



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 10:53 pm BST

PDB ID : 3EPS  
Title : The crystal structure of isocitrate dehydrogenase kinase/phosphatase from E. coli  
Authors : Zheng, J.; Jia, Z.; Montreal-Kingston Bacterial Structural Genomics Initiative (BSGI)  
Deposited on : 2008-09-29  
Resolution : 2.80 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](mailto: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.

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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 : 2.11  
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) : 2.11

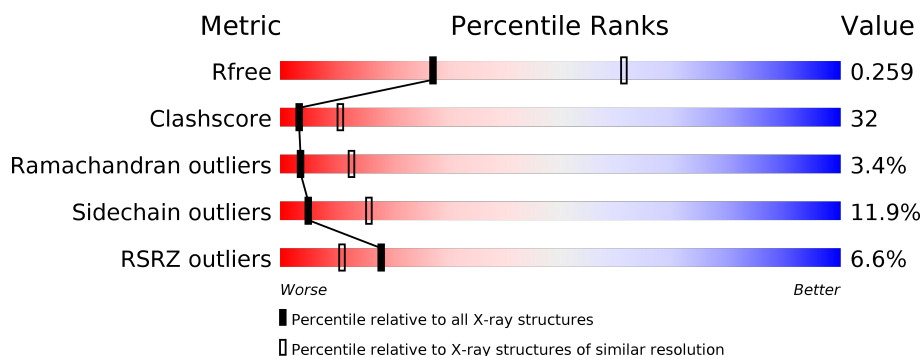
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	578	<div> <div>5%</div> <div> <div></div> <div>51%</div> <div>39%</div> <div>7%</div> <div>..</div> </div> </div>
1	B	578	<div> <div>7%</div> <div> <div></div> <div>44%</div> <div>42%</div> <div>11%</div> <div>..</div> </div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9467 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.

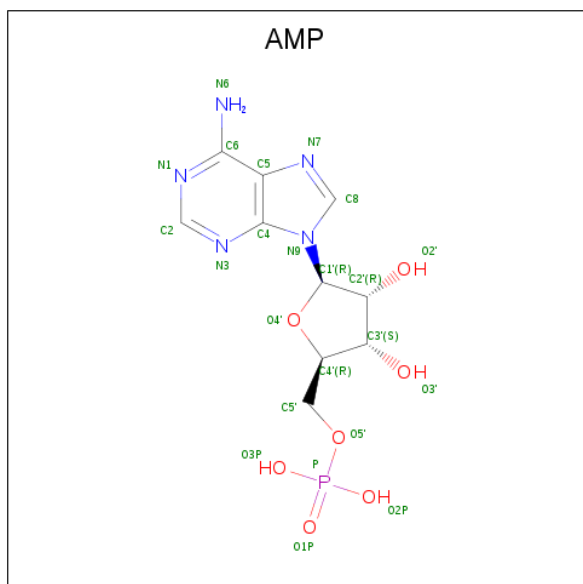
- Molecule 1 is a protein called Isocitrate dehydrogenase kinase/phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	566	Total	C	N	O	S	0	0	0
			4686	3013	827	825	21			
1	B	559	Total	C	N	O	S	0	0	0
			4621	2967	816	817	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP Q8X607
B	1	SER	-	expression tag	UNP Q8X607

- Molecule 2 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).



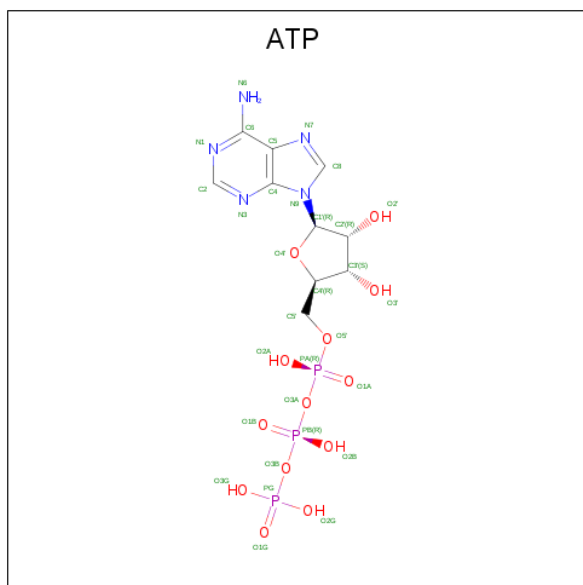
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is water.

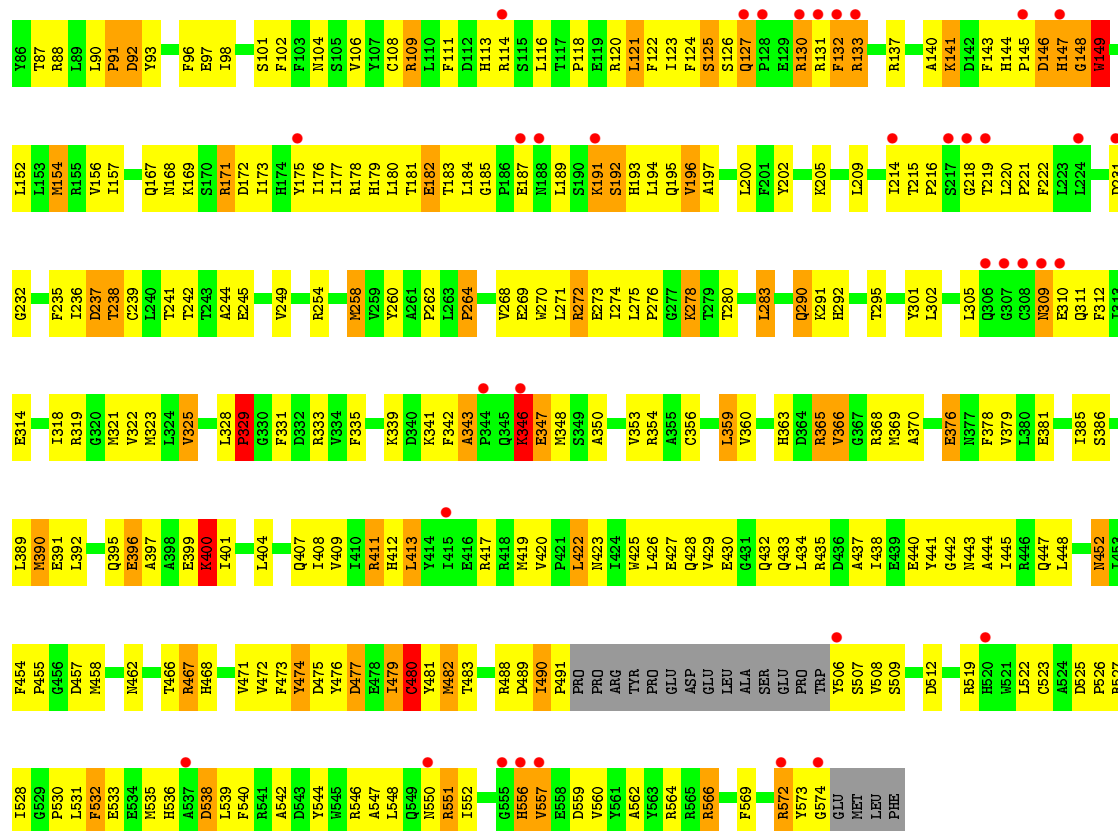
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	28	Total	O	0	0
			28	28		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	22	Total	O	0	0
			22	22		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.59 Å   124.59 Å   267.63 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	30.00 – 2.80 29.53 – 2.80	Depositor EDS
% Data completeness (in resolution range)	86.5 (30.00-2.80) 94.3 (29.53-2.80)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 2.80 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.233   ,   0.268 0.233   ,   0.259	Depositor DCC
$R_{free}$ test set	2527 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	80.5	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 60.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9467	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: AMP, 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	0.42	0/4815	0.68	3/6523 (0.0%)
1	B	0.39	0/4743	0.61	0/6421
All	All	0.41	0/9558	0.65	3/12944 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	359	LEU	CA-CB-CG	6.04	129.19	115.30
1	A	413	LEU	CA-CB-CG	5.40	127.71	115.30
1	A	147	HIS	N-CA-C	-5.10	97.24	111.00

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	4686	0	4603	282	0
1	B	4621	0	4542	324	0
2	A	23	0	12	2	0
2	B	23	0	12	2	0
3	A	31	0	12	5	0
3	B	31	0	12	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	28	0	0	2	0
5	B	22	0	0	4	0
All	All	9467	0	9193	604	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 32.

All (604) 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:A:242:THR:HB	1:A:245:GLU:HG3	1.22	1.11
1:B:242:THR:HB	1:B:245:GLU:HG3	1.23	1.11
1:B:143:PHE:HB3	1:B:152:LEU:HD11	1.21	1.07
1:A:143:PHE:HB3	1:A:152:LEU:HD11	1.44	0.99
1:A:135:ILE:H	1:A:135:ILE:HD12	1.26	0.99
1:B:566:ARG:HH21	1:B:566:ARG:HB3	1.30	0.96
1:A:368:ARG:HE	1:A:447:GLN:NE2	1.64	0.95
1:B:104:ASN:HD21	1:B:122:PHE:H	0.99	0.95
1:A:167:GLN:HB2	1:A:233:GLU:HB3	1.50	0.94
1:A:212:LYS:HG2	1:A:274:ILE:HD11	1.51	0.90
1:A:215:THR:HG22	1:A:217:SER:H	1.37	0.87
1:A:476:TYR:O	1:A:479:ILE:HG22	1.74	0.86
1:A:566:ARG:HH21	1:A:566:ARG:HB3	1.38	0.86
1:B:404:LEU:HD23	1:B:407:GLN:HE21	1.40	0.86
1:A:365:ARG:HG2	1:A:365:ARG:HH21	1.40	0.86
1:A:419:MET:HE2	1:A:466:THR:HG22	1.57	0.85
1:A:566:ARG:HA	1:A:571:VAL:HG11	1.58	0.85
1:A:551:ARG:HH11	1:A:551:ARG:HG2	1.42	0.84
1:B:466:THR:HG22	1:B:468:HIS:H	1.41	0.84
1:B:148:GLY:HA2	1:B:152:LEU:H	1.44	0.83
1:B:454:PHE:HB2	1:B:482:MET:HE3	1.61	0.82
1:B:28:THR:HA	1:B:258:MET:HE2	1.59	0.82
1:B:452:ASN:HD21	1:B:483:THR:H	1.28	0.82
1:A:208:TRP:CH2	1:A:225:PRO:HG3	2.16	0.81
1:B:452:ASN:HD22	1:B:482:MET:HB3	1.46	0.80
1:A:8:LEU:O	1:A:12:THR:HG23	1.82	0.80
1:A:237:ASP:O	1:A:238:THR:HG22	1.82	0.80
1:B:346:LYS:HE2	1:B:346:LYS:HA	1.64	0.79
1:A:411:ARG:CZ	1:B:507:SER:HB2	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:THR:CB	1:A:245:GLU:HG3	2.10	0.79
1:A:475:ASP:OD2	3:A:1605:ATP:O1G	1.99	0.79
1:A:76:ALA:HB1	1:A:120:ARG:HH12	1.48	0.78
1:B:145:PRO:HA	1:B:148:GLY:HA3	1.64	0.78
1:B:368:ARG:HE	1:B:447:GLN:HE21	1.31	0.78
1:A:419:MET:CE	1:A:472:VAL:HB	2.14	0.78
1:B:445:ILE:HD12	1:B:458:MET:HE2	1.66	0.78
1:B:348:MET:SD	1:B:477:ASP:OD1	2.43	0.77
1:B:417:ARG:HD2	5:B:585:HOH:O	1.84	0.77
1:A:124:PHE:O	1:A:125:SER:HB2	1.82	0.77
1:B:124:PHE:O	1:B:125:SER:HB3	1.84	0.77
1:B:477:ASP:HB3	3:B:1605:ATP:O1G	1.84	0.76
1:B:473:PHE:HE2	1:B:479:ILE:HD13	1.51	0.76
1:B:130:ARG:HB3	1:B:130:ARG:HH21	1.51	0.76
1:B:466:THR:HG23	1:B:467:ARG:NH1	2.01	0.76
1:B:310:GLU:HB3	1:B:329:PRO:HG2	1.68	0.75
1:B:221:PRO:HG3	1:B:274:ILE:HG23	1.67	0.75
1:B:141:LYS:HE3	1:B:141:LYS:HA	1.69	0.75
1:B:438:ILE:HD12	1:B:531:LEU:HD22	1.68	0.75
1:B:466:THR:HG21	5:B:586:HOH:O	1.85	0.75
1:B:272:ARG:NH1	1:B:280:THR:OG1	2.19	0.74
1:A:366:VAL:CG2	1:A:560:VAL:HG21	2.17	0.74
1:B:143:PHE:HB3	1:B:152:LEU:CD1	2.10	0.74
1:A:366:VAL:HG22	1:A:560:VAL:HG21	1.69	0.74
1:A:168:ASN:CG	1:A:171:ARG:HB2	2.07	0.74
1:A:510:PRO:HA	5:A:596:HOH:O	1.87	0.73
1:B:454:PHE:CD1	1:B:482:MET:HE1	2.22	0.73
1:B:33:GLN:O	1:B:37:GLN:HG2	1.89	0.73
1:B:542:ALA:O	1:B:546:ARG:HG3	1.88	0.73
1:A:453:ILE:HG23	1:A:479:ILE:HG13	1.70	0.73
1:B:111:PHE:O	1:B:114:ARG:HG2	1.89	0.72
1:A:9:ILE:HG23	1:A:65:LEU:HD21	1.70	0.72
1:B:475:ASP:OD2	3:B:1605:ATP:O1G	2.08	0.72
1:B:81:ARG:HB2	1:B:81:ARG:HH21	1.55	0.72
1:B:116:LEU:HB3	1:B:121:LEU:HD11	1.72	0.71
1:A:419:MET:HE1	1:A:472:VAL:HB	1.70	0.71
1:A:242:THR:HB	1:A:245:GLU:CG	2.12	0.71
1:B:143:PHE:CE2	1:B:156:VAL:HG12	2.26	0.71
1:B:473:PHE:CE2	1:B:479:ILE:HD13	2.26	0.70
1:A:152:LEU:O	1:A:156:VAL:HG13	1.90	0.70
1:B:87:THR:O	1:B:91:PRO:HD3	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:PHE:CE2	1:A:269:GLU:HG3	2.26	0.70
1:A:368:ARG:HE	1:A:447:GLN:HE21	1.37	0.69
1:B:466:THR:HG23	1:B:467:ARG:HH12	1.56	0.69
1:A:81:ARG:HG3	1:A:81:ARG:HH21	1.56	0.69
1:B:411:ARG:HH11	1:B:411:ARG:HB2	1.56	0.69
1:B:104:ASN:ND2	1:B:122:PHE:H	1.83	0.69
1:A:124:PHE:O	1:A:125:SER:CB	2.39	0.68
1:B:454:PHE:HB2	1:B:482:MET:CE	2.21	0.68
1:B:531:LEU:HD23	1:B:531:LEU:O	1.93	0.68
1:A:171:ARG:HB3	1:A:171:ARG:HH11	1.59	0.68
1:A:76:ALA:CB	1:A:120:ARG:HH22	2.06	0.68
1:B:275:LEU:N	1:B:276:PRO:HD3	2.09	0.68
1:B:350:ALA:O	1:B:354:ARG:HG3	1.93	0.68
1:B:574:GLY:HA3	5:B:584:HOH:O	1.93	0.68
1:B:572:ARG:HA	1:B:572:ARG:HE	1.57	0.68
1:B:137:ARG:HG3	1:B:137:ARG:HH21	1.57	0.68
1:B:72:GLN:H	1:B:72:GLN:CD	1.97	0.68
1:B:379:VAL:HG22	1:B:409:VAL:HG22	1.76	0.67
1:B:564:ARG:HD3	1:B:566:ARG:NH1	2.10	0.67
1:A:443:ASN:O	1:A:447:GLN:HG3	1.94	0.67
1:A:522:LEU:O	1:A:528:ILE:HD11	1.94	0.67
1:B:130:ARG:NH2	1:B:130:ARG:HB3	2.08	0.67
1:A:571:VAL:HG12	1:A:572:ARG:N	2.09	0.67
1:A:422:LEU:HD22	1:A:426:LEU:HG	1.76	0.66
1:B:149:TRP:O	1:B:177:ILE:HD11	1.95	0.66
1:A:324:LEU:HD12	1:A:324:LEU:C	2.15	0.66
1:B:489:ASP:O	1:B:490:ILE:HB	1.95	0.66
1:A:32:GLN:O	1:A:36:GLU:HG3	1.95	0.66
1:A:475:ASP:OD2	1:A:478:GLU:HG2	1.95	0.66
1:A:135:ILE:H	1:A:135:ILE:CD1	2.03	0.66
1:B:274:ILE:HG22	1:B:275:LEU:H	1.61	0.65
1:A:18:ASP:OD2	1:A:93:TYR:HE1	1.78	0.65
1:B:32:GLN:HA	1:B:202:TYR:CE2	2.31	0.65
1:B:260:TYR:CE1	1:B:262:PRO:HG3	2.32	0.65
1:A:157:ILE:HD12	1:A:173:ILE:HG12	1.78	0.65
1:A:365:ARG:CG	1:A:365:ARG:HH21	2.10	0.64
1:A:40:TRP:CD2	1:A:205:LYS:HG2	2.32	0.64
1:B:366:VAL:O	1:B:366:VAL:HG13	1.98	0.64
1:B:81:ARG:NH2	1:B:81:ARG:HB2	2.11	0.64
1:A:40:TRP:CZ3	1:A:205:LYS:HA	2.33	0.64
1:A:296:GLU:O	1:A:300:GLU:HG3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:VAL:HG13	1:B:283:LEU:HB3	1.78	0.63
1:B:400:LYS:H	1:B:400:LYS:HD2	1.63	0.63
1:B:397:ALA:O	1:B:401:ILE:HG22	1.98	0.63
1:A:208:TRP:CZ3	1:A:225:PRO:HG3	2.34	0.63
1:A:322:VAL:C	1:A:339:LYS:HD3	2.19	0.63
1:B:148:GLY:O	1:B:149:TRP:HB2	1.97	0.63
1:B:346:LYS:HD3	1:B:348:MET:HG2	1.80	0.63
1:A:33:GLN:O	1:A:37:GLN:HG2	1.98	0.63
1:A:519:ARG:HD3	1:A:540:PHE:CD2	2.34	0.63
1:A:149:TRP:O	1:A:150:GLU:HB2	1.99	0.62
1:A:113:HIS:HE1	2:A:1604:AMP:O2P	1.81	0.62
1:B:365:ARG:HH21	1:B:365:ARG:HG2	1.63	0.62
1:B:254:ARG:HH11	1:B:254:ARG:HG2	1.64	0.62
1:A:453:ILE:HG23	1:A:479:ILE:CG1	2.30	0.62
1:B:72:GLN:C	1:B:74:THR:H	2.02	0.62
1:B:88:ARG:O	1:B:91:PRO:HD2	2.00	0.62
1:A:372:THR:HG22	1:A:416:GLU:HB3	1.81	0.61
1:A:528:ILE:HG13	1:A:529:GLY:N	2.15	0.61
1:A:145:PRO:HA	1:A:148:GLY:HA3	1.83	0.61
1:A:138:PRO:O	1:A:139:LEU:HB3	1.98	0.61
1:A:140:ALA:O	1:A:141:LYS:HE2	2.00	0.61
1:B:309:ASN:N	1:B:309:ASN:ND2	2.45	0.61
1:B:443:ASN:O	1:B:447:GLN:HG3	2.00	0.61
1:A:219:THR:HG21	1:A:273:GLU:OE2	2.01	0.61
1:B:191:LYS:C	1:B:191:LYS:HE2	2.20	0.61
1:B:547:ALA:HA	1:B:550:ASN:HD22	1.64	0.61
1:B:566:ARG:HB3	1:B:566:ARG:NH2	2.11	0.61
1:A:171:ARG:HD2	1:A:175:TYR:CE2	2.36	0.61
1:A:551:ARG:NH1	1:A:551:ARG:HG2	2.15	0.61
1:A:215:THR:HG23	1:A:216:PRO:HD2	1.82	0.61
1:A:178:ARG:HD2	1:A:573:TYR:CZ	2.35	0.61
1:B:169:LYS:O	1:B:173:ILE:HG13	2.00	0.61
1:B:79:LEU:HD13	1:B:111:PHE:HZ	1.65	0.61
1:A:21:TYR:OH	1:A:264:PRO:HG3	2.00	0.60
1:A:422:LEU:HD22	1:A:422:LEU:O	2.01	0.60
1:A:440:GLU:HG3	1:A:471:VAL:HG23	1.83	0.60
1:A:167:GLN:HG2	1:A:233:GLU:OE2	2.01	0.60
1:A:542:ALA:O	1:A:546:ARG:HG3	2.01	0.60
1:B:173:ILE:O	1:B:177:ILE:HG12	2.01	0.60
1:B:572:ARG:O	1:B:573:TYR:HD2	1.83	0.60
1:A:76:ALA:HB2	1:A:120:ARG:HH22	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:LEU:O	1:B:156:VAL:HG13	2.02	0.60
1:A:449:ALA:HB1	1:A:482:MET:HE1	1.84	0.60
1:A:441:TYR:CE1	1:A:532:PHE:HZ	2.20	0.60
1:A:76:ALA:HB1	1:A:120:ARG:NH1	2.16	0.60
1:B:452:ASN:ND2	1:B:482:MET:HB3	2.15	0.60
1:A:221:PRO:HA	1:A:274:ILE:HD12	1.83	0.60
1:B:21:TYR:OH	1:B:264:PRO:HG3	2.02	0.60
1:B:391:GLU:O	1:B:395:GLN:HG3	2.02	0.59
1:A:143:PHE:CE2	1:A:156:VAL:HG12	2.37	0.59
1:A:375:PHE:HB2	1:A:413:LEU:CD2	2.32	0.59
1:B:441:TYR:O	1:B:445:ILE:HG12	2.02	0.59
1:A:548:LEU:O	1:A:552:ILE:HG12	2.01	0.59
1:B:171:ARG:HH11	1:B:171:ARG:HB3	1.67	0.59
1:B:466:THR:HG22	1:B:468:HIS:N	2.14	0.59
1:A:356:CYS:O	1:A:360:VAL:HG12	2.03	0.59
1:A:359:LEU:HD21	1:A:481:TYR:CZ	2.37	0.59
1:B:28:THR:HA	1:B:258:MET:CE	2.31	0.59
1:B:440:GLU:HB3	1:B:471:VAL:HG23	1.84	0.59
1:A:149:TRP:HB3	1:A:177:ILE:HD12	1.84	0.59
1:B:168:ASN:OD1	1:B:171:ARG:HB2	2.03	0.59
1:A:209:LEU:HD23	1:A:210:VAL:N	2.18	0.58
1:B:566:ARG:HH21	1:B:566:ARG:CB	2.11	0.58
1:A:341:LYS:HE2	1:B:347:GLU:OE2	2.04	0.58
1:B:531:LEU:HD21	1:B:535:MET:CE	2.33	0.58
1:B:274:ILE:HG22	1:B:275:LEU:N	2.18	0.58
1:B:126:SER:O	1:B:127:GLN:HB3	2.04	0.58
1:B:145:PRO:C	1:B:147:HIS:H	2.06	0.58
1:B:241:THR:HG22	1:B:241:THR:O	2.03	0.58
1:B:242:THR:HG22	1:B:244:ALA:H	1.68	0.58
1:A:275:LEU:HD12	1:A:275:LEU:O	2.04	0.58
1:B:455:PRO:HB2	1:B:458:MET:HE3	1.86	0.58
1:A:140:ALA:C	1:A:141:LYS:HE2	2.24	0.57
1:A:254:ARG:NH1	1:A:367:GLY:HA3	2.18	0.57
1:B:339:LYS:HE3	1:B:396:GLU:HG3	1.86	0.57
1:B:149:TRP:HA	1:B:149:TRP:CE3	2.39	0.57
1:B:149:TRP:NE1	1:B:189:LEU:HG	2.19	0.57
1:B:195:GLN:NE2	1:B:270:TRP:HE1	2.02	0.57
1:A:477:ASP:OD2	3:A:1605:ATP:O2G	2.21	0.57
1:B:309:ASN:HD22	1:B:309:ASN:N	2.00	0.57
1:B:76:ALA:O	1:B:80:LEU:HB2	2.04	0.57
1:A:466:THR:HB	1:A:467:ARG:NH2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:ALA:N	1:B:476:TYR:OH	2.38	0.57
1:A:163:ARG:O	1:A:164:LEU:HD23	2.04	0.57
1:A:244:ALA:O	1:A:248:ILE:HD12	2.04	0.57
1:A:475:ASP:OD2	3:A:1605:ATP:PG	2.62	0.57
1:B:309:ASN:HD22	1:B:309:ASN:H	1.52	0.57
1:B:325:VAL:HG11	3:B:1605:ATP:O4'	2.04	0.57
1:A:571:VAL:CG1	1:A:572:ARG:HE	2.17	0.56
1:B:454:PHE:HD1	1:B:482:MET:HE1	1.68	0.56
1:A:167:GLN:O	1:A:168:ASN:HB3	2.05	0.56
1:B:254:ARG:NH1	1:B:254:ARG:HG2	2.21	0.56
1:B:85:HIS:O	1:B:88:ARG:HB2	2.05	0.56
1:A:135:ILE:N	1:A:135:ILE:HD12	2.10	0.56
1:B:149:TRP:HA	1:B:149:TRP:HE3	1.71	0.56
1:A:413:LEU:HD23	1:A:413:LEU:C	2.25	0.56
1:A:145:PRO:CB	1:A:148:GLY:HA3	2.35	0.56
1:A:209:LEU:HD13	1:A:224:LEU:HD12	1.88	0.56
1:A:54:TYR:CD1	1:A:291:LYS:HG3	2.41	0.56
1:B:120:ARG:C	1:B:121:LEU:HD23	2.26	0.56
1:B:359:LEU:O	1:B:363:HIS:HB2	2.05	0.56
1:B:378:PHE:HB2	1:B:413:LEU:HD11	1.88	0.56
1:B:432:GLN:HE21	1:B:432:GLN:HA	1.71	0.56
1:B:476:TYR:O	1:B:479:ILE:HB	2.06	0.56
1:B:531:LEU:HD21	1:B:535:MET:HE1	1.86	0.56
1:A:209:LEU:C	1:A:209:LEU:HD23	2.26	0.55
1:A:429:VAL:HG13	1:A:433:GLN:HB3	1.88	0.55
1:A:145:PRO:CA	1:A:148:GLY:HA3	2.36	0.55
1:B:339:LYS:HE3	1:B:396:GLU:CG	2.37	0.55
1:B:81:ARG:CB	1:B:81:ARG:HH21	2.18	0.55
1:A:81:ARG:HG3	1:A:81:ARG:NH2	2.19	0.55
1:B:131:ARG:O	1:B:132:PHE:O	2.25	0.55
1:B:40:TRP:CE2	1:B:205:LYS:HG2	2.42	0.55
1:B:123:ILE:HD11	1:B:124:PHE:CE2	2.42	0.55
1:A:143:PHE:CD2	1:A:156:VAL:HG12	2.41	0.55
1:A:23:ARG:NE	5:A:588:HOH:O	2.35	0.55
1:B:22:GLY:O	1:B:26:GLU:HG2	2.07	0.55
1:B:109:ARG:CG	1:B:109:ARG:HH11	2.20	0.55
1:B:311:GLN:OE1	1:B:386:SER:HA	2.07	0.55
1:B:525:ASP:HB3	1:B:528:ILE:HG12	1.88	0.55
1:A:50:ARG:HD2	1:A:258:MET:CE	2.37	0.54
1:B:146:ASP:O	1:B:147:HIS:CG	2.60	0.54
1:B:411:ARG:NH1	1:B:411:ARG:HB2	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:PRO:O	1:A:241:THR:HA	2.08	0.54
1:A:513:VAL:O	1:A:515:PRO:HD3	2.08	0.54
1:A:322:VAL:O	1:A:339:LYS:HD3	2.07	0.54
1:A:184:LEU:HD11	1:A:213:LEU:HD21	1.89	0.54
1:A:441:TYR:HE1	1:A:532:PHE:HZ	1.54	0.54
1:B:113:HIS:CD2	1:B:376:GLU:HG3	2.43	0.54
1:B:140:ALA:HB2	1:B:197:ALA:HA	1.90	0.54
1:A:160:LEU:H	1:A:160:LEU:HD22	1.71	0.53
1:B:477:ASP:C	1:B:477:ASP:OD2	2.45	0.53
1:B:231:ASP:OD1	1:B:232:GLY:N	2.42	0.53
1:B:23:ARG:HA	1:B:23:ARG:HE	1.73	0.53
1:B:353:VAL:HG22	1:B:477:ASP:OD1	2.08	0.53
1:B:171:ARG:HD3	1:B:175:TYR:CE2	2.44	0.53
1:A:157:ILE:CD1	1:A:173:ILE:HG12	2.39	0.53
1:A:274:ILE:O	1:A:275:LEU:C	2.45	0.53
1:B:219:THR:HG21	1:B:273:GLU:OE2	2.08	0.53
1:B:96:PHE:CE1	1:B:127:GLN:HG2	2.43	0.53
1:A:139:LEU:C	1:A:139:LEU:HD23	2.28	0.53
1:A:168:ASN:ND2	1:A:171:ARG:H	2.07	0.53
1:B:422:LEU:HD22	1:B:426:LEU:HG	1.90	0.53
1:B:360:VAL:HG11	1:B:476:TYR:CD2	2.43	0.53
1:B:427:GLU:HA	1:B:427:GLU:OE2	2.08	0.53
1:A:149:TRP:O	1:A:150:GLU:CB	2.56	0.53
1:A:171:ARG:NH1	1:A:171:ARG:HB3	2.24	0.52
1:A:237:ASP:O	1:A:238:THR:CG2	2.54	0.52
1:B:104:ASN:HD21	1:B:122:PHE:N	1.84	0.52
1:B:321:MET:HE3	1:B:343:ALA:HB3	1.91	0.52
1:B:551:ARG:HE	1:B:551:ARG:HA	1.74	0.52
1:A:157:ILE:HG21	1:A:169:LYS:HD2	1.91	0.52
1:A:488:ARG:HB2	1:A:514:PHE:CD1	2.44	0.52
1:B:552:ILE:HG23	1:B:556:HIS:HB3	1.92	0.52
1:A:178:ARG:O	1:A:182:GLU:HG3	2.10	0.52
1:A:490:ILE:O	1:A:490:ILE:HD13	2.09	0.52
1:B:101:SER:OG	1:B:292:HIS:HD2	1.92	0.52
1:A:565:ARG:HH21	1:A:565:ARG:HG2	1.75	0.52
1:B:359:LEU:HD21	1:B:481:TYR:CZ	2.44	0.52
1:A:142:ASP:OD1	1:A:195:GLN:HG3	2.09	0.52
1:B:124:PHE:O	1:B:125:SER:CB	2.56	0.52
1:B:156:VAL:HG23	1:B:157:ILE:N	2.25	0.52
1:B:278:LYS:N	1:B:278:LYS:HE2	2.25	0.52
1:A:96:PHE:O	1:A:100:GLU:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:PHE:CE2	1:A:417:ARG:HG2	2.44	0.52
1:A:571:VAL:CG1	1:A:572:ARG:N	2.73	0.52
1:B:171:ARG:HB3	1:B:171:ARG:NH1	2.25	0.52
1:A:376:GLU:O	2:A:1604:AMP:N6	2.42	0.52
1:A:229:THR:HG22	1:A:230:ASP:N	2.25	0.52
1:A:24:PHE:HA	1:A:53:LEU:HD23	1.90	0.51
1:A:427:GLU:OE2	1:A:427:GLU:HA	2.10	0.51
1:A:278:LYS:HB3	1:A:283:LEU:HD22	1.93	0.51
1:A:404:LEU:HB2	1:A:407:GLN:O	2.10	0.51
1:B:97:GLU:HG2	1:B:98:ILE:N	2.25	0.51
1:A:339:LYS:HG2	1:A:396:GLU:HG3	1.93	0.51
1:A:401:ILE:C	1:A:401:ILE:HD12	2.30	0.51
1:B:413:LEU:HD22	1:B:413:LEU:C	2.31	0.51
1:A:419:MET:HE2	1:A:466:THR:CG2	2.34	0.51
1:B:390:MET:HE1	1:B:408:ILE:HG21	1.93	0.51
1:B:3:ARG:HB3	1:B:3:ARG:HH11	1.75	0.51
1:B:368:ARG:NE	1:B:447:GLN:HE21	2.06	0.51
1:A:54:TYR:CG	1:A:291:LYS:HG3	2.46	0.51
1:B:143:PHE:O	1:B:193:HIS:HB2	2.11	0.51
1:B:305:LEU:HD13	1:B:328:LEU:HD11	1.92	0.51
1:A:97:GLU:HG2	1:A:98:ILE:N	2.26	0.51
1:B:413:LEU:HD13	1:B:413:LEU:N	2.26	0.51
1:A:123:ILE:HD12	1:A:123:ILE:O	2.10	0.51
1:A:456:GLY:HA3	1:A:478:GLU:HB3	1.93	0.51
1:B:132:PHE:O	1:B:133:ARG:HB2	2.11	0.51
1:B:333:ARG:NH1	5:B:579:HOH:O	2.44	0.51
1:B:430:GLU:OE1	1:B:527:ARG:NH2	2.42	0.51
1:A:477:ASP:OD1	3:A:1605:ATP:O1G	2.29	0.50
1:A:566:ARG:HH21	1:A:566:ARG:CB	2.17	0.50
1:A:356:CYS:O	1:A:359:LEU:HB3	2.12	0.50
1:A:385:ILE:HG21	1:A:390:MET:HG2	1.94	0.50
1:A:467:ARG:H	1:A:467:ARG:CZ	2.24	0.50
1:B:342:PHE:O	1:B:343:ALA:C	2.49	0.50
1:A:127:GLN:HG3	1:A:128:PRO:HD2	1.92	0.50
1:A:229:THR:CG2	1:A:230:ASP:N	2.74	0.50
1:A:394:LEU:O	1:A:398:ALA:HB2	2.12	0.50
1:B:5:LEU:O	1:B:9:ILE:HD13	2.12	0.50
1:A:272:ARG:NH1	1:A:280:THR:OG1	2.45	0.50
1:A:123:ILE:HD11	1:A:124:PHE:CZ	2.47	0.50
1:A:124:PHE:CZ	1:A:302:LEU:HD23	2.47	0.50
1:A:419:MET:HE3	1:A:472:VAL:HB	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:GLU:HA	1:B:381:GLU:OE2	2.11	0.50
1:B:531:LEU:HD21	1:B:535:MET:SD	2.52	0.50
1:B:72:GLN:N	1:B:72:GLN:CD	2.66	0.50
1:A:314:GLU:OE1	1:A:319:ARG:HG3	2.12	0.50
1:A:442:GLY:HA3	1:A:536:HIS:CD2	2.47	0.50
1:B:242:THR:HB	1:B:245:GLU:CG	2.16	0.50
1:B:356:CYS:O	1:B:359:LEU:HB3	2.12	0.49
1:B:519:ARG:HB2	1:B:540:PHE:CD2	2.47	0.49
1:B:432:GLN:NE2	1:B:432:GLN:HA	2.27	0.49
1:B:462:ASN:OD1	1:B:475:ASP:OD1	2.30	0.49
1:B:214:ILE:HD13	1:B:219:THR:HB	1.95	0.49
1:B:522:LEU:HB3	1:B:532:PHE:CE1	2.47	0.49
1:A:167:GLN:O	1:A:168:ASN:CB	2.61	0.49
1:B:346:LYS:CA	1:B:346:LYS:HE2	2.40	0.49
1:B:90:LEU:O	1:B:92:ASP:N	2.45	0.49
1:A:229:THR:HG22	1:A:231:ASP:H	1.77	0.49
1:B:168:ASN:HB3	1:B:171:ARG:HB3	1.93	0.49
1:A:74:THR:HG22	1:A:74:THR:O	2.13	0.49
1:B:442:GLY:HA3	1:B:536:HIS:CE1	2.47	0.49
1:B:249:VAL:HA	1:B:562:ALA:HB1	1.94	0.49
1:A:229:THR:HB	1:A:233:GLU:HB2	1.95	0.48
1:B:76:ALA:O	1:B:80:LEU:HD23	2.13	0.48
1:B:85:HIS:HA	1:B:88:ARG:HG3	1.94	0.48
1:A:72:GLN:O	1:A:75:ASP:HB3	2.13	0.48
1:B:179:HIS:O	1:B:183:THR:HG22	2.13	0.48
1:B:70:ASN:HA	1:B:73:SER:CB	2.43	0.48
1:B:149:TRP:CZ3	1:B:152:LEU:HD23	2.47	0.48
1:A:312:PHE:CE2	1:A:328:LEU:HG	2.48	0.48
1:A:457:ASP:HB3	1:A:462:ASN:ND2	2.29	0.48
1:B:488:ARG:O	1:B:542:ALA:HB2	2.13	0.48
1:A:104:ASN:HD21	1:A:122:PHE:H	1.61	0.48
1:A:519:ARG:NE	1:A:533:GLU:OE2	2.45	0.48
1:A:7:LEU:HD21	1:A:85:HIS:CD2	2.49	0.48
1:B:171:ARG:CD	1:B:175:TYR:CE2	2.96	0.48
1:B:467:ARG:CZ	1:B:467:ARG:H	2.25	0.48
1:B:523:CYS:C	1:B:525:ASP:H	2.17	0.48
1:B:88:ARG:HH11	1:B:88:ARG:HG3	1.79	0.48
1:A:449:ALA:HB1	1:A:482:MET:CE	2.44	0.48
1:A:479:ILE:HD13	1:A:480:CYS:N	2.29	0.48
1:A:488:ARG:HB2	1:A:514:PHE:CE1	2.49	0.48
1:B:475:ASP:OD2	3:B:1605:ATP:PG	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:479:ILE:HG23	1:B:480:CYS:N	2.29	0.47
1:A:411:ARG:NH2	1:B:507:SER:HB2	2.29	0.47
1:B:322:VAL:HG22	1:B:323:MET:HG2	1.96	0.47
1:A:91:PRO:HA	1:A:127:GLN:HE22	1.78	0.47
1:B:466:THR:CG2	1:B:467:ARG:N	2.77	0.47
1:A:47:MET:O	1:A:51:ILE:HG13	2.14	0.47
1:B:137:ARG:HG3	1:B:137:ARG:NH2	2.25	0.47
1:A:108:CYS:HB3	1:A:113:HIS:CE1	2.49	0.47
1:A:278:LYS:HG3	1:A:282:GLU:HB3	1.96	0.47
1:A:519:ARG:HG2	1:A:519:ARG:HH11	1.79	0.47
1:B:149:TRP:H	1:B:152:LEU:CB	2.28	0.47
1:B:538:ASP:HB3	1:B:544:TYR:CG	2.49	0.47
1:B:556:HIS:O	1:B:557:VAL:C	2.53	0.47
1:A:143:PHE:HB3	1:A:152:LEU:CD1	2.30	0.47
1:A:50:ARG:HD2	1:A:258:MET:HE2	1.97	0.47
1:A:77:GLU:HG3	1:A:81:ARG:NH1	2.30	0.47
1:B:385:ILE:HG21	1:B:390:MET:HG2	1.96	0.47
1:B:452:ASN:HD22	1:B:482:MET:CB	2.20	0.47
1:B:47:MET:O	1:B:51:ILE:HG13	2.15	0.47
1:A:466:THR:HB	1:A:467:ARG:HH22	1.80	0.47
1:A:519:ARG:HG2	1:A:519:ARG:NH1	2.30	0.47
1:B:241:THR:CG2	1:B:241:THR:O	2.63	0.47
1:B:314:GLU:OE1	1:B:319:ARG:HG2	2.15	0.47
1:B:490:ILE:HD11	1:B:506:TYR:CD1	2.49	0.47
1:A:160:LEU:HD22	1:A:160:LEU:N	2.30	0.47
1:A:229:THR:CB	1:A:233:GLU:HB2	2.45	0.47
1:B:154:MET:HG2	1:B:173:ILE:CD1	2.45	0.47
1:B:328:LEU:HB2	1:B:331:PHE:HB2	1.96	0.47
1:A:368:ARG:NE	1:A:447:GLN:NE2	2.48	0.47
1:B:171:ARG:HD3	1:B:175:TYR:CZ	2.50	0.47
1:B:194:LEU:HD23	1:B:196:VAL:HG12	1.96	0.47
1:A:129:GLU:HG2	1:A:131:ARG:HG2	1.97	0.46
1:A:519:ARG:HD3	1:A:540:PHE:CE2	2.50	0.46
1:B:194:LEU:HD11	1:B:222:PHE:CE1	2.50	0.46
1:B:314:GLU:OE2	1:B:319:ARG:NH2	2.48	0.46
1:B:531:LEU:C	1:B:531:LEU:HD23	2.35	0.46
1:A:324:LEU:CD1	1:A:324:LEU:C	2.83	0.46
1:A:536:HIS:HB3	1:A:539:LEU:HD12	1.97	0.46
1:B:108:CYS:HB3	1:B:113:HIS:CE1	2.50	0.46
1:B:215:THR:HG22	1:B:218:GLY:O	2.15	0.46
1:A:475:ASP:OD2	3:A:1605:ATP:O3G	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:VAL:CG1	1:B:434:LEU:N	2.79	0.46
1:B:278:LYS:HE2	1:B:278:LYS:H	1.79	0.46
1:A:168:ASN:OD1	1:A:171:ARG:HB2	2.15	0.46
1:B:140:ALA:CB	1:B:197:ALA:HA	2.45	0.46
1:A:96:PHE:CZ	1:A:127:GLN:HG2	2.50	0.46
1:A:168:ASN:ND2	1:A:171:ARG:HB2	2.30	0.46
1:A:64:GLN:O	1:A:68:ILE:HG12	2.16	0.46
1:B:519:ARG:O	1:B:523:CYS:HB2	2.16	0.46
1:A:325:VAL:HA	1:A:335:PHE:O	2.16	0.46
1:A:69:THR:HG23	1:A:70:ASN:H	1.80	0.46
1:B:419:MET:HE3	1:B:472:VAL:HG21	1.98	0.46
1:A:335:PHE:CD1	1:A:335:PHE:N	2.84	0.46
1:B:475:ASP:CG	3:B:1605:ATP:O1B	2.54	0.46
1:A:132:PHE:N	1:A:132:PHE:CD2	2.77	0.46
1:B:176:ILE:HG22	1:B:180:LEU:HD12	1.98	0.46
1:B:191:LYS:HE2	1:B:192:SER:N	2.30	0.46
1:B:238:THR:OG1	1:B:239:CYS:N	2.49	0.46
1:A:149:TRP:H	1:A:152:LEU:HB3	1.80	0.45
1:B:434:LEU:HD11	1:B:528:ILE:HG22	1.96	0.45
1:A:368:ARG:HG2	1:A:444:ALA:HA	1.98	0.45
1:B:156:VAL:CG2	1:B:157:ILE:N	2.79	0.45
1:A:315:ALA:HB3	1:A:325:VAL:HG22	1.97	0.45
1:A:425:TRP:HZ3	1:A:437:ALA:HB2	1.81	0.45
1:B:71:GLY:C	1:B:73:SER:H	2.19	0.45
1:A:310:GLU:HA	1:A:310:GLU:OE1	2.17	0.45
1:A:425:TRP:CZ3	1:A:437:ALA:HB2	2.52	0.45
1:B:399:GLU:C	1:B:401:ILE:H	2.20	0.45
1:A:157:ILE:CG2	1:A:169:LYS:HD2	2.46	0.45
1:B:102:PHE:O	1:B:106:VAL:HG23	2.17	0.45
1:B:359:LEU:C	1:B:359:LEU:HD13	2.37	0.45
1:A:413:LEU:HD23	1:A:413:LEU:O	2.17	0.45
1:A:40:TRP:O	1:A:44:GLN:HG3	2.17	0.45
1:B:400:LYS:N	1:B:400:LYS:HD2	2.30	0.45
1:B:295:THR:HG1	2:B:1604:AMP:HO3'	1.64	0.45
1:B:441:TYR:OH	1:B:458:MET:HB2	2.16	0.45
1:B:490:ILE:HD12	1:B:491:PRO:HD2	1.99	0.45
1:B:69:THR:C	1:B:71:GLY:H	2.21	0.45
1:A:127:GLN:HG3	1:A:128:PRO:CD	2.46	0.45
1:A:192:SER:HB3	1:A:215:THR:HA	1.99	0.45
1:B:235:PHE:HE1	1:B:237:ASP:OD2	1.99	0.45
1:B:429:VAL:HG13	1:B:433:GLN:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:531:LEU:CD2	1:B:535:MET:CE	2.94	0.45
1:A:76:ALA:HB1	1:A:120:ARG:HH22	1.80	0.45
1:B:429:VAL:CG1	1:B:430:GLU:N	2.80	0.45
1:B:473:PHE:CE2	1:B:479:ILE:CD1	2.99	0.45
1:A:49:ASN:O	1:A:53:LEU:HD13	2.17	0.44
1:B:109:ARG:CG	1:B:109:ARG:NH1	2.80	0.44
1:B:325:VAL:HA	1:B:335:PHE:O	2.17	0.44
1:A:50:ARG:HA	1:A:53:LEU:HD22	2.00	0.44
1:B:185:GLY:C	1:B:187:GLU:N	2.70	0.44
1:A:172:ASP:HA	1:A:175:TYR:HD2	1.81	0.44
1:B:183:THR:HG23	1:B:184:LEU:HG	1.99	0.44
1:B:237:ASP:O	1:B:569:PHE:CD2	2.71	0.44
1:B:50:ARG:CZ	1:B:258:MET:HE3	2.47	0.44
1:A:149:TRP:CZ3	1:A:152:LEU:HD23	2.52	0.44
1:A:422:LEU:HD13	1:A:460:PHE:HB3	2.00	0.44
1:B:318:ILE:HD13	1:B:423:ASN:ND2	2.33	0.44
1:B:425:TRP:HZ3	1:B:437:ALA:HB2	1.81	0.44
1:A:474:TYR:HA	1:A:476:TYR:CE1	2.53	0.44
1:B:269:GLU:O	1:B:272:ARG:HB2	2.17	0.44
1:B:368:ARG:NE	1:B:444:ALA:HA	2.33	0.44
1:A:256:TYR:OH	1:A:290:GLN:HG3	2.18	0.44
1:A:356:CYS:SG	1:A:477:ASP:HA	2.57	0.44
1:A:482:MET:HE1	1:A:545:TRP:CE3	2.52	0.44
1:B:14:LEU:HD21	1:B:93:TYR:CZ	2.53	0.44
1:B:482:MET:HA	1:B:482:MET:CE	2.48	0.44
1:B:557:VAL:O	1:B:557:VAL:HG23	2.17	0.44
1:A:401:ILE:HA	1:A:409:VAL:O	2.18	0.44
1:B:178:ARG:O	1:B:182:GLU:HG3	2.17	0.44
1:B:221:PRO:HD2	1:B:241:THR:O	2.18	0.44
1:B:533:GLU:OE1	1:B:533:GLU:HA	2.17	0.44
1:A:370:ALA:N	1:A:476:TYR:OH	2.51	0.44
1:A:78:PHE:O	1:A:82:VAL:HG23	2.17	0.44
1:B:366:VAL:HG22	1:B:560:VAL:HG21	2.00	0.44
1:B:84:GLU:O	1:B:88:ARG:HG2	2.18	0.44
1:A:219:THR:HG21	1:A:273:GLU:CD	2.37	0.44
1:A:322:VAL:HG22	1:A:323:MET:HG2	1.99	0.44
1:A:123:ILE:HD11	1:A:124:PHE:CE2	2.52	0.43
1:A:100:GLU:OE2	1:A:125:SER:O	2.36	0.43
1:A:254:ARG:HG2	1:A:254:ARG:NH1	2.33	0.43
1:B:176:ILE:HD11	1:B:236:ILE:HD13	2.00	0.43
1:B:435:ARG:HH11	1:B:435:ARG:HG3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:PHE:HD2	1:A:132:PHE:H	1.60	0.43
1:B:219:THR:O	1:B:220:LEU:HD12	2.18	0.43
1:B:301:TYR:CZ	1:B:305:LEU:HD22	2.53	0.43
1:B:8:LEU:HD11	1:B:68:ILE:HD13	2.00	0.43
1:A:157:ILE:O	1:A:160:LEU:HD23	2.19	0.43
1:A:220:LEU:HG	1:A:221:PRO:HD2	2.00	0.43
1:A:40:TRP:HA	1:A:40:TRP:CE3	2.53	0.43
1:A:490:ILE:C	1:A:490:ILE:HD13	2.39	0.43
1:A:491:PRO:HA	1:A:492:PRO:HD3	1.89	0.43
1:B:519:ARG:HA	1:B:540:PHE:HE2	1.82	0.43
1:A:167:GLN:NE2	1:A:233:GLU:HG2	2.33	0.43
1:B:181:THR:C	1:B:183:THR:H	2.21	0.43
1:B:474:TYR:HA	1:B:476:TYR:CE1	2.54	0.43
1:A:150:GLU:O	1:A:154:MET:HB2	2.18	0.43
1:A:494:ARG:O	1:A:495:TYR:HB2	2.19	0.43
1:B:221:PRO:CG	1:B:274:ILE:HG23	2.43	0.43
1:B:274:ILE:C	1:B:276:PRO:HD3	2.38	0.43
1:B:359:LEU:C	1:B:359:LEU:CD1	2.87	0.43
1:B:366:VAL:CG1	1:B:366:VAL:O	2.66	0.43
1:B:144:HIS:HA	1:B:145:PRO:HD3	1.86	0.43
1:A:440:GLU:CG	1:A:471:VAL:HG23	2.48	0.43
1:B:148:GLY:CA	1:B:152:LEU:HB2	2.47	0.43
1:B:113:HIS:HE1	2:B:1604:AMP:O2P	2.01	0.43
1:B:72:GLN:C	1:B:74:THR:N	2.71	0.43
1:B:69:THR:HB	1:B:70:ASN:H	1.57	0.43
1:A:442:GLY:HA3	1:A:536:HIS:CE1	2.54	0.43
1:B:39:ASP:O	1:B:43:VAL:HG23	2.18	0.43
1:B:50:ARG:NE	1:B:258:MET:HE3	2.33	0.43
1:A:281:ALA:HB2	1:A:296:GLU:HB2	2.01	0.43
1:A:365:ARG:O	1:A:366:VAL:HG12	2.19	0.43
1:B:172:ASP:O	1:B:176:ILE:HG13	2.19	0.43
1:A:168:ASN:HD22	1:A:168:ASN:C	2.22	0.42
1:A:339:LYS:HG2	1:A:396:GLU:CG	2.49	0.42
1:A:489:ASP:CG	1:A:546:ARG:HH22	2.21	0.42
1:B:118:PRO:HG3	1:B:123:ILE:HD11	1.99	0.42
1:B:215:THR:OG1	1:B:216:PRO:HD2	2.19	0.42
1:B:242:THR:HG22	1:B:244:ALA:N	2.34	0.42
1:B:428:GLN:O	1:B:429:VAL:HG23	2.19	0.42
1:B:143:PHE:CD2	1:B:156:VAL:HG12	2.54	0.42
1:B:185:GLY:O	1:B:187:GLU:N	2.51	0.42
1:B:312:PHE:CE1	1:B:328:LEU:HD21	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:547:ALA:O	1:B:550:ASN:HB2	2.19	0.42
1:B:78:PHE:O	1:B:82:VAL:HG23	2.19	0.42
1:A:279:THR:O	1:A:283:LEU:HD22	2.19	0.42
1:A:483:THR:O	1:A:484:GLU:HB2	2.19	0.42
1:B:62:VAL:HG21	1:B:109:ARG:HB3	2.01	0.42
1:B:219:THR:C	1:B:220:LEU:HD12	2.40	0.42
1:B:88:ARG:HG3	1:B:88:ARG:NH1	2.33	0.42
1:A:375:PHE:HB2	1:A:413:LEU:HD22	2.01	0.42
1:A:6:GLU:OE2	1:A:81:ARG:HG3	2.19	0.42
1:B:32:GLN:HB2	1:B:202:TYR:OH	2.19	0.42
1:B:275:LEU:N	1:B:276:PRO:CD	2.81	0.42
1:B:526:PRO:O	1:B:530:PRO:HD2	2.19	0.42
1:A:476:TYR:O	1:A:479:ILE:CG2	2.57	0.42
1:B:490:ILE:HD12	1:B:491:PRO:CD	2.49	0.42
1:A:229:THR:OG1	1:A:233:GLU:HB2	2.19	0.42
1:A:164:LEU:HB2	1:A:234:LEU:HG	2.01	0.42
1:A:314:GLU:OE2	1:A:319:ARG:NH2	2.52	0.42
1:A:467:ARG:HB2	1:A:467:ARG:HH11	1.84	0.42
1:B:556:HIS:CG	1:B:557:VAL:H	2.38	0.42
1:A:9:ILE:HG23	1:A:65:LEU:CD2	2.44	0.42
1:B:167:GLN:OE1	1:B:171:ARG:NH2	2.52	0.42
1:B:8:LEU:CD1	1:B:68:ILE:HD13	2.50	0.42
1:A:420:VAL:HG13	1:A:465:VAL:HB	2.01	0.42
1:A:72:GLN:O	1:A:75:ASP:N	2.52	0.42
1:B:40:TRP:NE1	1:B:205:LYS:HE3	2.35	0.42
1:B:310:GLU:CB	1:B:329:PRO:HG2	2.45	0.42
1:A:154:MET:SD	1:A:169:LYS:NZ	2.89	0.41
1:A:324:LEU:HD12	1:A:325:VAL:N	2.34	0.41
1:B:40:TRP:CZ3	1:B:205:LYS:HA	2.55	0.41
1:A:149:TRP:H	1:A:152:LEU:CB	2.32	0.41
1:A:169:LYS:O	1:A:170:SER:C	2.58	0.41
1:A:201:PHE:O	1:A:208:TRP:HB2	2.20	0.41
1:A:495:TYR:N	1:A:496:PRO:CD	2.82	0.41
1:A:93:TYR:HA	1:A:94:PRO:HD3	1.65	0.41
1:A:365:ARG:NH2	1:A:365:ARG:CG	2.75	0.41
1:B:32:GLN:O	1:B:36:GLU:HG3	2.20	0.41
1:B:368:ARG:CD	1:B:444:ALA:HA	2.51	0.41
1:B:399:GLU:O	1:B:401:ILE:N	2.53	0.41
1:B:429:VAL:O	1:B:527:ARG:NH2	2.53	0.41
1:B:551:ARG:HE	1:B:551:ARG:CA	2.33	0.41
1:A:164:LEU:HD12	1:A:234:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ILE:HG22	1:A:275:LEU:N	2.35	0.41
1:A:390:MET:CE	1:A:390:MET:HA	2.51	0.41
1:A:456:GLY:HA3	1:A:478:GLU:O	2.20	0.41
1:A:453:ILE:CG2	1:A:479:ILE:HG13	2.46	0.41
1:A:130:ARG:O	1:A:133:ARG:NH2	2.53	0.41
1:A:222:PHE:O	1:A:223:LEU:HD23	2.20	0.41
1:A:452:ASN:ND2	1:A:481:TYR:CD1	2.88	0.41
1:B:290:GLN:HB3	1:B:290:GLN:HE21	1.60	0.41
1:B:457:ASP:OD1	1:B:457:ASP:C	2.58	0.41
1:A:229:THR:HB	1:A:233:GLU:H	1.85	0.41
1:A:533:GLU:OE1	1:A:533:GLU:HA	2.20	0.41
1:B:109:ARG:HG3	1:B:109:ARG:NH1	2.35	0.41
1:B:310:GLU:HG3	1:B:329:PRO:HB2	2.01	0.41
1:B:366:VAL:CG2	1:B:560:VAL:HG21	2.51	0.41
1:A:169:LYS:O	1:A:173:ILE:HG13	2.21	0.41
1:A:519:ARG:CG	1:A:519:ARG:HH11	2.33	0.41
1:B:149:TRP:H	1:B:152:LEU:HB3	1.84	0.41
1:B:347:GLU:OE1	1:B:348:MET:N	2.53	0.41
1:B:429:VAL:HG13	1:B:433:GLN:CB	2.51	0.41
1:A:382:LYS:HD2	1:A:405:GLY:O	2.20	0.41
1:A:188:ASN:HD22	1:A:188:ASN:N	2.17	0.41
1:A:365:ARG:HG2	1:A:369:MET:O	2.21	0.41
1:A:40:TRP:CE2	1:A:205:LYS:HG2	2.54	0.41
1:A:252:PHE:HE2	1:A:467:ARG:HH22	1.69	0.41
3:B:1605:ATP:O2B	3:B:1605:ATP:O1A	2.39	0.41
1:B:209:LEU:HD23	1:B:209:LEU:C	2.41	0.41
1:B:368:ARG:HD2	1:B:444:ALA:HA	2.02	0.40
1:B:312:PHE:O	1:B:389:LEU:HD23	2.21	0.40
1:A:157:ILE:HA	1:A:160:LEU:CD2	2.51	0.40
1:B:141:LYS:O	1:B:195:GLN:HA	2.21	0.40
1:B:378:PHE:CB	1:B:413:LEU:HD11	2.50	0.40
1:B:428:GLN:HE21	1:B:428:GLN:HB2	1.61	0.40
1:B:20:GLN:HG3	1:B:21:TYR:N	2.36	0.40
1:B:291:LYS:HD2	1:B:291:LYS:HA	1.89	0.40
1:A:333:ARG:HH12	1:A:373:GLN:HE22	1.70	0.40
1:A:551:ARG:NH2	1:A:556:HIS:CE1	2.89	0.40
1:B:180:LEU:C	1:B:183:THR:HG22	2.41	0.40
1:B:23:ARG:HA	1:B:26:GLU:HG3	2.03	0.40
1:B:305:LEU:CD1	1:B:328:LEU:HD11	2.51	0.40
1:B:466:THR:CG2	1:B:468:HIS:H	2.24	0.40
1:B:508:VAL:HG13	1:B:512:ASP:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:MET:HG3	1:B:448:LEU:HD21	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	562/578 (97%)	494 (88%)	54 (10%)	14 (2%)	5	19
1	B	555/578 (96%)	458 (82%)	73 (13%)	24 (4%)	2	8
All	All	1117/1156 (97%)	952 (85%)	127 (11%)	38 (3%)	3	13

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	PHE
1	A	138	PRO
1	A	484	GLU
1	B	132	PHE
1	B	133	ARG
1	B	147	HIS
1	B	148	GLY
1	B	238	THR
1	A	125	SER
1	A	148	GLY
1	A	150	GLU
1	A	168	ASN
1	B	70	ASN
1	B	346	LYS
1	B	400	LYS
1	B	556	HIS
1	B	559	ASP

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Mol	Chain	Res	Type
1	B	125	SER
1	B	192	SER
1	A	147	HIS
1	A	238	THR
1	B	91	PRO
1	B	146	ASP
1	B	149	TRP
1	B	182	GLU
1	B	480	CYS
1	B	539	LEU
1	B	557	VAL
1	A	230	ASP
1	A	365	ARG
1	A	366	VAL
1	B	127	GLN
1	B	329	PRO
1	B	343	ALA
1	A	38	ALA
1	A	187	GLU
1	B	264	PRO
1	B	490	ILE

### 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	497/508 (98%)	442 (89%)	55 (11%)	6	19
1	B	490/508 (96%)	428 (87%)	62 (13%)	4	14
All	All	987/1016 (97%)	870 (88%)	117 (12%)	5	16

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	8	LEU

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Mol	Chain	Res	Type
1	A	53	LEU
1	A	60	LEU
1	A	65	LEU
1	A	69	THR
1	A	79	LEU
1	A	80	LEU
1	A	84	GLU
1	A	123	ILE
1	A	137	ARG
1	A	138	PRO
1	A	139	LEU
1	A	141	LYS
1	A	167	GLN
1	A	168	ASN
1	A	171	ARG
1	A	200	LEU
1	A	230	ASP
1	A	258	MET
1	A	271	LEU
1	A	283	LEU
1	A	290	GLN
1	A	302	LEU
1	A	324	LEU
1	A	325	VAL
1	A	329	PRO
1	A	337	VAL
1	A	359	LEU
1	A	360	VAL
1	A	365	ARG
1	A	366	VAL
1	A	368	ARG
1	A	381	GLU
1	A	390	MET
1	A	392	LEU
1	A	394	LEU
1	A	401	ILE
1	A	406	GLU
1	A	413	LEU
1	A	422	LEU
1	A	425	TRP
1	A	429	VAL
1	A	467	ARG

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Mol	Chain	Res	Type
1	A	474	TYR
1	A	479	ILE
1	A	480	CYS
1	A	482	MET
1	A	485	VAL
1	A	490	ILE
1	A	519	ARG
1	A	528	ILE
1	A	532	PHE
1	A	548	LEU
1	A	566	ARG
1	B	3	ARG
1	B	7	LEU
1	B	20	GLN
1	B	23	ARG
1	B	37	GLN
1	B	60	LEU
1	B	70	ASN
1	B	78	PHE
1	B	79	LEU
1	B	80	LEU
1	B	92	ASP
1	B	109	ARG
1	B	121	LEU
1	B	130	ARG
1	B	141	LYS
1	B	149	TRP
1	B	154	MET
1	B	171	ARG
1	B	191	LYS
1	B	196	VAL
1	B	200	LEU
1	B	237	ASP
1	B	258	MET
1	B	271	LEU
1	B	272	ARG
1	B	278	LYS
1	B	283	LEU
1	B	290	GLN
1	B	302	LEU
1	B	309	ASN
1	B	325	VAL

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Mol	Chain	Res	Type
1	B	329	PRO
1	B	341	LYS
1	B	346	LYS
1	B	347	GLU
1	B	359	LEU
1	B	365	ARG
1	B	366	VAL
1	B	376	GLU
1	B	390	MET
1	B	392	LEU
1	B	396	GLU
1	B	400	LYS
1	B	411	ARG
1	B	412	HIS
1	B	413	LEU
1	B	420	VAL
1	B	422	LEU
1	B	452	ASN
1	B	467	ARG
1	B	474	TYR
1	B	477	ASP
1	B	479	ILE
1	B	480	CYS
1	B	482	MET
1	B	509	SER
1	B	532	PHE
1	B	538	ASP
1	B	548	LEU
1	B	551	ARG
1	B	566	ARG
1	B	572	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	41	HIS
1	A	57	HIS
1	A	64	GLN
1	A	104	ASN
1	A	113	HIS
1	A	127	GLN

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Mol	Chain	Res	Type
1	A	167	GLN
1	A	168	ASN
1	A	179	HIS
1	A	188	ASN
1	A	193	HIS
1	A	290	GLN
1	A	292	HIS
1	A	352	HIS
1	A	373	GLN
1	A	377	ASN
1	A	395	GLN
1	A	407	GLN
1	A	428	GLN
1	A	432	GLN
1	A	447	GLN
1	A	549	GLN
1	B	15	GLN
1	B	32	GLN
1	B	64	GLN
1	B	70	ASN
1	B	72	GLN
1	B	104	ASN
1	B	113	HIS
1	B	195	GLN
1	B	198	ASN
1	B	204	ASN
1	B	228	GLN
1	B	290	GLN
1	B	292	HIS
1	B	309	ASN
1	B	352	HIS
1	B	373	GLN
1	B	377	ASN
1	B	407	GLN
1	B	428	GLN
1	B	432	GLN
1	B	447	GLN
1	B	452	ASN
1	B	549	GLN
1	B	550	ASN

### 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 carbohydrates 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$
3	ATP	B	1605	4	26,33,33	1.11	2 (7%)	31,52,52	2.77	6 (19%)
2	AMP	A	1604	-	22,25,25	2.16	2 (9%)	25,38,38	1.96	6 (24%)
3	ATP	A	1605	4	26,33,33	1.18	2 (7%)	31,52,52	2.81	8 (25%)
2	AMP	B	1604	-	22,25,25	2.37	2 (9%)	25,38,38	1.86	6 (24%)

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
3	ATP	B	1605	4	-	0/18/38/38	0/3/3/3
2	AMP	A	1604	-	-	0/6/26/26	0/3/3/3
3	ATP	A	1605	4	-	0/18/38/38	0/3/3/3
2	AMP	B	1604	-	-	0/6/26/26	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1604	AMP	C2-N3	9.30	1.47	1.32
2	A	1604	AMP	C2-N3	8.62	1.46	1.32
2	B	1604	AMP	O4'-C1'	4.38	1.47	1.41
2	A	1604	AMP	O4'-C1'	3.66	1.46	1.41
3	A	1605	ATP	O4'-C1'	3.38	1.45	1.41
3	B	1605	ATP	O4'-C1'	2.60	1.44	1.41
3	B	1605	ATP	C8-N7	-2.44	1.30	1.34
3	A	1605	ATP	C8-N7	-2.35	1.30	1.34

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1605	ATP	PA-O3A-PB	-9.71	99.52	132.83
3	B	1605	ATP	PA-O3A-PB	-9.22	101.20	132.83
3	A	1605	ATP	PB-O3B-PG	-8.89	102.33	132.83
3	B	1605	ATP	PB-O3B-PG	-8.69	103.00	132.83
2	B	1604	AMP	N3-C2-N1	-5.48	120.12	128.68
2	A	1604	AMP	N3-C2-N1	-5.32	120.37	128.68
2	A	1604	AMP	P-O5'-C5'	-4.91	104.78	118.30
3	B	1605	ATP	N3-C2-N1	-4.58	121.53	128.68
3	A	1605	ATP	N3-C2-N1	-4.44	121.74	128.68
2	B	1604	AMP	P-O5'-C5'	-4.27	106.54	118.30
3	B	1605	ATP	C3'-C2'-C1'	3.48	106.21	100.98
3	A	1605	ATP	C3'-C2'-C1'	3.11	105.66	100.98
3	B	1605	ATP	PA-O5'-C5'	-3.02	103.96	121.68
2	A	1604	AMP	C5'-C4'-C3'	-2.84	104.55	115.18
3	A	1605	ATP	PA-O5'-C5'	-2.80	105.27	121.68
2	A	1604	AMP	O4'-C4'-C3'	2.67	110.39	105.11
3	B	1605	ATP	O3G-PG-O3B	2.58	113.30	104.64
2	B	1604	AMP	C3'-C2'-C1'	2.52	104.77	100.98
2	B	1604	AMP	C4-C5-N7	-2.42	106.88	109.40
3	A	1605	ATP	C4-C5-N7	-2.31	107.00	109.40
3	A	1605	ATP	C2'-C3'-C4'	2.23	106.98	102.64
3	A	1605	ATP	O3G-PG-O3B	2.22	112.07	104.64
2	A	1604	AMP	C4-C5-N7	-2.19	107.12	109.40
2	B	1604	AMP	C5'-C4'-C3'	-2.12	107.25	115.18
2	A	1604	AMP	C3'-C2'-C1'	2.12	104.16	100.98
2	B	1604	AMP	C2'-C3'-C4'	2.04	106.60	102.64

There are no chirality outliers.

There are no torsion outliers.

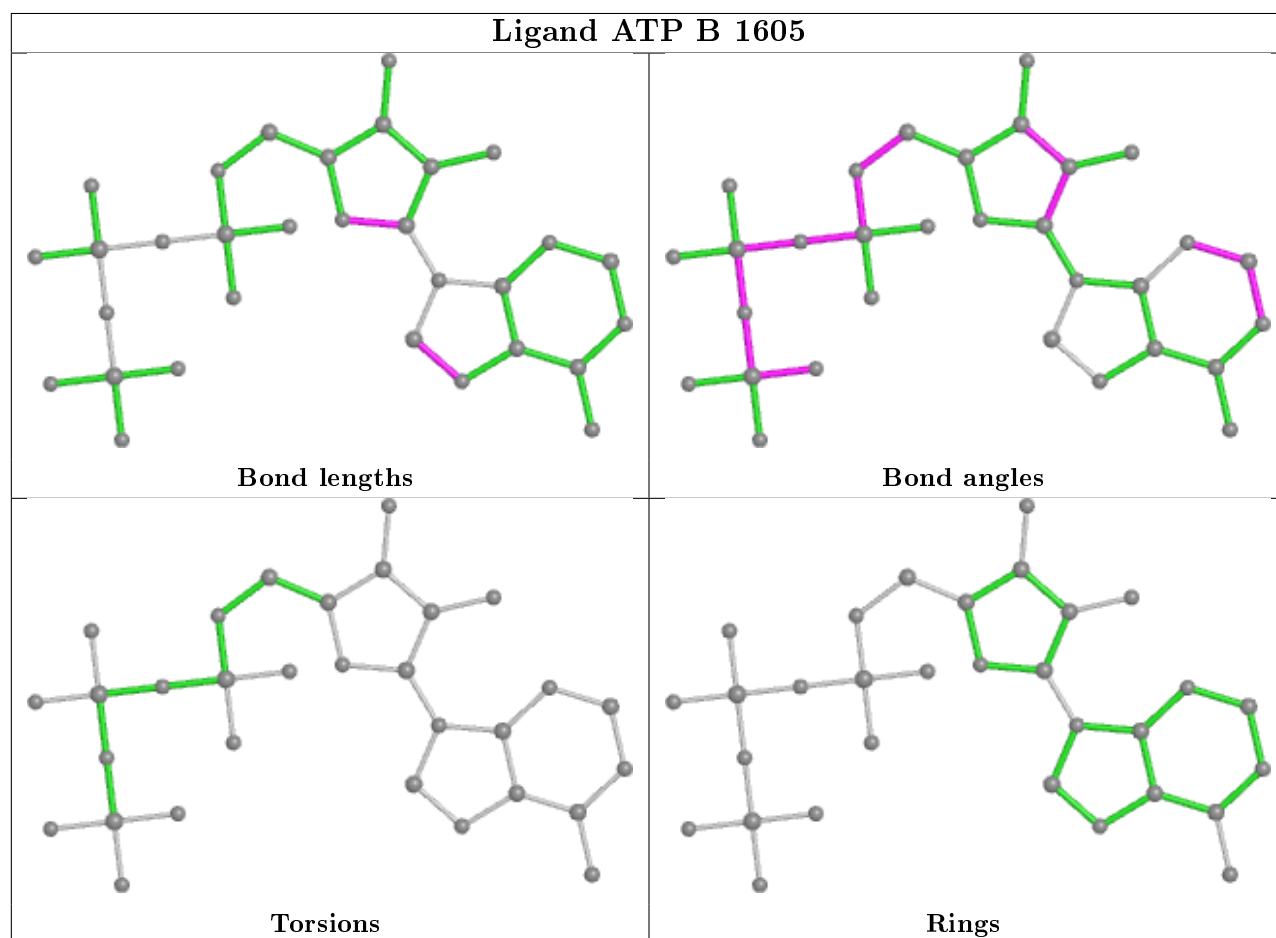


There are no ring outliers.

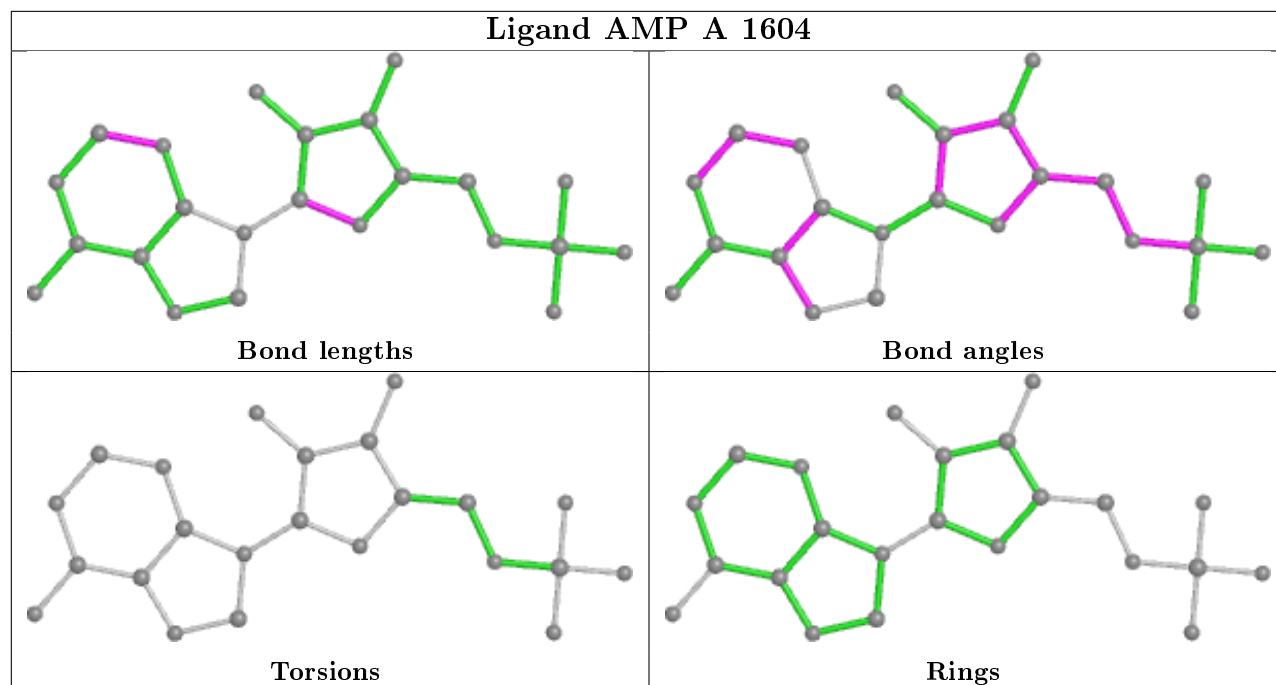
4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1605	ATP	6	0
2	A	1604	AMP	2	0
3	A	1605	ATP	5	0
2	B	1604	AMP	2	0

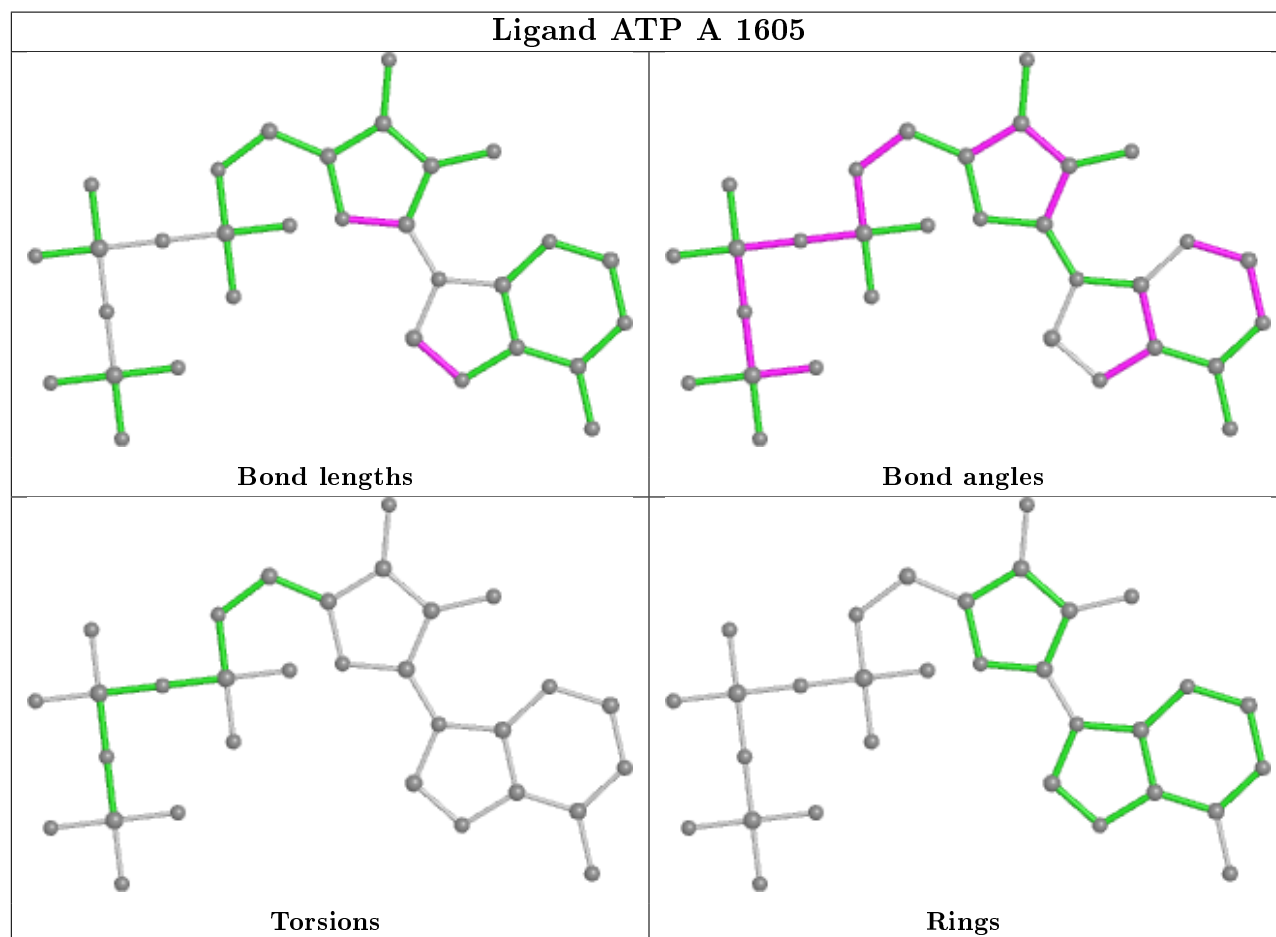
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

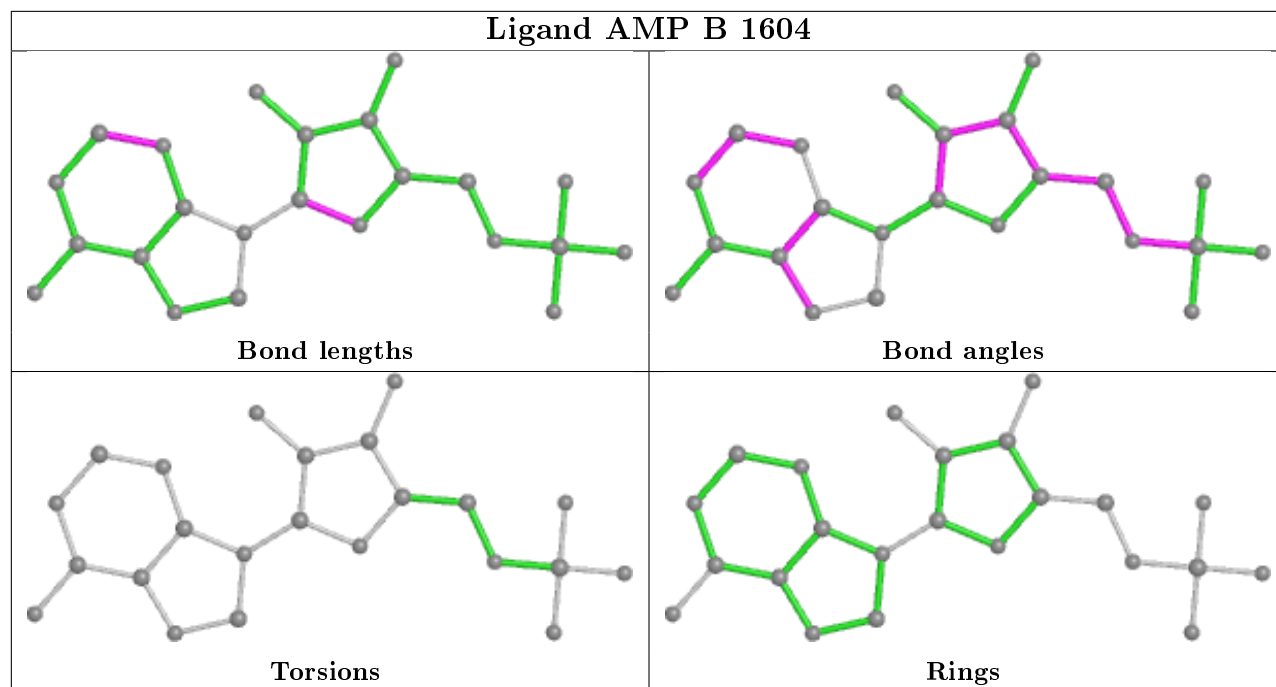


## Ligand AMP A 1604



## Ligand ATP A 1605





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	566/578 (97%)	0.23	31 (5%) 25 16	46, 68, 104, 144	0
1	B	559/578 (96%)	0.44	43 (7%) 13 7	46, 79, 117, 139	0
All	All	1125/1156 (97%)	0.33	74 (6%) 18 11	46, 74, 112, 144	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	74	THR	6.5
1	B	73	SER	5.8
1	A	496	PRO	5.7
1	B	556	HIS	5.5
1	B	308	CYS	5.1
1	B	309	ASN	5.0
1	A	76	ALA	4.8
1	B	131	ARG	4.7
1	B	132	PHE	4.6
1	B	555	GLY	4.4
1	A	495	TYR	4.3
1	B	3	ARG	4.3
1	A	72	GLN	3.9
1	A	131	ARG	3.8
1	A	132	PHE	3.7
1	B	574	GLY	3.7
1	B	2	PRO	3.6
1	B	218	GLY	3.5
1	A	133	ARG	3.5
1	A	70	ASN	3.5
1	B	188	ASN	3.5
1	B	114	ARG	3.4
1	A	309	ASN	3.4
1	B	145	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	130	ARG	3.3
1	B	537	ALA	3.2
1	B	128	PRO	3.1
1	A	165	HIS	3.1
1	B	344	PRO	3.1
1	A	130	ARG	3.0
1	A	494	ARG	3.0
1	B	191	LYS	3.0
1	B	572	ARG	2.9
1	B	70	ASN	2.9
1	A	572	ARG	2.9
1	B	310	GLU	2.9
1	B	415	ILE	2.9
1	B	217	SER	2.9
1	B	520	HIS	2.9
1	B	127	GLN	2.8
1	B	71	GLY	2.7
1	A	167	GLN	2.7
1	B	557	VAL	2.7
1	B	219	THR	2.6
1	A	233	GLU	2.6
1	B	307	GLY	2.5
1	A	71	GLY	2.5
1	A	74	THR	2.5
1	B	214	ILE	2.5
1	A	187	GLU	2.4
1	B	175	TYR	2.4
1	A	191	LYS	2.4
1	B	133	ARG	2.4
1	B	147	HIS	2.4
1	B	550	ASN	2.4
1	B	224	LEU	2.3
1	B	306	GLN	2.3
1	A	308	CYS	2.3
1	A	129	GLU	2.3
1	A	504	PRO	2.3
1	B	506	TYR	2.3
1	A	216	PRO	2.2
1	A	184	LEU	2.2
1	A	12	THR	2.2
1	A	531	LEU	2.2
1	A	573	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	13	ILE	2.1
1	B	187	GLU	2.1
1	A	231	ASP	2.1
1	A	223	LEU	2.1
1	B	346	LYS	2.1
1	A	458	MET	2.1
1	B	231	ASP	2.0
1	A	188	ASN	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 carbohydrates in this entry.

## 6.4 Ligands ⓘ

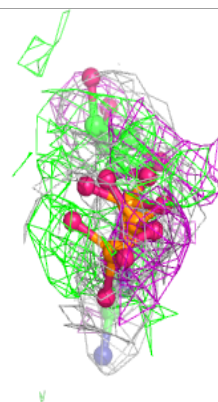
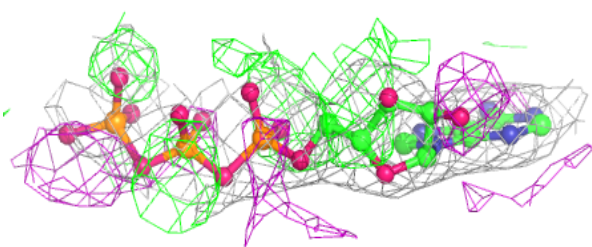
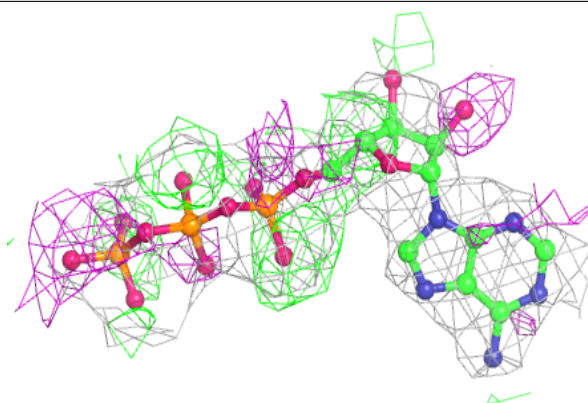
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	ATP	B	1605	31/31	0.89	0.25	47,59,77,77	0
3	ATP	A	1605	31/31	0.92	0.22	43,51,77,77	0
4	MG	A	1606	1/1	0.93	0.29	44,44,44,44	0
4	MG	B	1606	1/1	0.94	0.39	53,53,53,53	0
2	AMP	B	1604	23/23	0.95	0.21	63,68,77,82	0
2	AMP	A	1604	23/23	0.96	0.21	49,55,57,61	0

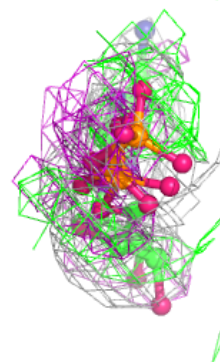
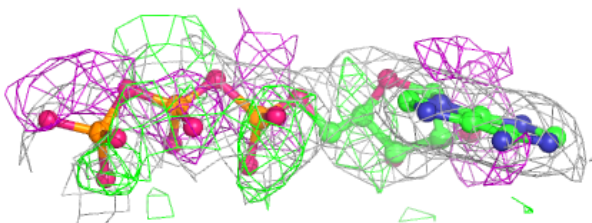
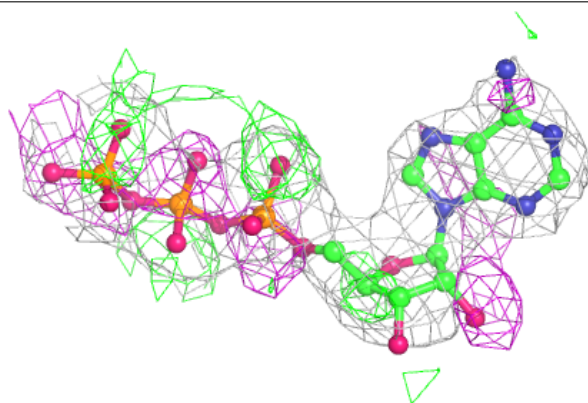
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ATP B 1605:**

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

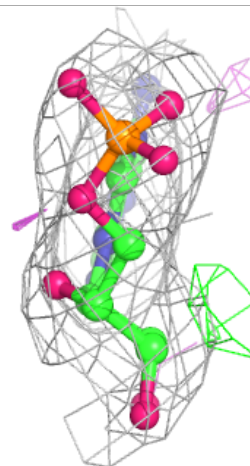
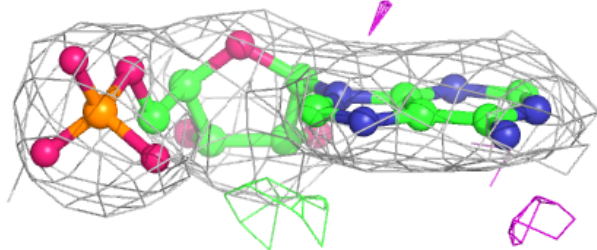
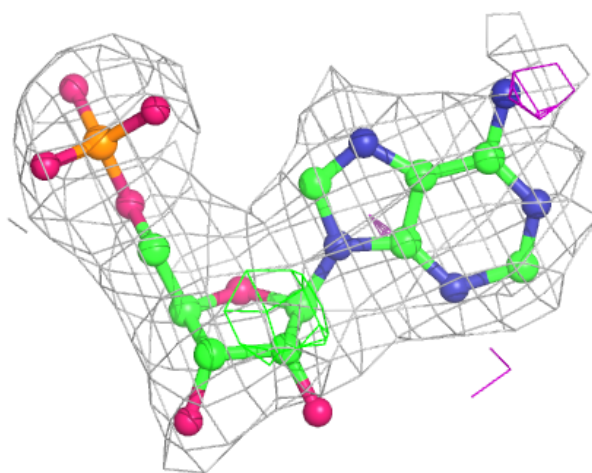
**Electron density around ATP A 1605:**

$2mF_o-DF_c$  (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:**

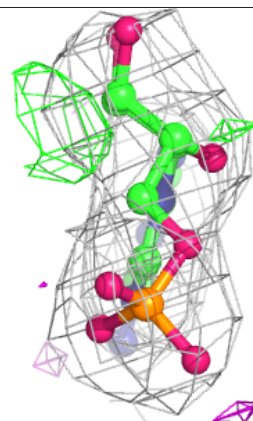
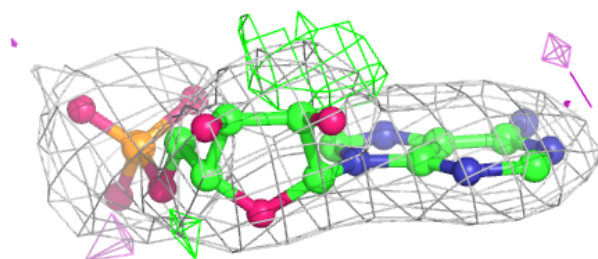
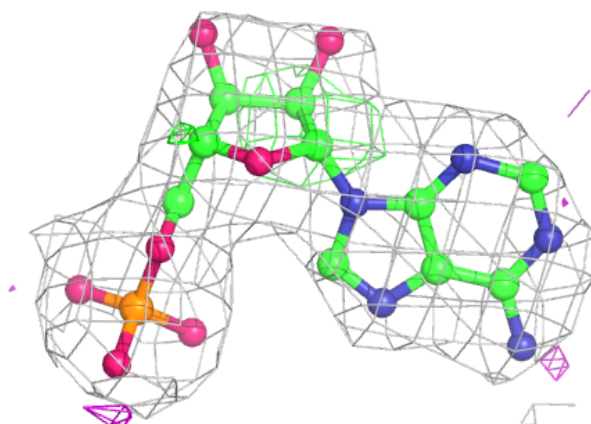
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**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 ⓘ

There are no such residues in this entry.