48
1:B:152:LEU:O	1:B:155:ARG:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:528:ILE:HA	1:B:531:LEU:HD12	1.96	0.47
2:D:100:LYS:NZ	2:D:115:ASN:OD1	2.44	0.47
1:B:51:ILE:HG13	1:B:290:GLN:NE2	2.29	0.47
1:B:113:HIS:CE1	3:B:1604:AMP:O2P	2.65	0.47
2:C:173:GLU:O	2:C:177:LYS:HB2	2.13	0.47
2:C:130:PRO:HA	2:C:150:VAL:HA	1.95	0.47
2:C:185:VAL:O	2:C:186:LYS:CB	2.57	0.47
2:D:159:ILE:CD1	2:D:199:LYS:HB2	2.45	0.47
1:B:205:LYS:HD2	1:B:559:ASP:OD1	2.15	0.47
2:C:154:GLU:HB2	2:C:209:LEU:HD22	1.97	0.47
2:D:242:LYS:HB3	2:D:242:LYS:HE3	1.75	0.47
1:B:94:PRO:HB2	1:B:263:LEU:CD1	2.44	0.47
1:B:104:ASN:ND2	1:B:122:PHE:H	2.03	0.47
2:D:178:PHE:O	2:D:182:GLU:HB2	2.15	0.47
1:A:303:VAL:O	1:A:306:GLN:HG2	2.14	0.47
2:C:185:VAL:C	2:C:186:LYS:HG2	2.34	0.47
1:A:117:THR:C	1:A:120:ARG:CZ	2.83	0.47
2:C:160:TYR:OH	2:D:230:LYS:HD2	2.15	0.47
1:B:9:ILE:HG13	1:B:65:LEU:HD22	1.96	0.47
2:D:96:ARG:HD3	2:D:331:GLU:O	2.15	0.47
4:A:1760:ATP:O1B	4:A:1760:ATP:H5'2	2.15	0.46
1:B:325:VAL:HG11	4:B:1761:ATP:H1'	1.97	0.46
1:B:425:TRP:CZ3	1:B:437:ALA:HB2	2.49	0.46
2:C:349:ASP:O	2:C:404:LYS:HB3	2.15	0.46
1:B:180:LEU:HD12	1:B:181:THR:N	2.30	0.46
1:A:18:ASP:HB3	1:B:19:ALA:HA	1.96	0.46
1:A:118:PRO:O	1:A:121:LEU:O	2.32	0.46
1:B:152:LEU:H	1:B:155:ARG:NH2	2.12	0.46
1:A:215:THR:HG23	1:A:216:PRO:HD2	1.98	0.46
1:B:570:SER:O	1:B:570:SER:OG	2.30	0.46
1:A:168:ASN:HB3	1:A:171:ARG:HB2	1.97	0.46
1:A:411:ARG:CG	1:A:411:ARG:NH1	2.63	0.46
1:B:324:LEU:HD21	1:B:392:LEU:HD13	1.98	0.46
1:A:561:TYR:CD2	1:A:561:TYR:N	2.84	0.46
1:B:177:ILE:HA	1:B:180:LEU:CD1	2.46	0.46
1:A:85:HIS:O	1:A:88:ARG:HG2	2.16	0.45
1:A:172:ASP:HA	1:A:175:TYR:HD2	1.81	0.45
2:C:128:LEU:HD11	2:C:150:VAL:CG1	2.46	0.45
1:A:77:GLU:O	1:A:81:ARG:HD2	2.17	0.45
1:A:378:PHE:HB3	1:A:413:LEU:HD11	1.97	0.45
1:B:153:LEU:O	1:B:156:VAL:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1761:ATP:O2A	4:B:1761:ATP:H4'	2.16	0.45
2:D:133:TYR:CD1	2:D:144:PRO:HB2	2.52	0.45
2:D:395:ARG:HB2	2:D:395:ARG:NH1	2.32	0.45
1:B:171:ARG:HG3	1:B:175:TYR:CE2	2.51	0.45
1:B:466:THR:HG22	1:B:467:ARG:N	2.31	0.45
2:D:78:TYR:OH	2:D:87:GLU:OE1	2.28	0.45
1:A:227:HIS:O	1:A:234:LEU:HA	2.16	0.45
1:B:365:ARG:CG	1:B:365:ARG:NH2	2.67	0.45
2:D:365:ARG:HG3	2:D:370:THR:HG22	1.99	0.45
1:A:119:GLU:N	1:A:120:ARG:CZ	2.79	0.45
1:A:314:GLU:OE1	1:A:319:ARG:HG3	2.16	0.45
1:B:174:HIS:HA	1:B:177:ILE:HG13	1.99	0.45
1:B:432:GLN:HA	1:B:435:ARG:HG3	1.98	0.45
4:B:1761:ATP:H5'2	4:B:1761:ATP:C8	2.51	0.45
1:B:91:PRO:HA	1:B:127:GLN:HE22	1.80	0.45
1:B:215:THR:HB	1:B:216:PRO:HD2	1.99	0.45
1:B:177:ILE:HA	1:B:180:LEU:CG	2.46	0.45
1:B:20:GLN:HG3	1:B:21:TYR:N	2.32	0.45
1:B:109:ARG:CG	1:B:109:ARG:NH1	2.79	0.45
1:B:133:ARG:H	1:B:133:ARG:CD	2.07	0.45
2:D:10:GLN:O	2:D:26:ASN:OD1	2.35	0.45
1:B:520:HIS:NE2	2:C:72:GLU:HG3	2.32	0.44
1:A:274:ILE:O	1:A:275:LEU:C	2.53	0.44
1:B:156:VAL:C	1:B:159:ASP:OD2	2.56	0.44
1:A:215:THR:CG2	1:A:216:PRO:HD2	2.46	0.44
1:A:390:MET:O	1:A:394:LEU:HB2	2.18	0.44
1:B:141:LYS:HD2	1:B:143:PHE:CZ	2.53	0.44
1:A:491:PRO:HA	1:A:492:PRO:HD3	1.91	0.44
2:C:131:VAL:HG11	2:C:313:LEU:HB3	2.00	0.44
2:D:380:MET:O	2:D:384:ILE:HG12	2.17	0.44
2:D:113:SER:CB	2:D:116:VAL:HG12	2.48	0.44
1:A:561:TYR:O	1:A:563:TYR:N	2.50	0.44
1:A:137:ARG:NH1	1:A:137:ARG:CG	2.78	0.43
1:B:442:GLY:HA3	1:B:536:HIS:CE1	2.53	0.43
1:A:231:ASP:N	1:A:231:ASP:OD2	2.52	0.43
1:A:417:ARG:HH11	1:A:417:ARG:HB2	1.81	0.43
1:B:176:ILE:CD1	1:B:176:ILE:N	2.81	0.43
2:D:297:ASP:HB3	2:D:298:VAL:H	1.59	0.43
2:D:357:ILE:O	2:D:360:ALA:HB3	2.19	0.43
1:B:242:THR:HB	1:B:245:GLU:OE2	2.17	0.43
1:B:439:GLU:HA	1:B:536:HIS:HE2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:126:ILE:O	2:D:327:ASN:HA	2.18	0.43
1:B:109:ARG:NH1	1:B:109:ARG:HG3	2.33	0.43
1:B:466:THR:HG22	1:B:468:HIS:H	1.83	0.43
2:D:409:GLY:HA2	2:D:412:ILE:HD12	2.01	0.43
2:D:72:GLU:O	2:D:75:THR:HB	2.19	0.43
1:B:359:LEU:HD12	1:B:359:LEU:C	2.39	0.43
1:A:119:GLU:HG3	1:A:120:ARG:NH2	2.33	0.43
1:B:335:PHE:N	1:B:335:PHE:CD1	2.87	0.43
1:B:139:LEU:HD11	1:B:266:ALA:HB1	2.00	0.43
1:B:154:MET:H	1:B:155:ARG:NH2	2.16	0.43
1:B:201:PHE:HB2	1:B:208:TRP:HB2	2.01	0.43
1:A:168:ASN:CB	1:A:171:ARG:HB2	2.49	0.43
1:A:457:ASP:CB	1:A:462:ASN:ND2	2.82	0.43
1:B:170:SER:O	1:B:173:ILE:HG12	2.18	0.43
1:A:64:GLN:HE22	1:B:15:GLN:HE22	1.67	0.42
1:B:107:TYR:CD2	1:B:107:TYR:C	2.92	0.42
1:B:173:ILE:HG12	1:B:173:ILE:H	1.29	0.42
1:B:174:HIS:C	1:B:174:HIS:HD1	2.20	0.42
1:B:176:ILE:HD12	1:B:176:ILE:H	1.82	0.42
2:D:83:TRP:HB3	2:D:114:LEU:HD11	2.01	0.42
2:D:361:GLU:OE1	2:D:365:ARG:NH2	2.48	0.42
1:A:490:ILE:CD1	1:A:506:TYR:OH	2.67	0.42
1:B:420:VAL:HG13	1:B:465:VAL:HB	2.00	0.42
1:B:424:ILE:O	1:B:427:GLU:HB2	2.19	0.42
2:D:177:LYS:O	2:D:181:GLU:HG2	2.19	0.42
1:B:229:THR:C	1:B:230:ASP:O	2.49	0.42
2:C:45:MET:HE1	2:C:99:ILE:HG21	2.01	0.42
2:C:55:LYS:HD3	2:C:375:LEU:HD13	2.02	0.42
2:C:387:LYS:HB3	2:C:400:ALA:HA	2.01	0.42
2:D:105:THR:HA	2:D:106:PRO:HD3	1.88	0.42
1:A:79:LEU:O	1:A:83:LYS:HB2	2.19	0.42
1:A:117:THR:CB	1:A:118:PRO:HD2	2.49	0.42
2:C:26:ASN:N	2:C:27:PRO:HD3	2.34	0.42
2:C:45:MET:HE3	2:C:360:ALA:HB2	2.01	0.42
1:B:179:HIS:CE1	1:B:241:THR:HG23	2.55	0.42
2:C:323:ALA:HA	2:C:324:PRO:HD3	1.88	0.42
1:B:420:VAL:HA	1:B:421:PRO:HD3	1.95	0.42
2:C:29:ILE:CG2	2:C:363:MET:HE1	2.50	0.42
1:A:40:TRP:CZ3	1:A:205:LYS:HA	2.54	0.42
1:B:457:ASP:CB	1:B:462:ASN:HD22	2.33	0.42
2:C:408:PHE:O	2:C:412:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:THR:HB	1:A:118:PRO:HD2	2.02	0.42
2:C:142:LYS:HE2	2:D:139:SER:O	2.20	0.42
1:B:109:ARG:HH11	1:B:109:ARG:HG3	1.85	0.41
1:B:172:ASP:O	1:B:176:ILE:HD12	2.16	0.41
1:A:504:PRO:HB3	1:A:506:TYR:CZ	2.55	0.41
1:B:525:ASP:HB3	1:B:528:ILE:CG1	2.48	0.41
1:B:104:ASN:ND2	1:B:121:LEU:HB2	2.34	0.41
1:B:459:LEU:CD2	1:B:521:TRP:HB3	2.51	0.41
2:C:165:TRP:HH2	2:D:179:LEU:HD23	1.85	0.41
2:D:268:ASN:HA	2:D:269:PRO:HD3	1.96	0.41
1:A:454:PHE:HD1	1:A:482:MET:HE1	1.85	0.41
1:A:250:PHE:O	1:A:278:LYS:HE3	2.20	0.41
1:B:336:LYS:NZ	4:B:1761:ATP:C8	2.88	0.41
2:C:133:TYR:CE2	2:C:135:GLN:HA	2.56	0.41
1:A:118:PRO:N	1:A:120:ARG:NH1	2.67	0.41
1:A:457:ASP:CB	1:A:462:ASN:HD22	2.33	0.41
1:B:151:SER:C	1:B:155:ARG:NE	2.74	0.41
1:B:147:HIS:O	1:B:151:SER:HB2	2.20	0.41
1:B:202:TYR:HB2	1:B:258:MET:HB2	2.02	0.41
1:B:381:GLU:HB2	1:B:384:HIS:ND1	2.34	0.41
1:B:411:ARG:HB2	1:B:411:ARG:NH1	2.36	0.41
2:D:169:SER:O	2:D:170:ALA:HB3	2.21	0.41
1:A:274:ILE:HG22	1:A:275:LEU:N	2.35	0.41
1:A:525:ASP:HA	1:A:526:PRO:HD3	1.88	0.41
1:A:562:ALA:C	1:A:563:TYR:CD2	2.94	0.41
1:B:94:PRO:HB2	1:B:263:LEU:HD13	2.03	0.41
1:B:318:ILE:HD13	2:C:81:ASP:HB2	2.03	0.41
2:D:170:ALA:O	2:D:174:LYS:N	2.36	0.41
1:A:104:ASN:HD21	1:A:122:PHE:N	2.08	0.41
1:A:290:GLN:HG3	1:A:291:LYS:N	2.36	0.41
1:A:439:GLU:HA	1:A:536:HIS:HE2	1.86	0.41
1:A:473:PHE:HE2	1:A:479:ILE:HD12	1.86	0.41
1:A:196:VAL:HA	1:A:211:GLY:HA2	2.03	0.40
1:A:322:VAL:HG13	4:A:1760:ATP:O2B	2.21	0.40
1:B:346:LYS:NZ	4:B:1761:ATP:O2G	2.48	0.40
1:B:151:SER:CA	1:B:155:ARG:CZ	2.99	0.40
1:B:177:ILE:HG12	1:B:177:ILE:H	1.07	0.40
2:D:13:LYS:HE3	2:D:94:GLU:HG2	2.03	0.40
2:D:259:ASP:C	2:D:261:GLY:H	2.24	0.40
1:A:157:ILE:HA	1:A:160:LEU:HD22	2.04	0.40
1:A:341:LYS:C	1:A:342:PHE:HD1	2.23	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:ARG:CD	1:A:467:ARG:N	2.83	0.40
2:D:159:ILE:HG12	2:D:199:LYS:HG3	2.04	0.40
2:C:281:ILE:H	2:C:281:ILE:HG12	1.63	0.40
1:A:119:GLU:H	1:A:120:ARG:CZ	2.33	0.40
1:B:151:SER:HA	1:B:155:ARG:CZ	2.51	0.40
1:B:170:SER:CA	1:B:173:ILE:HG12	2.51	0.40
1:B:320:GLY:CA	4:B:1761:ATP:O2A	2.65	0.40
2:D:37:ILE:HB	2:D:351:VAL:HG21	2.03	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	548/578 (95%)	523 (95%)	24 (4%)	1 (0%)	47	78
1	B	557/578 (96%)	536 (96%)	19 (3%)	2 (0%)	34	66
2	C	413/416 (99%)	389 (94%)	22 (5%)	2 (0%)	29	61
2	D	413/416 (99%)	389 (94%)	24 (6%)	0	100	100
All	All	1931/1988 (97%)	1837 (95%)	89 (5%)	5 (0%)	41	71

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	158	ASP
1	A	431	GLY
1	B	456	GLY
2	C	108	GLY
1	B	366	VAL

5.3.2　Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	486/508 (96%)	422 (87%)	64 (13%)	4	12
1	B	495/508 (97%)	420 (85%)	75 (15%)	3	8
2	C	337/338 (100%)	325 (96%)	12 (4%)	35	69
2	D	337/338 (100%)	314 (93%)	23 (7%)	16	42
All	All	1655/1692 (98%)	1481 (90%)	174 (10%)	7	21

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	7	LEU
1	A	8	LEU
1	A	20	GLN
1	A	50	ARG
1	A	60	LEU
1	A	66	ARG
1	A	77	GLU
1	A	78	PHE
1	A	83	LYS
1	A	84	GLU
1	A	89	LEU
1	A	97	GLU
1	A	117	THR
1	A	119	GLU
1	A	120	ARG
1	A	123	ILE
1	A	137	ARG
1	A	154	MET
1	A	160	LEU
1	A	167	GLN
1	A	178	ARG
1	A	189	LEU
1	A	191	LYS

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Mol	Chain	Res	Type
1	A	196	VAL
1	A	200	LEU
1	A	231	ASP
1	A	233	GLU
1	A	234	LEU
1	A	242	THR
1	A	247	SER
1	A	254	ARG
1	A	271	LEU
1	A	283	LEU
1	A	285	MET
1	A	322	VAL
1	A	324	LEU
1	A	325	VAL
1	A	336	LYS
1	A	337	VAL
1	A	342	PHE
1	A	364	ASP
1	A	381	GLU
1	A	390	MET
1	A	411	ARG
1	A	413	LEU
1	A	416	GLU
1	A	417	ARG
1	A	422	LEU
1	A	432	GLN
1	A	435	ARG
1	A	467	ARG
1	A	474	TYR
1	A	475	ASP
1	A	477	ASP
1	A	479	ILE
1	A	482	MET
1	A	490	ILE
1	A	507	SER
1	A	527	ARG
1	A	535	MET
1	A	549	GLN
1	A	559	ASP
1	A	571	VAL
1	B	6	GLU
1	B	8	LEU

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Mol	Chain	Res	Type
1	B	20	GLN
1	B	41	HIS
1	B	45	GLN
1	B	60	LEU
1	B	63	GLU
1	B	77	GLU
1	B	78	PHE
1	B	80	LEU
1	B	93	TYR
1	B	109	ARG
1	B	116	LEU
1	B	123	ILE
1	B	133	ARG
1	B	135	ILE
1	B	146	ASP
1	B	154	MET
1	B	155	ARG
1	B	159	ASP
1	B	160	LEU
1	B	167	GLN
1	B	170	SER
1	B	171	ARG
1	B	172	ASP
1	B	173	ILE
1	B	177	ILE
1	B	178	ARG
1	B	180	LEU
1	B	189	LEU
1	B	194	LEU
1	B	243	THR
1	B	271	LEU
1	B	283	LEU
1	B	290	GLN
1	B	302	LEU
1	B	306	GLN
1	B	309	ASN
1	B	337	VAL
1	B	345	GLN
1	B	348	MET
1	B	359	LEU
1	B	365	ARG
1	B	372	THR

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Mol	Chain	Res	Type
1	B	383	ARG
1	B	392	LEU
1	B	396	GLU
1	B	401	ILE
1	B	402	THR
1	B	404	LEU
1	B	407	GLN
1	B	411	ARG
1	B	413	LEU
1	B	417	ARG
1	B	422	LEU
1	B	425	TRP
1	B	429	VAL
1	B	430	GLU
1	B	435	ARG
1	B	457	ASP
1	B	474	TYR
1	B	479	ILE
1	B	485	VAL
1	B	488	ARG
1	B	489	ASP
1	B	508	VAL
1	B	509	SER
1	B	522	LEU
1	B	538	ASP
1	B	543	ASP
1	B	549	GLN
1	B	556	HIS
1	B	565	ARG
1	B	566	ARG
1	B	568	ARG
2	C	17	GLN
2	C	18	ASN
2	C	58	LYS
2	C	82	VAL
2	C	119	ARG
2	C	242	LYS
2	C	267	LYS
2	C	280	VAL
2	C	281	ILE
2	C	297	ASP
2	C	303	ASN

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Mol	Chain	Res	Type
2	C	361	GLU
2	D	2	GLU
2	D	5	VAL
2	D	6	VAL
2	D	10	GLN
2	D	12	LYS
2	D	13	LYS
2	D	26	ASN
2	D	54	GLU
2	D	60	GLU
2	D	77	VAL
2	D	116	VAL
2	D	129	ARG
2	D	171	ASP
2	D	230	LYS
2	D	234	MET
2	D	256	GLU
2	D	263	TRP
2	D	267	LYS
2	D	331	GLU
2	D	336	GLU
2	D	361	GLU
2	D	385	ASN
2	D	394	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	32	GLN
1	A	52	HIS
1	A	57	HIS
1	A	64	GLN
1	A	104	ASN
1	A	113	HIS
1	A	167	GLN
1	A	188	ASN
1	A	193	HIS
1	A	292	HIS
1	A	373	GLN
1	A	377	ASN
1	A	428	GLN

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Mol	Chain	Res	Type
1	A	443	ASN
1	A	549	GLN
1	B	32	GLN
1	B	37	GLN
1	B	64	GLN
1	B	70	ASN
1	B	85	HIS
1	B	104	ASN
1	B	113	HIS
1	B	127	GLN
1	B	204	ASN
1	B	292	HIS
1	B	306	GLN
1	B	309	ASN
1	B	352	HIS
1	B	373	GLN
1	B	377	ASN
1	B	549	GLN
2	C	17	GLN
2	C	76	GLN
2	C	80	GLN
2	C	120	GLN
2	C	288	GLN
2	C	303	ASN
2	C	366	HIS
2	D	26	ASN
2	D	76	GLN
2	D	193	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 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	$\#|Z| > 2$
4	ATP	B	1761	5	26,33,33	1.22	3 (11%)	31,52,52	2.11	9 (29%)
4	ATP	A	1760	5	26,33,33	1.00	2 (7%)	31,52,52	1.20	2 (6%)
3	AMP	A	1604	-	22,25,25	0.99	1 (4%)	25,38,38	1.27	2 (8%)
3	AMP	B	1604	-	22,25,25	1.02	1 (4%)	25,38,38	1.39	3 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	B	1761	5	-	5/18/38/38	0/3/3/3
4	ATP	A	1760	5	-	1/18/38/38	0/3/3/3
3	AMP	A	1604	-	-	0/6/26/26	0/3/3/3
3	AMP	B	1604	-	-	0/6/26/26	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1761	ATP	O4'-C1'	3.11	1.45	1.41
3	B	1604	AMP	C5-C4	2.57	1.47	1.40
3	A	1604	AMP	C5-C4	2.56	1.47	1.40
4	B	1761	ATP	C5-C4	2.56	1.47	1.40
4	A	1760	ATP	C5-C4	2.48	1.47	1.40
4	B	1761	ATP	C2-N3	2.20	1.35	1.32
4	A	1760	ATP	C2-N3	2.13	1.35	1.32

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1761	ATP	PB-O3B-PG	-6.73	109.72	132.83
4	B	1761	ATP	PA-O3A-PB	-4.47	117.49	132.83
3	B	1604	AMP	N3-C2-N1	-3.50	123.21	128.68
4	B	1761	ATP	O5'-C5'-C4'	3.39	120.65	108.99
3	A	1604	AMP	N3-C2-N1	-3.24	123.61	128.68
4	A	1760	ATP	N3-C2-N1	-3.18	123.71	128.68
4	B	1761	ATP	N3-C2-N1	-3.10	123.84	128.68
4	B	1761	ATP	C2'-C3'-C4'	3.06	108.59	102.64
4	B	1761	ATP	C3'-C2'-C1'	2.79	105.17	100.98
3	B	1604	AMP	C4-C5-N7	-2.72	106.56	109.40
4	A	1760	ATP	C4-C5-N7	-2.59	106.70	109.40
3	A	1604	AMP	C4-C5-N7	-2.32	106.98	109.40
4	B	1761	ATP	N6-C6-N1	2.19	123.12	118.57
4	B	1761	ATP	O3G-PG-O2G	2.19	115.99	107.64
4	B	1761	ATP	C4-C5-N7	-2.08	107.23	109.40
3	B	1604	AMP	C2-N1-C6	2.03	122.22	118.75

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1761	ATP	C4'-C5'-O5'-PA
4	B	1761	ATP	C3'-C4'-C5'-O5'
4	B	1761	ATP	O4'-C4'-C5'-O5'
4	A	1760	ATP	C4'-C5'-O5'-PA
4	B	1761	ATP	PA-O3A-PB-O2B
4	B	1761	ATP	PB-O3A-PA-O2A

There are no ring outliers.

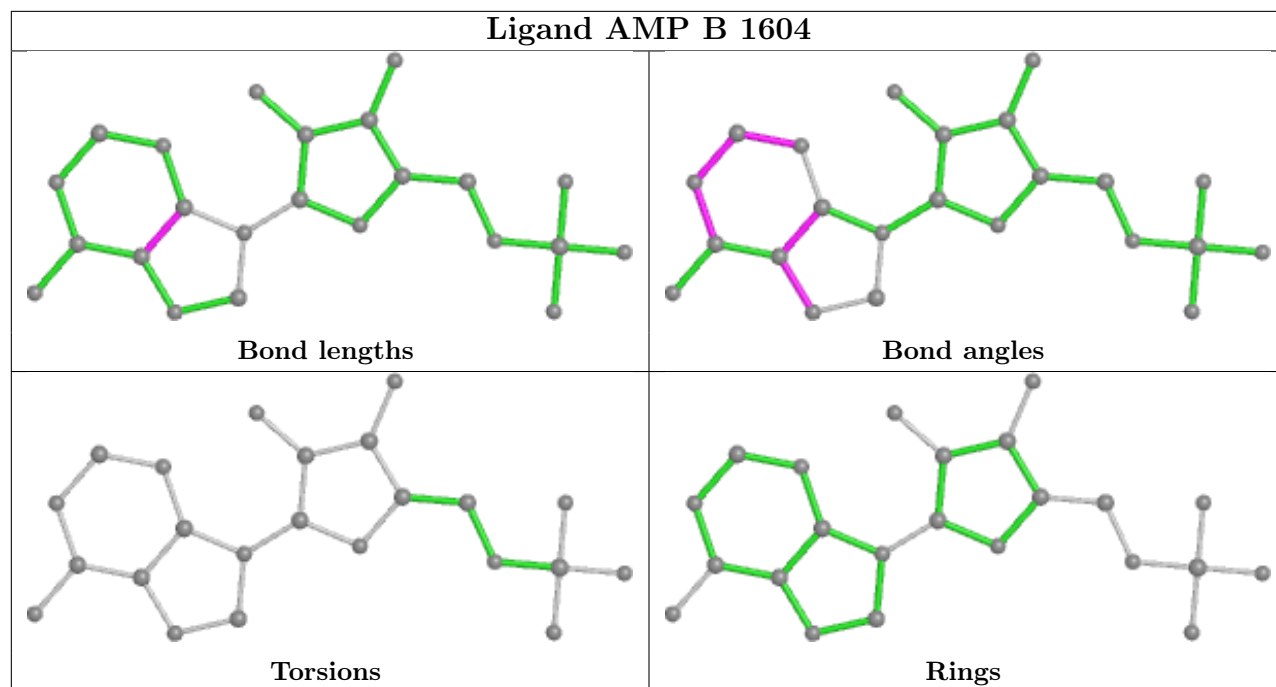3 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1761	ATP	12	0
4	A	1760	ATP	6	0
3	B	1604	AMP	2	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ATP B 1761

Bond lengths — Bond angles — Torsions — Rings

Ligand ATP A 1760

Bond lengths

Bond angles

Torsions

Rings

Ligand AMP A 1604

Bond lengths

Bond angles

Torsions

Rings

Ligand AMP B 1604
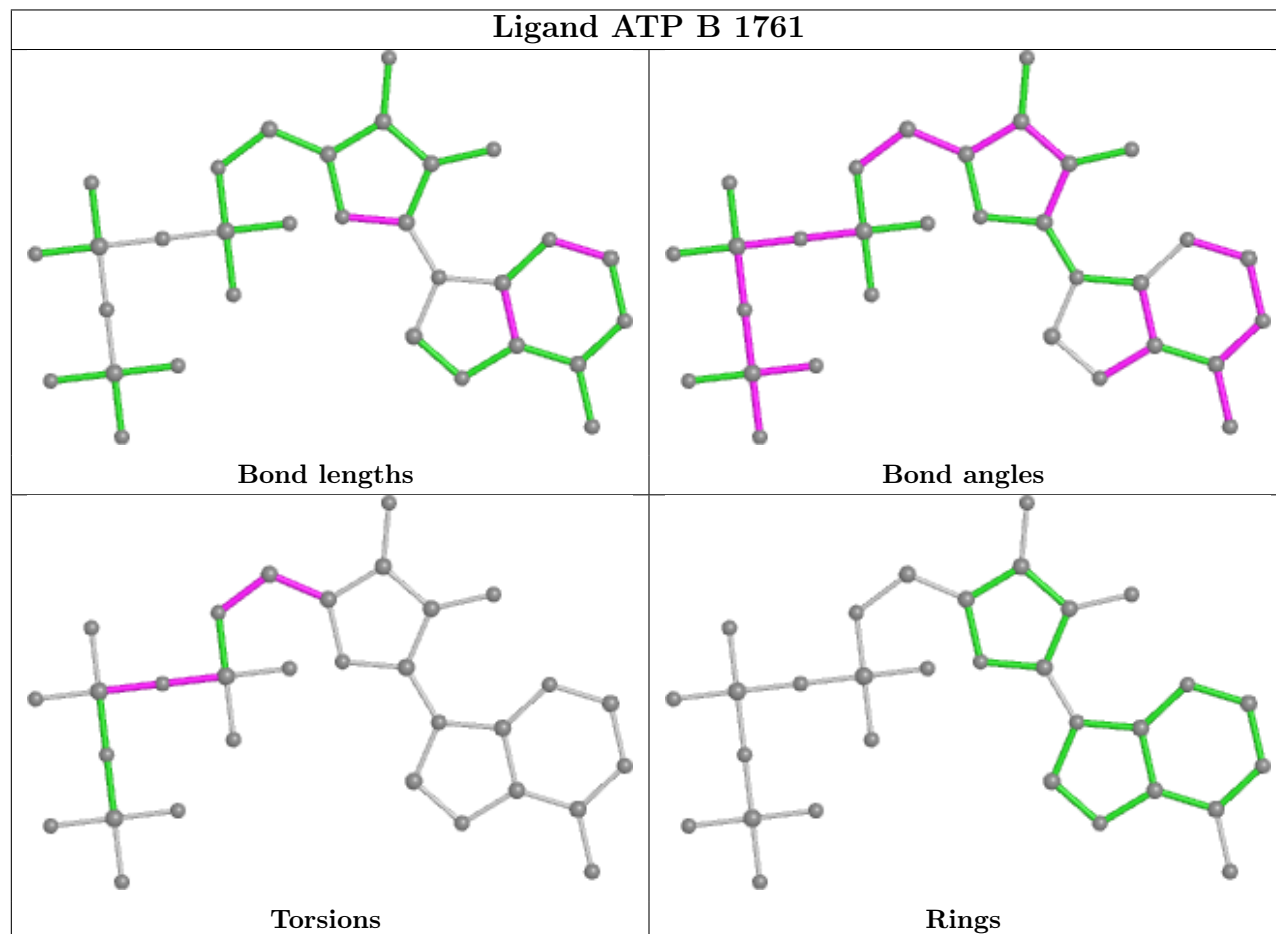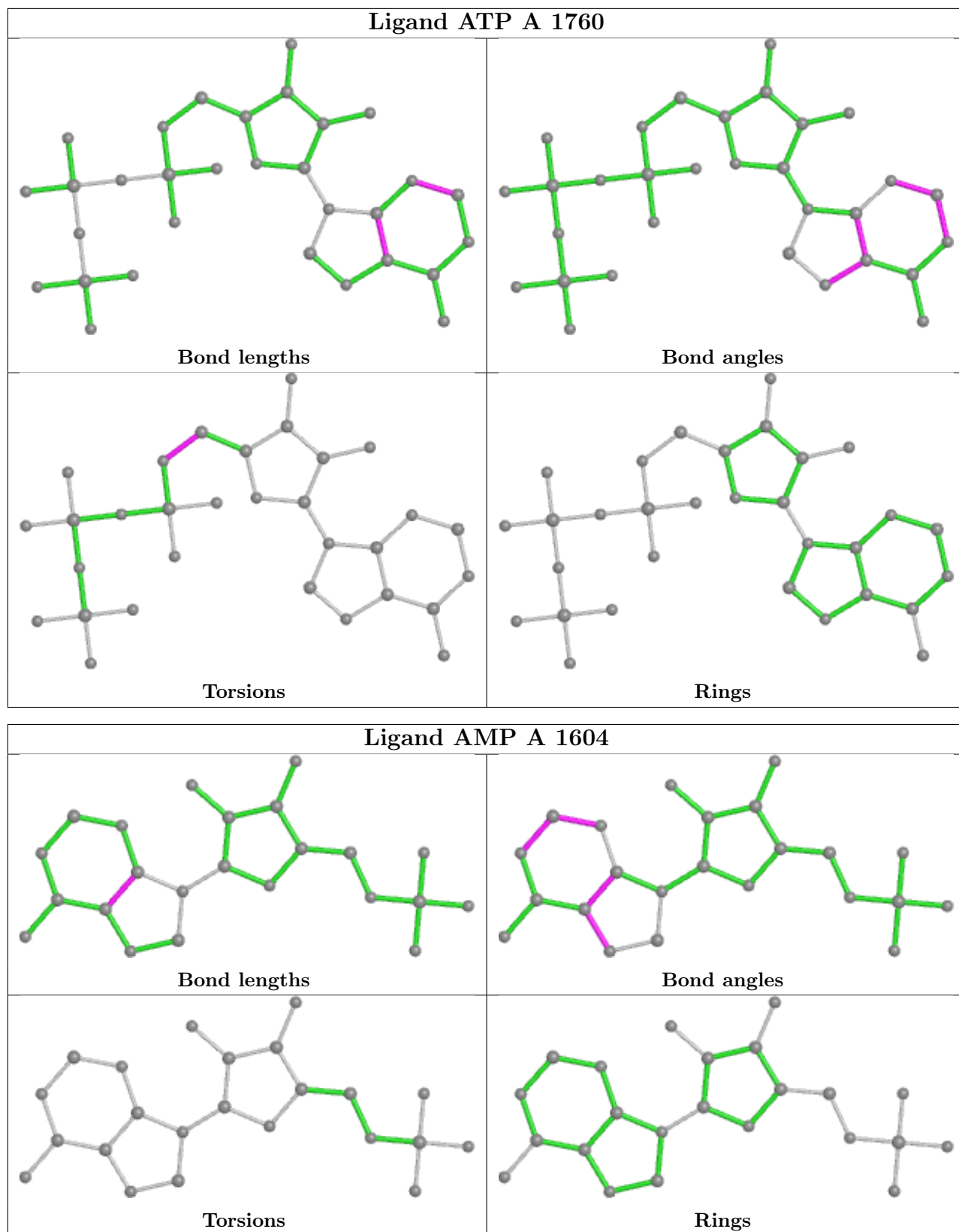
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	554/578 (95%)	0.17	19 (3%)	45	40	54, 74, 105, 124	0
1	B	561/578 (97%)	0.17	17 (3%)	50	45	50, 70, 107, 129	0
2	C	415/416 (99%)	-0.06	6 (1%)	75	75	44, 58, 86, 96	0
2	D	415/416 (99%)	0.01	7 (1%)	70	69	50, 66, 83, 108	0
All	All	1945/1988 (97%)	0.09	49 (2%)	57	55	44, 68, 100, 129	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	133	ARG	4.4
1	B	130	ARG	4.0
1	B	147	HIS	3.9
1	B	131	ARG	3.8
1	B	132	PHE	3.8
2	D	18	ASN	3.7
2	C	17	GLN	3.4
1	A	566	ARG	3.4
1	B	191	LYS	3.2
1	A	174	HIS	3.1
2	C	19	GLY	3.1
1	B	174	HIS	3.1
1	A	342	PHE	3.0
1	B	52	HIS	2.9
2	D	17	GLN	2.8
1	B	467	ARG	2.8
1	A	52	HIS	2.7
1	B	134	THR	2.7
2	C	16	LEU	2.7
2	D	58	LYS	2.7
1	A	306	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	349	SER	2.6
1	B	41	HIS	2.5
1	A	41	HIS	2.5
1	A	146	ASP	2.4
1	B	534	GLU	2.4
1	A	218	GLY	2.4
2	C	18	ASN	2.3
2	C	272	GLY	2.3
2	D	9	ALA	2.3
1	A	399	GLU	2.3
1	A	308	CYS	2.3
1	A	148	GLY	2.3
1	B	107	TYR	2.3
1	B	351	ALA	2.2
1	A	114	ARG	2.2
1	A	70	ASN	2.2
1	A	445	ILE	2.2
1	A	185	GLY	2.2
1	A	458	MET	2.2
2	D	362	MET	2.2
1	B	569	PHE	2.1
2	D	260	GLY	2.1
2	C	2	GLU	2.1
1	A	430	GLU	2.0
2	D	16	LEU	2.0
1	A	341	LYS	2.0
1	B	405	GLY	2.0
1	A	571	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 monosaccharides 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
4	ATP	B	1761	31/31	0.88	0.22	55,57,67,68	0
4	ATP	A	1760	31/31	0.93	0.17	63,65,70,70	0
5	MG	A	579	1/1	0.94	0.15	79,79,79,79	0
5	MG	B	579	1/1	0.94	0.11	72,72,72,72	0
3	AMP	B	1604	23/23	0.96	0.21	62,65,66,66	0
3	AMP	A	1604	23/23	0.98	0.17	64,66,67,68	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 B 1761:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)
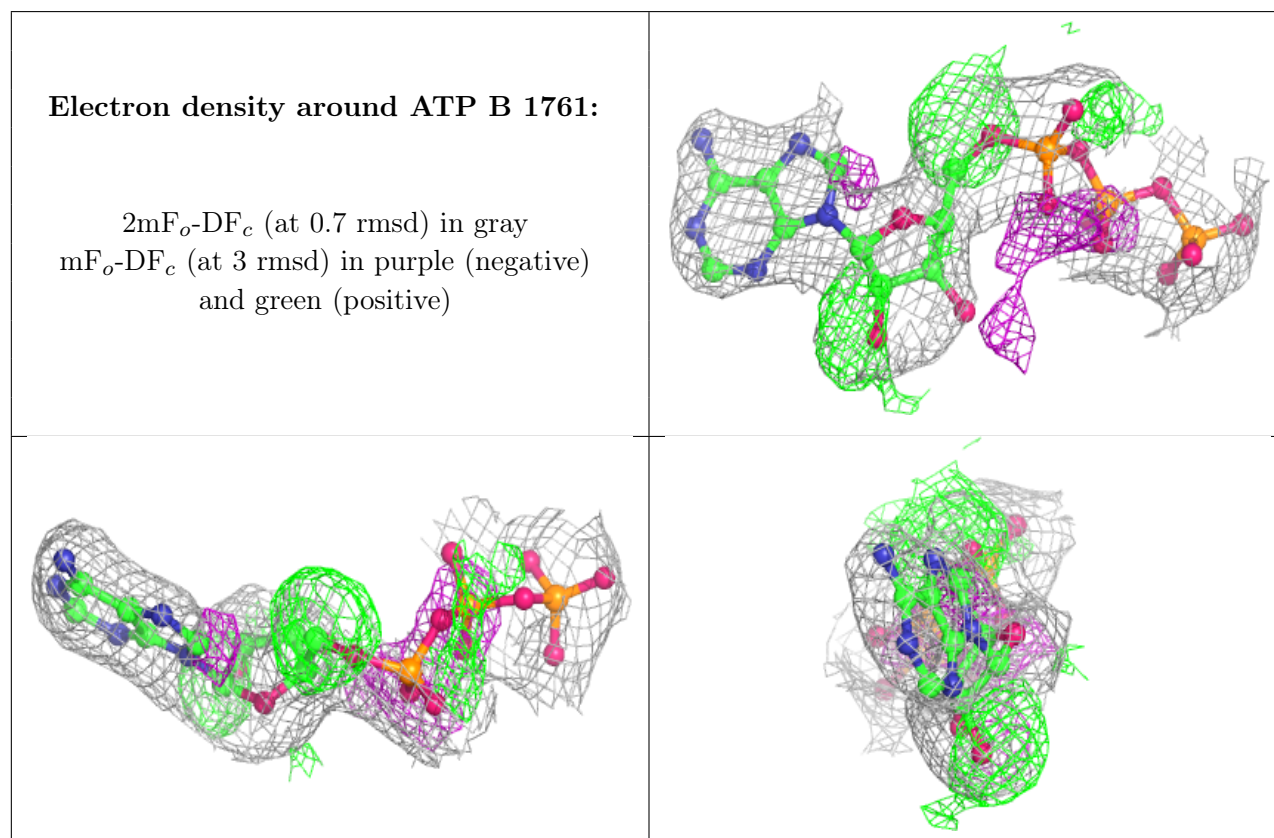
Electron density around ATP A 1760:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
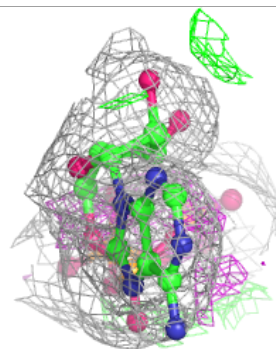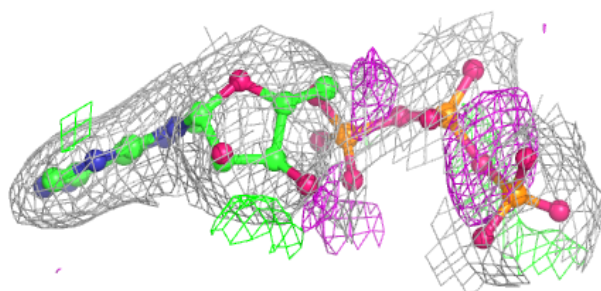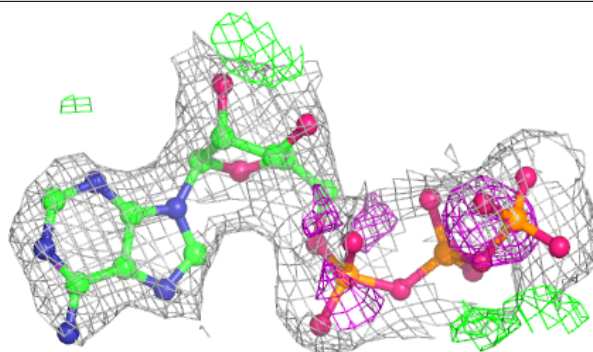
Electron density around AMP B 1604:

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

Electron density around AMP A 1604:

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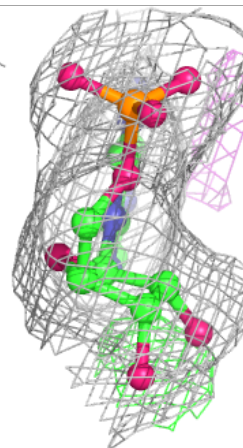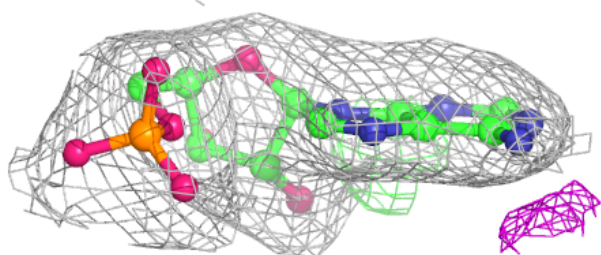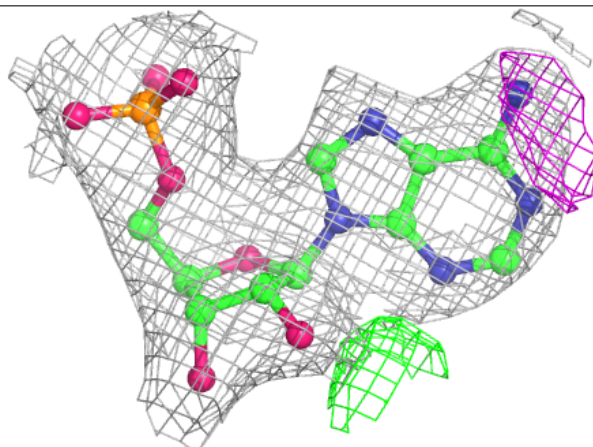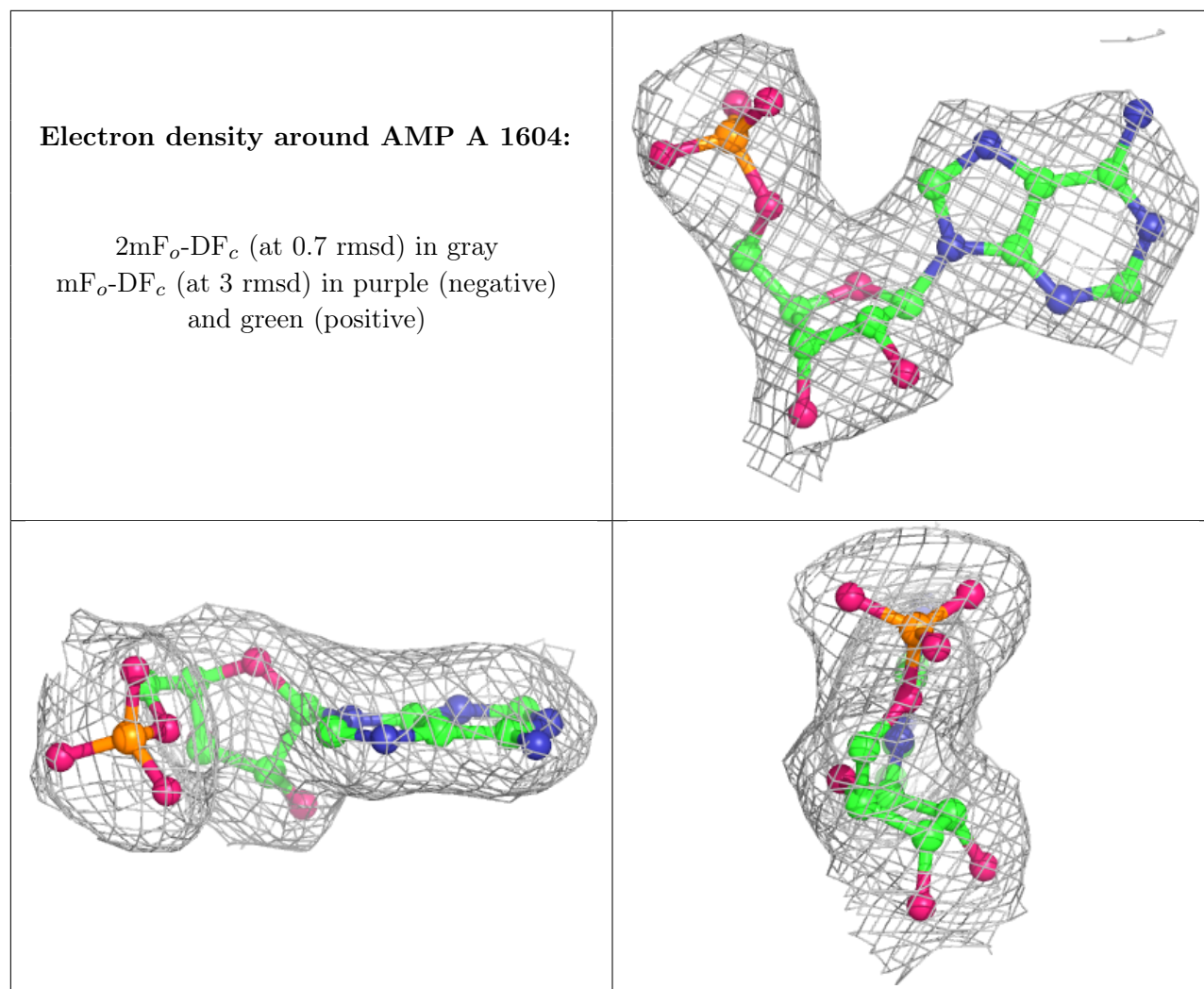
6.5 Other polymers (i)

There are no such residues in this entry.