



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:11 AM UTC

PDB ID : 3EPS / pdb_00003eps
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

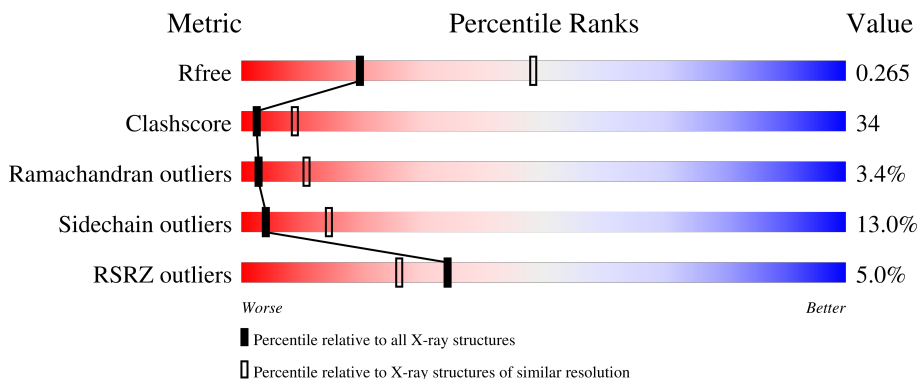
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	578	
1	B	578	

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.

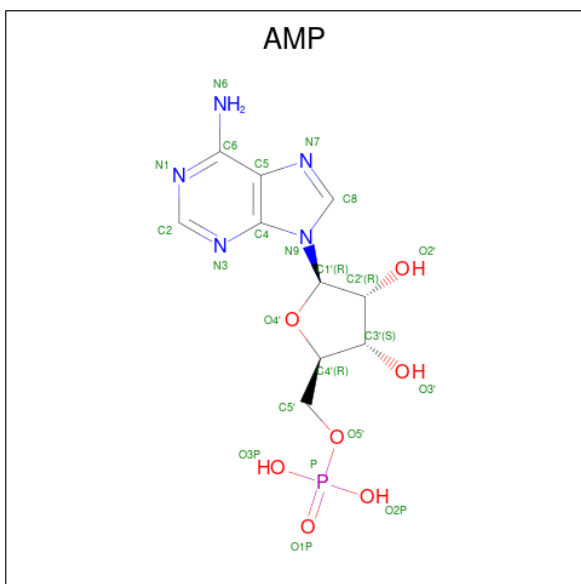
- Molecule 1 is a protein called Isocitrate dehydrogenase kinase/phosphatase.

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

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 (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



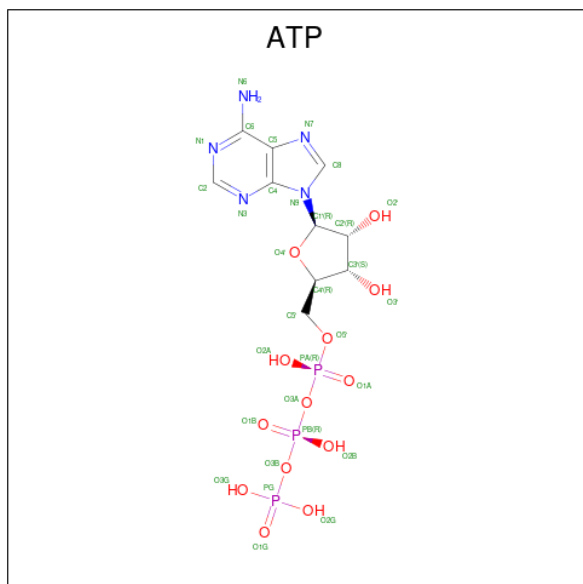
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total 23	C 10	N 5	O 7	P 1	0	0

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

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



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

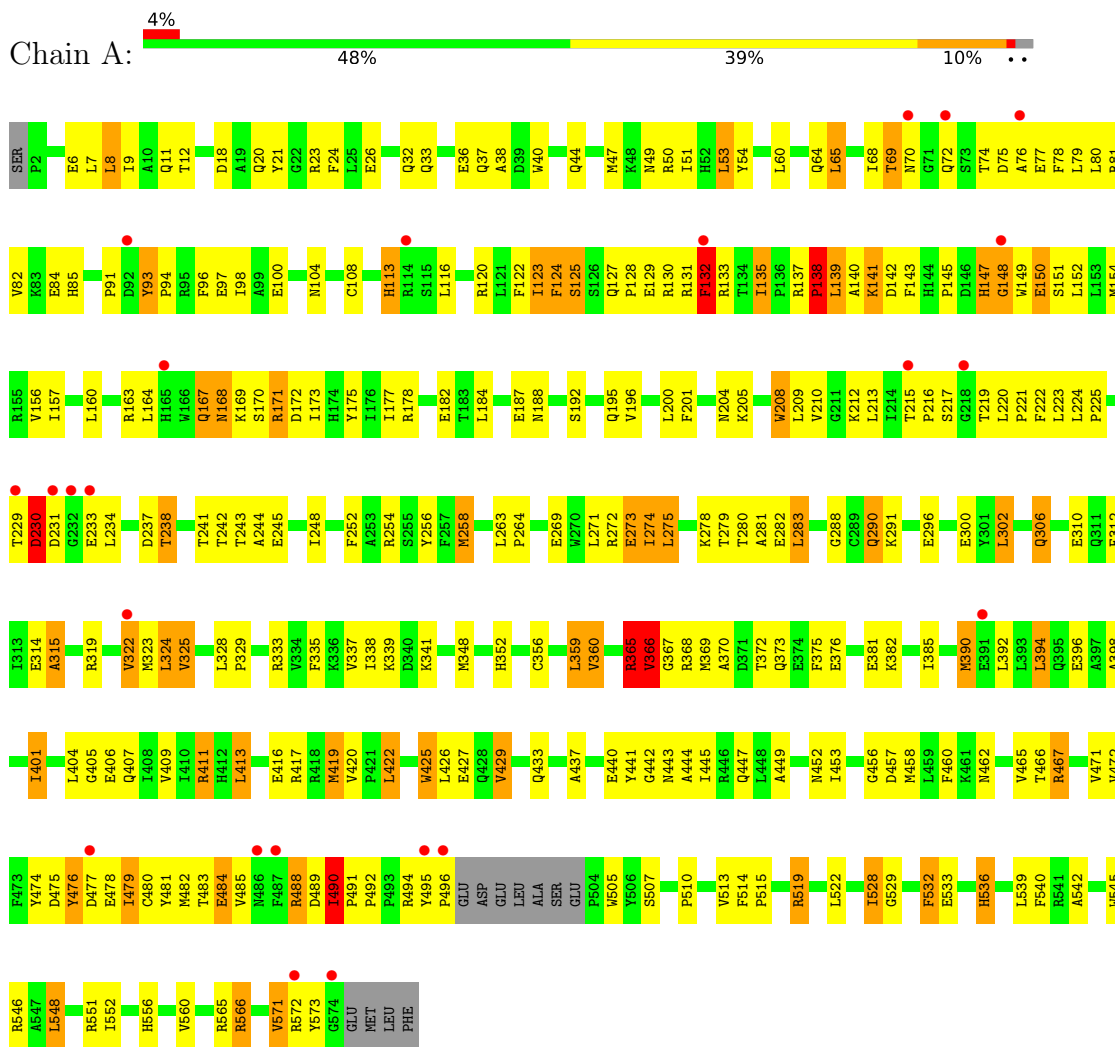
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	28	28	28	0	0
5	B	22	22	22	0	0

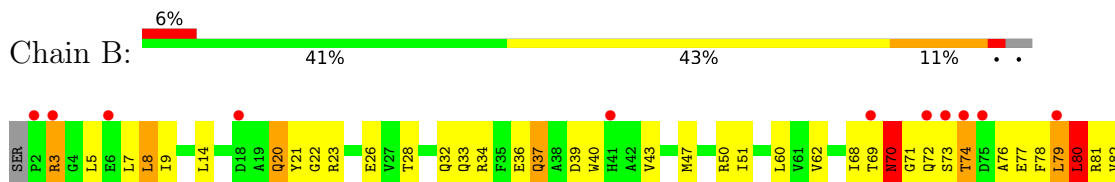
3 Residue-property plots

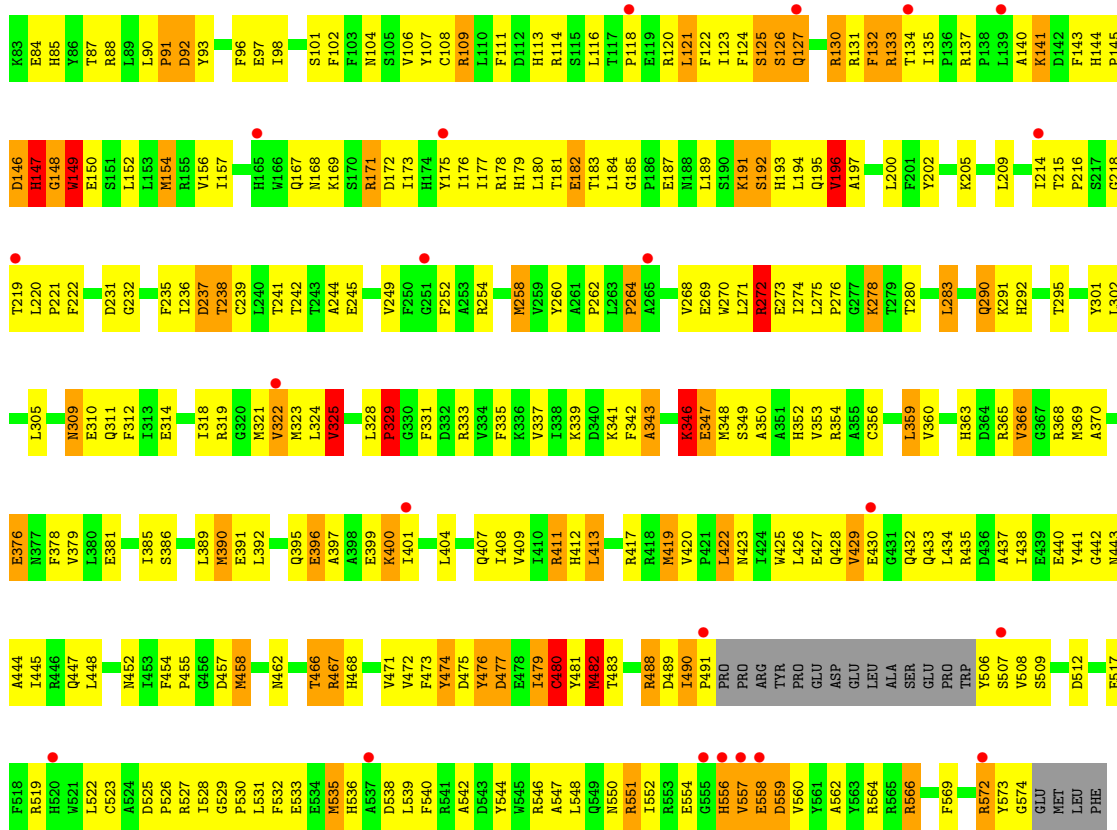
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Isocitrate dehydrogenase kinase/phosphatase



- Molecule 1: Isocitrate dehydrogenase kinase/phosphatase





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	124.59Å 124.59Å 267.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 30.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	86.5 (30.00-2.80) 94.2 (30.00-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.80Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.233 , 0.268 0.236 , 0.265	Depositor DCC
R_{free} test set	2527 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	80.5	Xtrriage
Anisotropy	0.047	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 64.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9467	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, AMP, 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	0.51	1/4815 (0.0%)	1.05	28/6523 (0.4%)
1	B	0.46	1/4743 (0.0%)	0.95	15/6421 (0.2%)
All	All	0.49	2/9558 (0.0%)	1.00	43/12944 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	419	MET	SD-CE	-7.43	1.60	1.79
1	B	482	MET	SD-CE	-6.12	1.64	1.79

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	490	ILE	CA-C-N	10.45	127.29	119.66
1	A	490	ILE	C-N-CA	10.45	127.29	119.66
1	A	476	TYR	N-CA-C	9.61	122.97	111.82
1	A	137	ARG	CA-C-N	8.52	130.49	119.84
1	A	137	ARG	C-N-CA	8.52	130.49	119.84
1	B	150	GLU	N-CA-C	-8.40	103.55	113.88
1	B	74	THR	N-CA-C	-7.89	105.62	114.62
1	A	26	GLU	N-CA-C	-7.58	103.09	111.36
1	A	113	HIS	N-CA-C	6.63	120.69	112.47
1	A	274	ILE	N-CA-C	-6.59	102.76	110.21
1	B	80	LEU	N-CA-C	-6.46	105.04	113.12
1	A	147	HIS	N-CA-C	-6.37	97.24	110.80
1	A	204	ASN	CB-CA-C	-6.22	109.38	116.54
1	A	490	ILE	N-CA-C	6.14	114.64	107.77
1	B	196	VAL	N-CA-C	6.08	116.68	108.17
1	A	93	TYR	CA-C-N	5.93	125.81	119.28
1	A	93	TYR	C-N-CA	5.93	125.81	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	517	GLU	N-CA-C	-5.91	105.90	114.12
1	B	126	SER	N-CA-C	-5.88	101.24	110.36
1	A	132	PHE	N-CA-C	5.87	123.31	110.80
1	A	124	PHE	N-CA-C	5.79	120.84	113.55
1	B	419	MET	CA-C-N	-5.64	117.16	123.02
1	B	419	MET	C-N-CA	-5.64	117.16	123.02
1	A	419	MET	CA-C-N	-5.58	117.91	123.04
1	A	419	MET	C-N-CA	-5.58	117.91	123.04
1	B	529	GLY	CA-C-N	5.58	125.04	119.24
1	B	529	GLY	C-N-CA	5.58	125.04	119.24
1	B	488	ARG	N-CA-C	5.53	118.70	109.96
1	A	411	ARG	N-CA-C	5.48	116.94	111.07
1	B	476	TYR	N-CA-C	5.48	119.06	112.38
1	B	325	VAL	N-CA-C	5.42	115.70	108.11
1	B	272	ARG	N-CA-C	5.39	117.85	111.33
1	A	263	LEU	CA-C-N	5.32	126.48	119.84
1	A	263	LEU	C-N-CA	5.32	126.48	119.84
1	A	507	SER	N-CA-C	5.32	117.88	109.96
1	B	147	HIS	N-CA-C	-5.29	99.54	110.80
1	A	315	ALA	CA-C-N	5.28	125.53	119.83
1	A	315	ALA	C-N-CA	5.28	125.53	119.83
1	A	536	HIS	N-CA-C	5.21	117.13	110.61
1	A	151	SER	N-CA-C	-5.12	105.87	112.68
1	A	288	GLY	N-CA-C	5.11	120.80	114.37
1	A	208	TRP	N-CA-C	5.08	118.48	109.96
1	A	505	TRP	N-CA-C	-5.04	106.64	112.89

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	294	0
1	B	4621	0	4542	350	0
2	A	23	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	23	0	12	1	0
3	A	31	0	12	5	0
3	B	31	0	12	7	0
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	642	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 34.

All (642) 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:A:419:MET:HE1	1:A:472:VAL:HB	1.23	1.08
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:419:MET:HE1	1:A:472:VAL:CB	2.02	0.89
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:HB3	1:A:566:ARG:HH21	1.38	0.86
1:B:404:LEU:HD23	1:B:407:GLN:HE21	1.40	0.86
1:A:365:ARG:HH21	1:A:365:ARG:HG2	1.40	0.86
1:A:566:ARG:HA	1:A:571:VAL:HG11	1.58	0.85
1:A:551:ARG:HG2	1:A:551:ARG:HH11	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:168:ASN:CG	1:A:171:ARG:HB2	2.07	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:50:ARG:HD2	1:A:258:MET:HE2	1.64	0.78
1:B:348:MET:SD	1:B:477:ASP:OD1	2.43	0.77
1:A:252:PHE:HZ	1:A:419:MET:HE3	1.47	0.77
1:B:454:PHE:CD1	1:B:482:MET:HE1	2.19	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:454:PHE:HB2	1:B:482:MET:HE3	1.66	0.76
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:HA	1:B:141:LYS:HE3	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:252:PHE:HZ	1:B:419:MET:HE3	1.51	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:510:PRO:HA	5:A:596:HOH:O	1.87	0.73
1:B:50:ARG:NE	1:B:258:MET:HE3	2.04	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:B:72:GLN:CD	1:B:72:GLN:H	1.97	0.72
1:A:9:ILE:HG23	1:A:65:LEU:HD21	1.70	0.72
1:A:419:MET:CE	1:A:472:VAL:HB	2.14	0.72
1:B:475:ASP:OD2	3:B:1605:ATP:O1G	2.08	0.72
1:B:81:ARG:HH21	1:B:81:ARG:HB2	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:LEU:HB3	1:B:121:LEU:HD11	1.72	0.71
1:A:324:LEU:HD12	1:A:324:LEU:C	2.15	0.71
1:B:419:MET:HE1	1:B:472:VAL:CG2	2.21	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:445:ILE:HD12	1:B:458:MET:HE2	1.73	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
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:HH21	1:A:81:ARG:HG3	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:76:ALA:CB	1:A:120:ARG:HH22	2.06	0.68
1:A:171:ARG:HB3	1:A:171:ARG:HH11	1.59	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:72:GLN:C	1:B:74:THR:H	2.02	0.68
1:B:572:ARG:HE	1:B:572:ARG:HA	1.57	0.68
1:A:322:VAL:C	1:A:339:LYS:HD3	2.19	0.68
1:B:137:ARG:HH21	1:B:137:ARG:HG3	1.57	0.68
1:B:379:VAL:HG22	1:B:409:VAL:HG22	1.76	0.67
1:B:419:MET:HE1	1:B:472:VAL:HG21	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:HB3	1:B:130:ARG:NH2	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: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:B:191:LYS:HE2	1:B:191:LYS:C	2.20	0.66
1:A:135:ILE:H	1:A:135:ILE:CD1	2.03	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH21	1:A:365:ARG:CG	2.10	0.64
1:A:40:TRP:CD2	1:A:205:LYS:HG2	2.32	0.64
1:A:390:MET:HE2	1:A:390:MET:HA	1.79	0.64
1:B:366:VAL:O	1:B:366:VAL:HG13	1.98	0.64
1:B:81:ARG:HB2	1:B:81:ARG:NH2	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
1:B:268:VAL:HG13	1:B:283:LEU:HB3	1.78	0.63
1:B:321:MET:HE3	1:B:343:ALA:HB3	1.80	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: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:B:145:PRO:C	1:B:147:HIS:H	2.06	0.63
1:A:113:HIS:HE1	2:A:1604:AMP:O2P	1.81	0.62
1:B:365:ARG:HG2	1:B:365:ARG:HH21	1.63	0.62
1:B:254:ARG:HG2	1:B:254:ARG:HH11	1.64	0.62
1:A:453:ILE:HG23	1:A:479:ILE:CG1	2.30	0.62
1:A:140:ALA:C	1:A:141:LYS:HE2	2.24	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:145:PRO:HA	1:A:148:GLY:HA3	1.83	0.61
1:B:454:PHE:HD1	1:B:482:MET:HE1	1.61	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:A:149:TRP:O	1:A:150:GLU:HB2	1.99	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:HG2	1:A:551:ARG:NH1	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ARG:HD2	1:A:573:TYR:CZ	2.35	0.61
1:A:215:THR:HG23	1:A:216:PRO:HD2	1.82	0.61
1:B:79:LEU:HD13	1:B:111:PHE:HZ	1.65	0.61
1:B:169:LYS:O	1:B:173:ILE:HG13	2.00	0.61
1:A:21:TYR:OH	1:A:264:PRO:HG3	2.00	0.60
1:A:413:LEU:C	1:A:413:LEU:HD23	2.25	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:120:ARG:C	1:B:121:LEU:HD23	2.26	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
1:A:209:LEU:C	1:A:209:LEU:HD23	2.26	0.60
1:B:152:LEU:O	1:B:156:VAL:HG13	2.02	0.60
1:A:441:TYR:CE1	1:A:532:PHE:HZ	2.20	0.60
1:B:28:THR:HA	1:B:258:MET:CE	2.31	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:346:LYS:NZ	1:B:348:MET:HE3	2.17	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:477:ASP:OD2	1:B:477:ASP:C	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:LEU:C	1:A:139:LEU:HD23	2.28	0.58
1:B:126:SER:O	1:B:127:GLN:HB3	2.04	0.58
1:B:242:THR:HG22	1:B:244:ALA:H	1.68	0.58
1:A:275:LEU:O	1:A:275:LEU:HD12	2.04	0.58
1:B:241:THR:O	1:B:241:THR:HG22	2.03	0.58
1:A:274:ILE:O	1:A:275:LEU:C	2.45	0.58
1:A:482:MET:HE1	1:A:545:TRP:CE3	2.39	0.58
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:76:ALA:O	1:B:80:LEU:HB2	2.04	0.57
1:B:309:ASN:N	1:B:309:ASN:HD22	2.00	0.57
1:A:466:THR:HB	1:A:467:ARG:NH2	2.19	0.57
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:A:348:MET:HE2	1:A:352:HIS:CD2	2.41	0.56
1:B:85:HIS:O	1:B:88:ARG:HB2	2.05	0.56
1:B:254:ARG:HG2	1:B:254:ARG:NH1	2.21	0.56
1:A:135:ILE:HD12	1:A:135:ILE:N	2.10	0.56
1:B:149:TRP:HA	1:B:149:TRP:HE3	1.71	0.56
1:A:528:ILE:HG13	1:A:529:GLY:N	2.15	0.56
1:B:413:LEU:C	1:B:413:LEU:HD22	2.31	0.56
1:A:252:PHE:CZ	1:A:419:MET:HE3	2.36	0.56
1:A:401:ILE:HD12	1:A:401:ILE:C	2.30	0.56
1:A:54:TYR:CD1	1:A:291:LYS:HG3	2.41	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:167:GLN:O	1:A:168:ASN:HB3	2.05	0.56
1:B:28:THR:HA	1:B:258:MET:HE1	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:81:ARG:HH21	1:B:81:ARG:CB	2.18	0.55
1:B:339:LYS:HE3	1:B:396:GLU:CG	2.37	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:342:PHE:O	1:B:343:ALA:C	2.49	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:23:ARG:NE	5:A:588:HOH:O	2.35	0.55
1:A:143:PHE:CD2	1:A:156:VAL:HG12	2.41	0.55
1:B:22:GLY:O	1:B:26:GLU:HG2	2.07	0.55
1:B:109:ARG:HH11	1:B:109:ARG:CG	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:455:PRO:HB2	1:B:458:MET:HE3	1.90	0.54
1:B:411:ARG:HB2	1:B:411:ARG:NH1	2.21	0.54
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:HD22	1:A:160:LEU:H	1.71	0.53
1:B:23:ARG:HE	1:B:23:ARG:HA	1.73	0.53
1:B:231:ASP:OD1	1:B:232:GLY:N	2.42	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:B:96:PHE:CE1	1:B:127:GLN:HG2	2.43	0.53
1:B:219:THR:HG21	1:B:273:GLU:OE2	2.08	0.53
1:A:168:ASN:ND2	1:A:171:ARG:H	2.07	0.53
1:B:360:VAL:HG11	1:B:476:TYR:CD2	2.43	0.53
1:B:422:LEU:HD22	1:B:426:LEU:HG	1.90	0.53
1:B:427:GLU:OE2	1:B:427:GLU:HA	2.08	0.53
1:A:149:TRP:O	1:A:150:GLU:CB	2.56	0.53
1:B:419:MET:HE1	1:B:472:VAL:HB	1.90	0.53
1:A:171:ARG:HB3	1:A:171:ARG:NH1	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:523:CYS:C	1:B:525:ASP:H	2.17	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:HD13	1:A:490:ILE:O	2.09	0.52
1:B:101:SER:OG	1:B:292:HIS:HD2	1.92	0.52
1:A:565:ARG:HG2	1:A:565:ARG:HH21	1.75	0.52
1:B:50:ARG:CZ	1:B:258:MET:HE3	2.39	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:72:GLN:CD	1:B:72:GLN:N	2.66	0.52
1:B:124:PHE:O	1:B:125:SER:CB	2.56	0.52
1:B:278:LYS:N	1:B:278:LYS:HE2	2.25	0.52
1:B:556:HIS:O	1:B:557:VAL:C	2.53	0.52
1:A:96:PHE:O	1:A:100:GLU:HG3	2.10	0.52
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:229:THR:HG22	1:A:230:ASP:N	2.25	0.52
1:A:376:GLU:O	2:A:1604:AMP:N6	2.42	0.52
1:A:24:PHE:HA	1:A:53:LEU:HD23	1.90	0.51
1:A:427:GLU:HA	1:A:427:GLU:OE2	2.10	0.51
1:B:419:MET:HE1	1:B:472:VAL:CB	2.39	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:B:156:VAL:HG23	1:B:157:ILE:N	2.25	0.51
1:A:339:LYS:HG2	1:A:396:GLU:HG3	1.93	0.51
1:B:531:LEU:HD23	1:B:531:LEU:C	2.35	0.51
1:B:3:ARG:HH11	1:B:3:ARG:HB3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CZ	1:A:467:ARG:H	2.24	0.50
1:B:475:ASP:CG	3:B:1605:ATP:O1B	2.54	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:324:LEU:C	1:A:324:LEU:CD1	2.83	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:B:71:GLY:C	1:B:73:SER:H	2.19	0.50
1:A:219:THR:HG21	1:A:273:GLU:CD	2.37	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:B:359:LEU:HD13	1:B:359:LEU:C	2.37	0.50
1:B:381:GLU:OE2	1:B:381:GLU:HA	2.11	0.50
1:B:531:LEU:HD21	1:B:535:MET:SD	2.52	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:399:GLU:C	1:B:401:ILE:H	2.20	0.49
1:B:519:ARG:HB2	1:B:540:PHE:CD2	2.47	0.49
1:B:69:THR:C	1:B:71:GLY:H	2.21	0.49
1:B:432:GLN:HA	1:B:432:GLN:NE2	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:90:LEU:O	1:B:92:ASP:N	2.45	0.49
1:B:185:GLY:C	1:B:187:GLU:N	2.70	0.49
1:B:346:LYS:HE2	1:B:346:LYS:CA	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:70:ASN:HA	1:B:73:SER:CB	2.43	0.48
1:B:179:HIS:O	1:B:183:THR:HG22	2.13	0.48
1:B:149:TRP:CZ3	1:B:152:LEU:HD23	2.47	0.48
1:B:252:PHE:CZ	1:B:419:MET:HE3	2.41	0.48
1:A:312:PHE:CE2	1:A:328:LEU:HG	2.48	0.48
1:A:348:MET:HE2	1:A:352:HIS:HD2	1.76	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:419:MET:CE	1:A:466:THR:HG22	2.43	0.48
1:A:490:ILE:HD13	1:A:490:ILE:C	2.39	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:A:449:ALA:HB1	1:A:482:MET:CE	2.44	0.48
1:B:171:ARG:CD	1:B:175:TYR:CE2	2.96	0.48
1:B:274:ILE:C	1:B:276:PRO:HD3	2.38	0.48
1:B:359:LEU:C	1:B:359:LEU:CD1	2.87	0.48
1:B:467:ARG:H	1:B:467:ARG:CZ	2.25	0.48
1:B:88:ARG:HG3	1:B:88:ARG:HH11	1.79	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
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:B:390:MET:HE1	1:B:408:ILE:HG21	1.96	0.47
1:A:91:PRO:HA	1:A:127:GLN:HE22	1.78	0.47
1:A:168:ASN:HD22	1:A:168:ASN:C	2.22	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:40:TRP:CD1	1:B:205:LYS:HZ1	2.32	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:489:ASP:CG	1:A:546:ARG:HH22	2.21	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:219:THR:C	1:B:220:LEU:HD12	2.40	0.47
1:B:482:MET:HE3	1:B:482:MET:HA	1.96	0.47
1:B:538:ASP:HB3	1:B:544:TYR:CG	2.49	0.47
1:A:77:GLU:HG3	1:A:81:ARG:NH1	2.30	0.47
1:A:143:PHE:HB3	1:A:152:LEU:CD1	2.30	0.47
1:B:47:MET:O	1:B:51:ILE:HG13	2.15	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: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:O	1:B:241:THR:CG2	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:181:THR:C	1:B:183:THR:H	2.21	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: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:169:LYS:O	1:A:170:SER:C	2.58	0.46
1:A:475:ASP:OD2	3:A:1605:ATP:O3G	2.34	0.46
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:B:140:ALA:CB	1:B:197:ALA:HA	2.45	0.46
1:A:64:GLN:O	1:A:68:ILE:HG12	2.16	0.46
1:A:96:PHE:CZ	1:A:127:GLN:HG2	2.50	0.46
1:B:519:ARG:O	1:B:523:CYS:HB2	2.16	0.46
1:A:69:THR:HG23	1:A:70:ASN:H	1.80	0.46
1:A:325:VAL:HA	1:A:335:PHE:O	2.16	0.46
1:A:335:PHE:N	1:A:335:PHE:CD1	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:PHE:CD2	1:A:132:PHE:N	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:A:482:MET:HE1	1:A:545:TRP:CZ3	2.51	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:28:THR:HA	1:B:258:MET:HE2	1.99	0.45
1:A:157:ILE:CG2	1:A:169:LYS:HD2	2.46	0.45
1:A:419:MET:HE3	1:A:466:THR:HG22	1.98	0.45
1:B:102:PHE:O	1:B:106:VAL:HG23	2.17	0.45
1:A:123:ILE:HD12	1:A:123:ILE:C	2.41	0.45
1:A:413:LEU:HD23	1:A:413:LEU:O	2.17	0.45
1:B:457:ASP:OD1	1:B:457:ASP:C	2.58	0.45
1:A:40:TRP:O	1:A:44:GLN:HG3	2.17	0.45
1:B:209:LEU:HD23	1:B:209:LEU:C	2.41	0.45
1:B:400:LYS:HD2	1:B:400:LYS:N	2.30	0.45
1:B:180:LEU:C	1:B:183:THR:HG22	2.41	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: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:A:449:ALA:HB1	1:A:482:MET:HE1	1.98	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
1:B:531:LEU:CD2	1:B:535:MET:CE	2.94	0.45
1:B:558:GLU:O	1:B:559:ASP:C	2.59	0.45
1:A:76:ALA:HB1	1:A:120:ARG:HH22	1.80	0.45
1:A:168:ASN:ND2	1:A:171:ARG:HB2	2.30	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:A:477:ASP:OD2	1:A:477:ASP:C	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ARG:HA	1:A:53:LEU:HD22	2.00	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: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:235:PHE:CD1	1:B:235:PHE:C	2.95	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:B:14:LEU:HD21	1:B:93:TYR:CZ	2.53	0.44
1:B:482:MET:CE	1:B:482:MET:HA	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:HA	1:B:533:GLU:OE1	2.17	0.44
1:A:78:PHE:O	1:A:82:VAL:HG23	2.17	0.44
1:A:168:ASN:OD1	1:A:171:ARG:HB2	2.15	0.44
1:A:370:ALA:N	1:A:476:TYR:OH	2.51	0.44
1:B:84:GLU:O	1:B:88:ARG:HG2	2.18	0.44
1:B:366:VAL:HG22	1:B:560:VAL:HG21	2.00	0.44
1:B:531:LEU:CD2	1:B:535:MET:HE3	2.47	0.44
1:A:322:VAL:HG22	1:A:323:MET:HG2	1.99	0.44
1:A:100:GLU:OE2	1:A:125:SER:O	2.36	0.43
1:A:123:ILE:HD11	1:A:124:PHE:CE2	2.52	0.43
1:A:254:ARG:NH1	1:A:254:ARG:HG2	2.33	0.43
1:B:176:ILE:HD11	1:B:236:ILE:HD13	2.00	0.43
1:B:413:LEU:C	1:B:413:LEU:CD2	2.91	0.43
1:B:435:ARG:HH11	1:B:435:ARG:HG3	1.83	0.43
1:A:132:PHE:H	1:A:132:PHE:HD2	1.60	0.43
1:B:8:LEU:HD11	1:B:68:ILE:HD13	2.00	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:A:40:TRP:HA	1:A:40:TRP:CE3	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:209:LEU:C	1:A:209:LEU:CD2	2.91	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:445:ILE:HD12	1:A:458:MET:HE3	1.99	0.43
1:B:107:TYR:CD2	1:B:107:TYR:C	2.96	0.43
1:B:221:PRO:CG	1:B:274:ILE:HG23	2.43	0.43
1:B:366:VAL:O	1:B:366:VAL:CG1	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:113:HIS:HE1	2:B:1604:AMP:O2P	2.01	0.43
1:B:148:GLY:CA	1:B:152:LEU:HB2	2.47	0.43
1:B:69:THR:HB	1:B:70:ASN:H	1.57	0.43
1:A:154:MET:SD	1:A:169:LYS:NZ	2.89	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: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:339:LYS:HG2	1:A:396:GLU:CG	2.49	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:272:ARG:NH1	1:B:280:THR:HG1	2.16	0.42
1:B:428:GLN:O	1:B:429:VAL:HG23	2.19	0.42
1:B:78:PHE:C	1:B:78:PHE:CD2	2.96	0.42
1:B:78:PHE:O	1:B:82:VAL:HG23	2.19	0.42
1:B:143:PHE:CD2	1:B:156:VAL:HG12	2.54	0.42
1:B:181:THR:C	1:B:183:THR:N	2.77	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
1:B:477:ASP:CG	3:B:1605:ATP:O2G	2.62	0.42
1:B:547:ALA:O	1:B:550:ASN:HB2	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:88:ARG:HG3	1:B:88:ARG:NH1	2.33	0.42
1:A:6:GLU:OE2	1:A:81:ARG:HG3	2.19	0.42
1:A:375:PHE:HB2	1:A:413:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:ILE:O	1:A:529:GLY:C	2.60	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:306:GLN:C	1:A:306:GLN:CD	2.87	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:164:LEU:HB2	1:A:234:LEU:HG	2.01	0.42
1:A:229:THR:OG1	1:A:233:GLU:HB2	2.19	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:A:494:ARG:O	1:A:495:TYR:HB2	2.19	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:78:PHE:C	1:B:80:LEU:H	2.27	0.42
1:B:167:GLN:OE1	1:B:171:ARG:NH2	2.52	0.42
1:B:445:ILE:HD12	1:B:458:MET:CE	2.47	0.42
1:B:8:LEU:CD1	1:B:68:ILE:HD13	2.50	0.42
1:A:72:GLN:O	1:A:75:ASP:N	2.52	0.42
1:A:420:VAL:HG13	1:A:465:VAL:HB	2.01	0.42
1:B:40:TRP:NE1	1:B:205:LYS:HE3	2.35	0.42
1:A:237:ASP:C	1:A:238:THR:HG22	2.42	0.42
1:B:72:GLN:C	1:B:74:THR:N	2.71	0.42
1:B:252:PHE:CD1	1:B:252:PHE:C	2.98	0.42
1:B:310:GLU:CB	1:B:329:PRO:HG2	2.45	0.42
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:93:TYR:HA	1:A:94:PRO:HD3	1.65	0.41
1:A:149:TRP:H	1:A:152:LEU:CB	2.32	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:365:ARG:CG	1:A:365:ARG:NH2	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
1:A:274:ILE:HG22	1:A:275:LEU:N	2.35	0.41
1:A:453:ILE:CG2	1:A:479:ILE:HG13	2.46	0.41
1:A:456:GLY:HA3	1:A:478:GLU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE21	1:B:290:GLN:HB3	1.60	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:77:GLU:N	1:B:77:GLU:CD	2.78	0.41
1:B:109:ARG:NH1	1:B:109:ARG:HG3	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:HH11	1:A:519:ARG:CG	2.33	0.41
1:B:149:TRP:H	1:B:152:LEU:HB3	1.84	0.41
1:B:346:LYS:HZ2	1:B:348:MET:HE3	1.86	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:40:TRP:CE2	1:A:205:LYS:HG2	2.54	0.41
1:A:188:ASN:N	1:A:188:ASN:HD22	2.17	0.41
1:A:365:ARG:HG2	1:A:369:MET:O	2.21	0.41
1:A:382:LYS:HD2	1:A:405:GLY:O	2.20	0.41
1:B:349:SER:O	1:B:350:ALA:C	2.63	0.41
1:B:352:HIS:O	1:B:353:VAL:C	2.63	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:134:THR:O	1:B:135:ILE:C	2.63	0.40
1:B:274:ILE:O	1:B:275:LEU:C	2.64	0.40
1:B:312:PHE:O	1:B:389:LEU:HD23	2.21	0.40
1:B:368:ARG:HD2	1:B:444:ALA:HA	2.02	0.40
1:A:157:ILE:HA	1:A:160:LEU:CD2	2.51	0.40
1:B:78:PHE:C	1:B:78:PHE:HD2	2.29	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:291:LYS:HA	1:B:291:LYS:HD2	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: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
1:B:20:GLN:HG3	1:B:21:TYR:N	2.36	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%)	4 16
1	B	555/578 (96%)	458 (82%)	73 (13%)	24 (4%)	2 7
All	All	1117/1156 (97%)	952 (85%)	127 (11%)	38 (3%)	3 11

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 [i](#)

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%)	436 (88%)	61 (12%)	4	16
1	B	490/508 (96%)	423 (86%)	67 (14%)	3	13
All	All	987/1016 (97%)	859 (87%)	128 (13%)	4	14

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	11	GLN

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Mol	Chain	Res	Type
1	A	20	GLN
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	116	LEU
1	A	123	ILE
1	A	135	ILE
1	A	138	PRO
1	A	139	LEU
1	A	141	LYS
1	A	167	GLN
1	A	171	ARG
1	A	196	VAL
1	A	200	LEU
1	A	230	ASP
1	A	243	THR
1	A	258	MET
1	A	271	LEU
1	A	273	GLU
1	A	275	LEU
1	A	283	LEU
1	A	290	GLN
1	A	302	LEU
1	A	306	GLN
1	A	322	VAL
1	A	324	LEU
1	A	325	VAL
1	A	329	PRO
1	A	337	VAL
1	A	338	ILE
1	A	359	LEU
1	A	360	VAL
1	A	365	ARG
1	A	366	VAL
1	A	381	GLU
1	A	390	MET
1	A	392	LEU
1	A	394	LEU

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Mol	Chain	Res	Type
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
1	A	479	ILE
1	A	485	VAL
1	A	488	ARG
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	A	571	VAL
1	B	3	ARG
1	B	7	LEU
1	B	8	LEU
1	B	20	GLN
1	B	34	ARG
1	B	37	GLN
1	B	60	LEU
1	B	70	ASN
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

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Mol	Chain	Res	Type
1	B	278	LYS
1	B	283	LEU
1	B	290	GLN
1	B	295	THR
1	B	302	LEU
1	B	309	ASN
1	B	322	VAL
1	B	324	LEU
1	B	325	VAL
1	B	329	PRO
1	B	337	VAL
1	B	341	LYS
1	B	346	LYS
1	B	347	GLU
1	B	359	LEU
1	B	366	VAL
1	B	376	GLU
1	B	390	MET
1	B	392	LEU
1	B	396	GLU
1	B	411	ARG
1	B	412	HIS
1	B	413	LEU
1	B	420	VAL
1	B	422	LEU
1	B	429	VAL
1	B	458	MET
1	B	466	THR
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	535	MET
1	B	548	LEU
1	B	551	ARG
1	B	554	GLU
1	B	558	GLU
1	B	566	ARG
1	B	572	ARG

Sometimes 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	64	GLN
1	A	104	ASN
1	A	113	HIS
1	A	127	GLN
1	A	167	GLN
1	A	168	ASN
1	A	179	HIS
1	A	188	ASN
1	A	193	HIS
1	A	204	ASN
1	A	228	GLN
1	A	290	GLN
1	A	292	HIS
1	A	373	GLN
1	A	377	ASN
1	A	384	HIS
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	70	ASN
1	B	72	GLN
1	B	85	HIS
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	306	GLN
1	B	309	ASN
1	B	373	GLN
1	B	377	ASN
1	B	407	GLN

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Mol	Chain	Res	Type
1	B	428	GLN
1	B	432	GLN
1	B	447	GLN
1	B	452	ASN
1	B	550	ASN
1	B	567	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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$
2	AMP	B	1604	-	25,25,25	1.84	3 (12%)	37,38,38	2.05	10 (27%)
2	AMP	A	1604	-	25,25,25	1.68	2 (8%)	37,38,38	2.01	9 (24%)
3	ATP	A	1605	4	32,33,33	2.84	4 (12%)	48,52,52	2.01	15 (31%)
3	ATP	B	1605	4	32,33,33	2.11	1 (3%)	48,52,52	2.00	15 (31%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AMP	B	1604	-	-	0/10/26/26	0/3/3/3
2	AMP	A	1604	-	-	0/10/26/26	0/3/3/3
3	ATP	A	1605	4	-	0/22/38/38	0/3/3/3
3	ATP	B	1605	4	-	0/22/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1605	ATP	PA-O3A	13.97	1.74	1.59
3	B	1605	ATP	PA-O3A	10.74	1.71	1.59
2	B	1604	AMP	C2-N3	7.42	1.47	1.33
2	A	1604	AMP	C2-N3	6.80	1.46	1.33
3	A	1605	ATP	PB-O3A	-5.23	1.53	1.59
3	A	1605	ATP	PB-O3B	-2.44	1.56	1.59
2	A	1604	AMP	C5-C4	2.35	1.43	1.39
2	B	1604	AMP	C5-C4	2.29	1.43	1.39
2	B	1604	AMP	O4'-C1'	2.25	1.47	1.42
3	A	1605	ATP	C6-N6	2.16	1.39	1.34

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1604	AMP	N3-C2-N1	-5.59	120.12	128.58
2	A	1604	AMP	N3-C2-N1	-5.43	120.37	128.58
2	B	1604	AMP	C5-C4-N3	-5.06	119.75	126.72
2	A	1604	AMP	C5-C4-N3	-4.84	120.05	126.72
3	B	1605	ATP	N3-C2-N1	-4.66	121.53	128.58
3	B	1605	ATP	C5-C4-N3	-4.66	120.30	126.72
3	A	1605	ATP	C5-C4-N3	-4.64	120.32	126.72
3	A	1605	ATP	N3-C2-N1	-4.52	121.74	128.58
3	B	1605	ATP	N3-C4-N9	4.25	134.40	127.17
2	B	1604	AMP	N3-C4-N9	4.09	134.13	127.17
3	A	1605	ATP	N3-C4-N9	4.03	134.02	127.17
2	A	1604	AMP	N3-C4-N9	3.82	133.66	127.17
2	B	1604	AMP	C5-N7-C8	3.76	109.36	103.45
3	A	1605	ATP	C5-N7-C8	3.75	109.35	103.45
3	B	1605	ATP	C5-N7-C8	3.64	109.17	103.45
3	A	1605	ATP	C2-N3-C4	3.63	120.70	111.83
3	B	1605	ATP	C2-N3-C4	3.54	120.48	111.83
2	A	1604	AMP	C5-N7-C8	3.30	108.63	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1604	AMP	C4-C5-N7	-3.24	106.88	110.58
3	A	1605	ATP	N9-C8-N7	-3.21	109.38	113.94
3	A	1605	ATP	O2B-PB-O3A	-3.17	98.71	107.27
3	A	1605	ATP	C4-C5-N7	-3.14	107.00	110.58
3	B	1605	ATP	N9-C8-N7	-3.12	109.52	113.94
3	B	1605	ATP	PA-O5'-C5'	-3.03	103.96	121.35
2	A	1604	AMP	C4-C5-N7	-3.03	107.12	110.58
2	B	1604	AMP	C2-N3-C4	3.02	119.20	111.83
2	A	1604	AMP	C5'-C4'-C3'	-2.96	104.55	115.21
2	A	1604	AMP	C2-N3-C4	2.84	118.78	111.83
3	A	1605	ATP	PA-O5'-C5'	-2.81	105.27	121.35
3	B	1605	ATP	O2B-PB-O3A	-2.80	99.70	107.27
3	A	1605	ATP	C2'-C1'-N9	-2.77	106.42	113.30
3	A	1605	ATP	C4-N9-C8	2.74	108.62	105.74
3	A	1605	ATP	O4'-C1'-N9	2.74	113.36	108.09
3	B	1605	ATP	C2'-C1'-N9	-2.69	106.62	113.30
3	B	1605	ATP	C4-C5-N7	-2.68	107.52	110.58
2	B	1604	AMP	N9-C8-N7	-2.67	110.15	113.94
2	A	1604	AMP	O4'-C4'-C3'	2.64	110.39	105.15
3	B	1605	ATP	C4-N9-C8	2.63	108.50	105.74
3	B	1605	ATP	O3G-PG-O3B	2.58	113.30	104.64
3	B	1605	ATP	C3'-C2'-C1'	2.51	106.21	101.46
2	A	1604	AMP	N9-C8-N7	-2.50	110.38	113.94
3	A	1605	ATP	C2'-C3'-C4'	2.26	106.98	102.61
3	A	1605	ATP	C3'-C2'-C1'	2.22	105.66	101.46
3	A	1605	ATP	O3G-PG-O3B	2.22	112.07	104.64
2	B	1604	AMP	C5'-C4'-C3'	-2.21	107.25	115.21
3	B	1605	ATP	O4'-C1'-N9	2.20	112.32	108.09
3	B	1605	ATP	O2B-PB-O3B	-2.14	101.50	107.27
2	B	1604	AMP	C2'-C3'-C4'	2.07	106.60	102.61
2	B	1604	AMP	C2-N1-C6	2.03	122.07	118.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 15 short contacts:

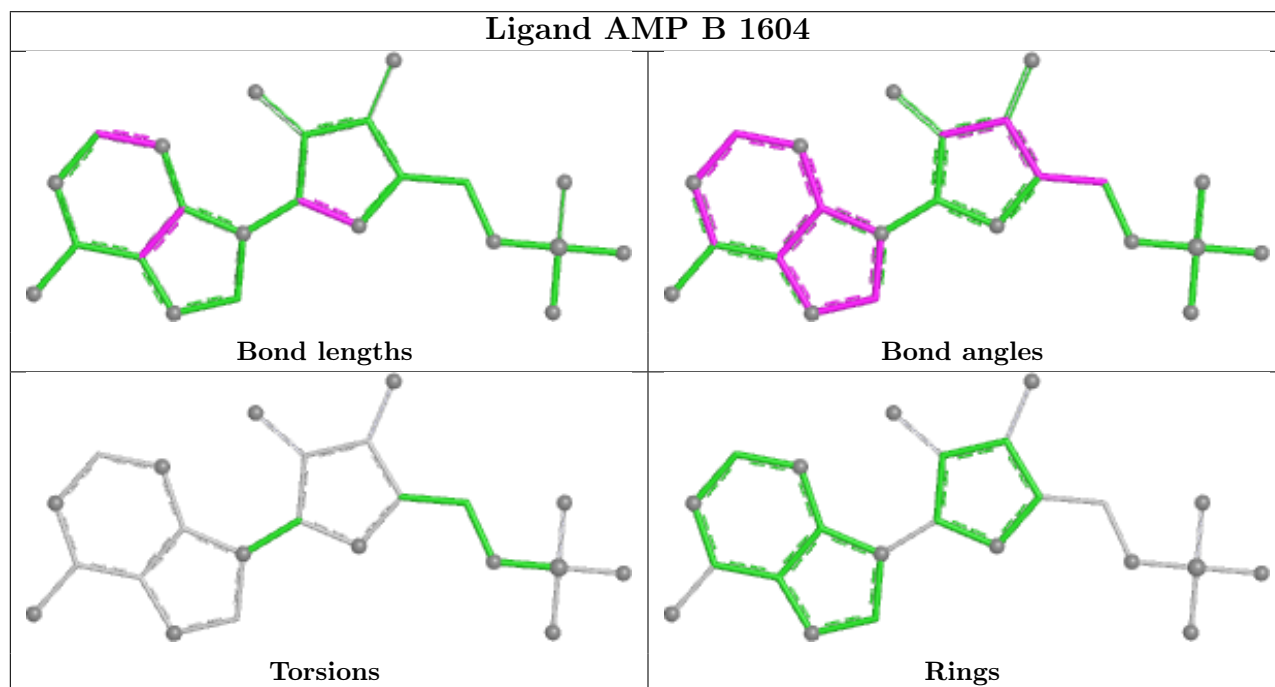
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1604	AMP	1	0
2	A	1604	AMP	2	0
3	A	1605	ATP	5	0

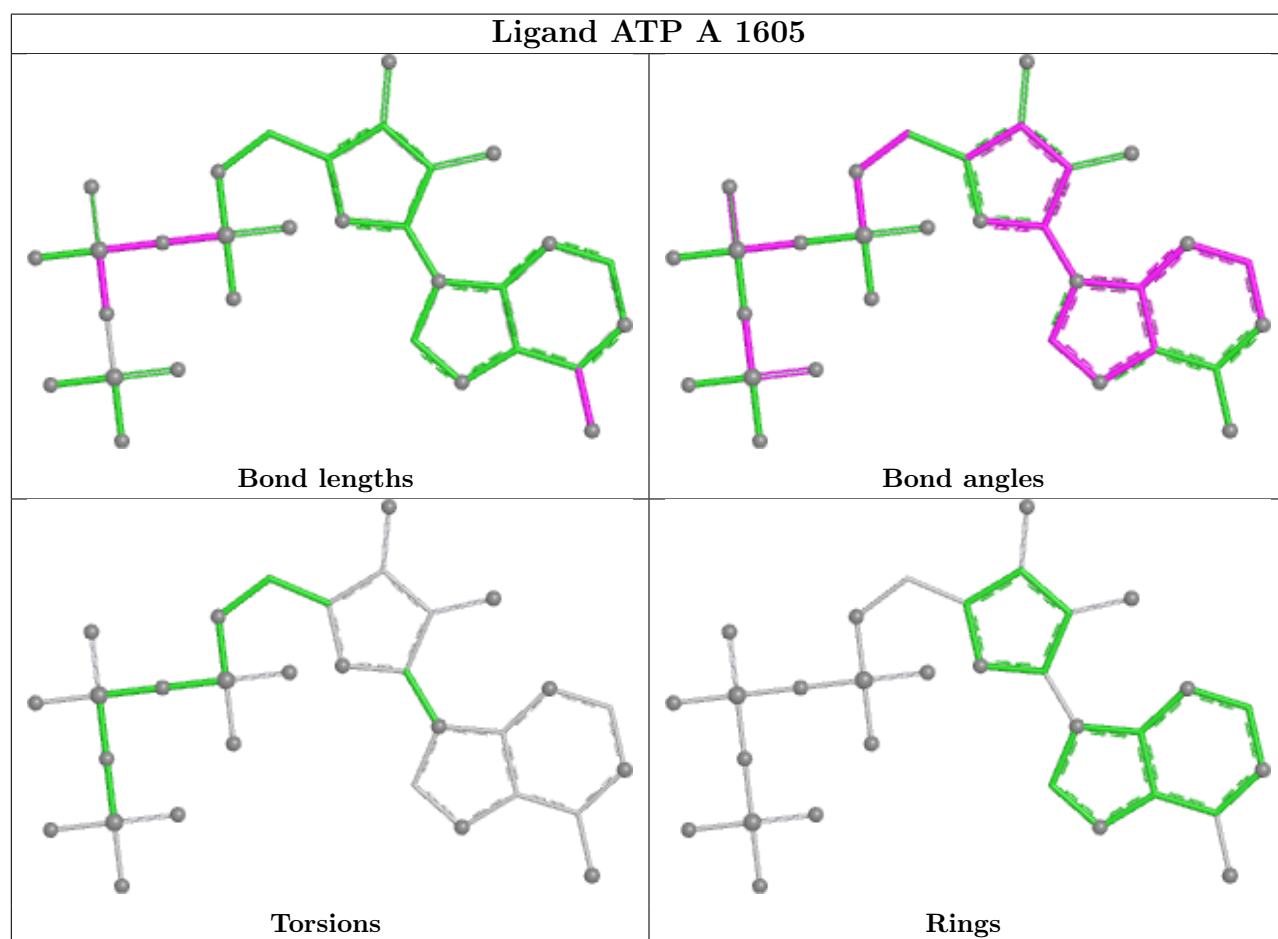
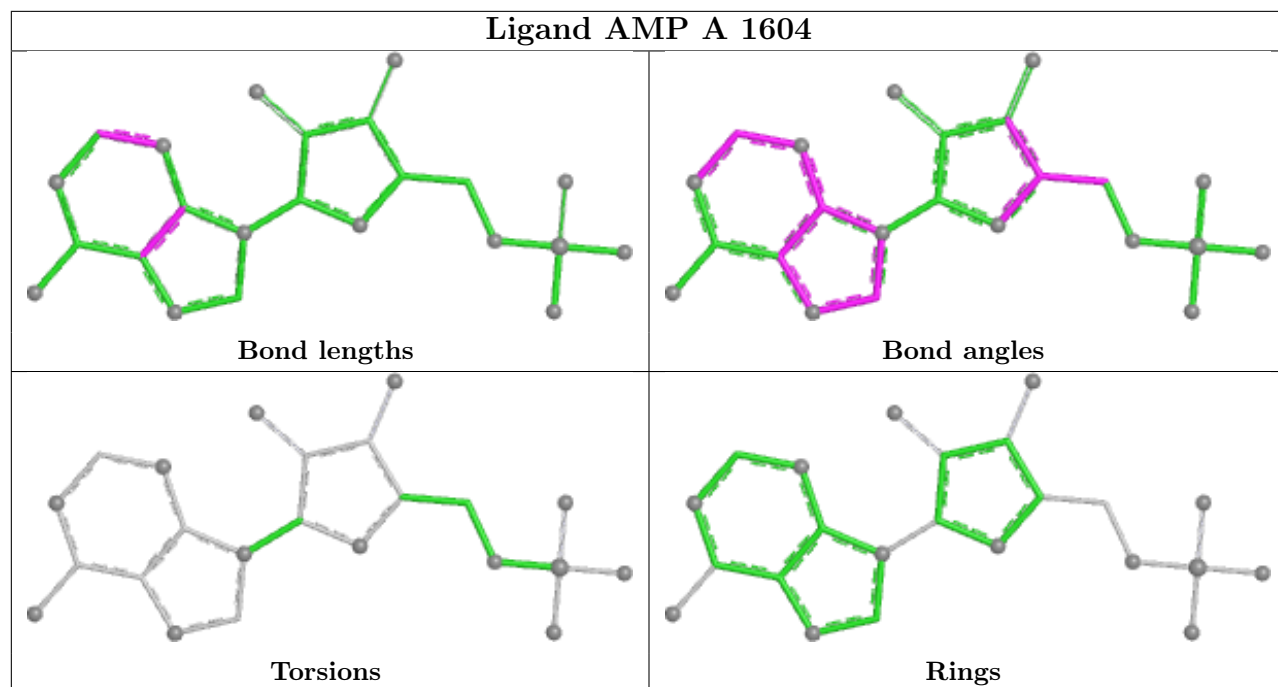
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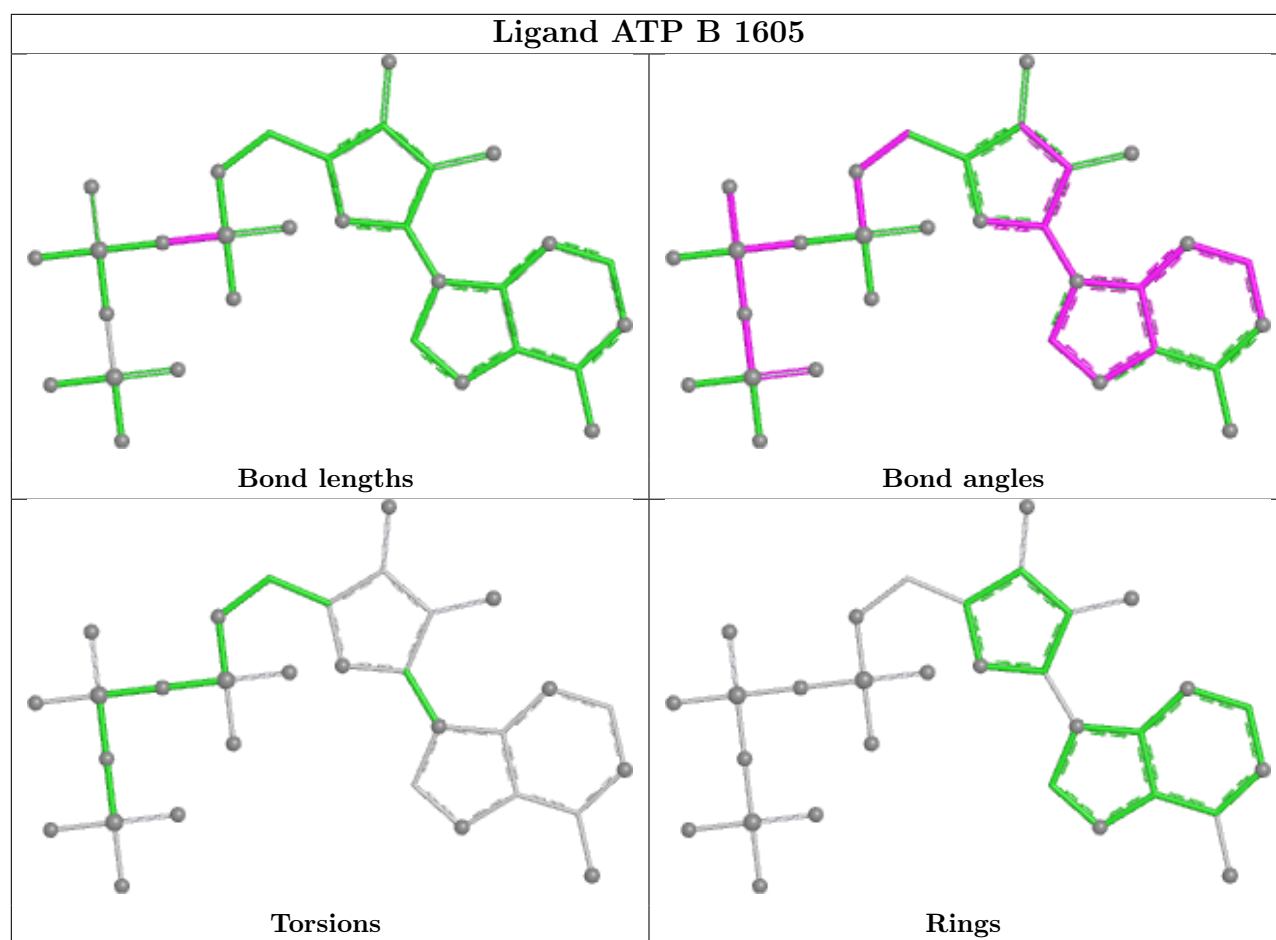
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1605	ATP	7	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	566/578 (97%)	0.25	23 (4%) 41 33	46, 68, 104, 144	0
1	B	559/578 (96%)	0.54	33 (5%) 28 21	46, 79, 117, 139	0
All	All	1125/1156 (97%)	0.40	56 (4%) 34 26	46, 74, 112, 144	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	PRO	5.0
1	B	557	VAL	4.6
1	A	496	PRO	3.8
1	B	73	SER	3.7
1	B	537	ALA	3.5
1	B	79	LEU	3.4
1	A	477	ASP	3.3
1	B	322	VAL	3.3
1	B	251	GLY	3.3
1	B	555	GLY	3.2
1	B	18	ASP	3.1
1	A	70	ASN	3.1
1	B	430	GLU	3.1
1	A	574	GLY	3.0
1	A	132	PHE	3.0
1	A	72	GLN	2.9
1	A	231	ASP	2.9
1	A	76	ALA	2.9
1	B	175	TYR	2.9
1	A	92	ASP	2.9
1	B	572	ARG	2.8
1	A	229	THR	2.8
1	B	72	GLN	2.7
1	B	74	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	148	GLY	2.7
1	A	165	HIS	2.6
1	A	322	VAL	2.5
1	A	486	ASN	2.5
1	B	41	HIS	2.5
1	B	556	HIS	2.5
1	B	219	THR	2.5
1	B	75	ASP	2.5
1	B	507	SER	2.4
1	A	233	GLU	2.4
1	A	215	THR	2.4
1	B	127	GLN	2.4
1	B	214	ILE	2.3
1	A	232	GLY	2.3
1	B	265	ALA	2.3
1	B	401	ILE	2.2
1	B	3	ARG	2.2
1	B	134	THR	2.2
1	A	495	TYR	2.2
1	B	118	PRO	2.2
1	B	491	PRO	2.2
1	A	218	GLY	2.2
1	B	558	GLU	2.2
1	A	572	ARG	2.2
1	B	139	LEU	2.2
1	A	391	GLU	2.2
1	B	520	HIS	2.1
1	B	165	HIS	2.1
1	B	69	THR	2.1
1	A	114	ARG	2.1
1	B	6	GLU	2.1
1	A	487	PHE	2.1

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

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

6.3 Carbohydrates [i](#)

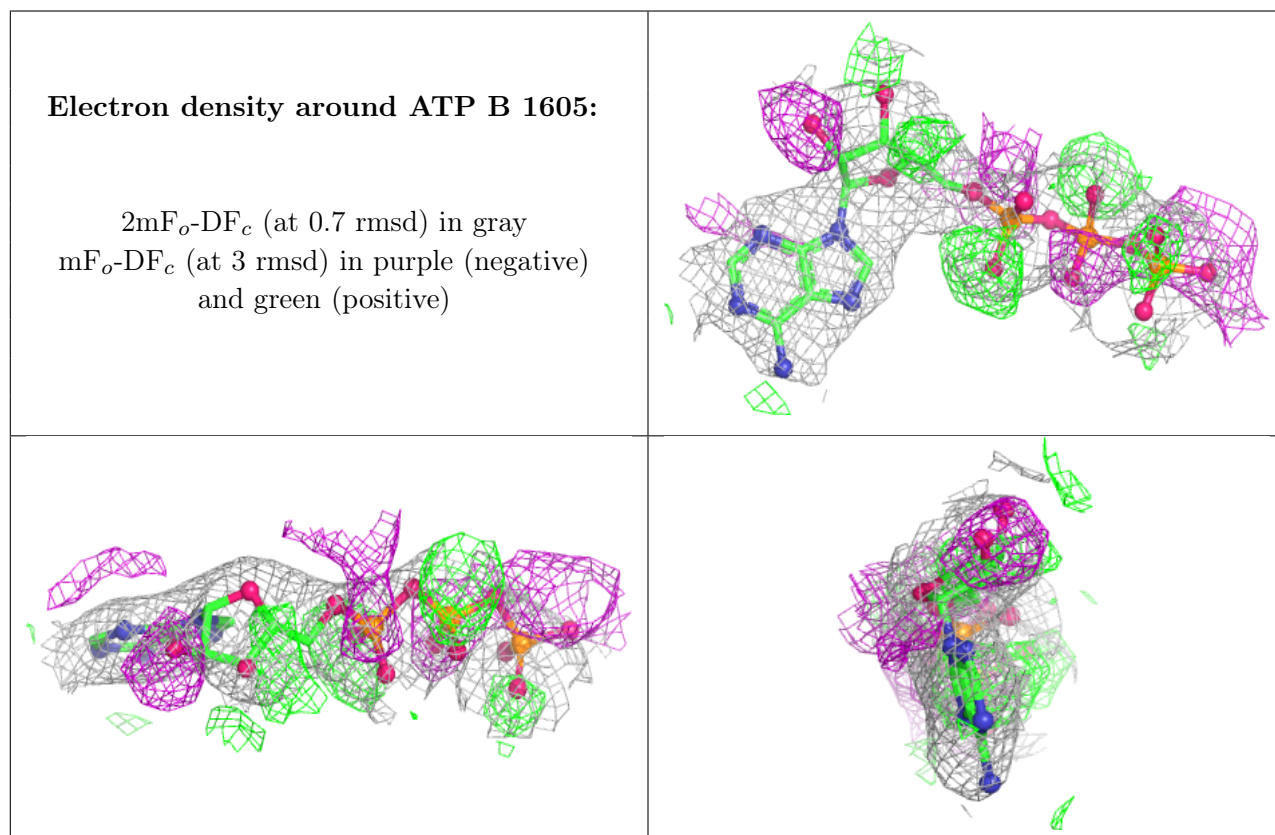
There are no oligosaccharides in this entry.

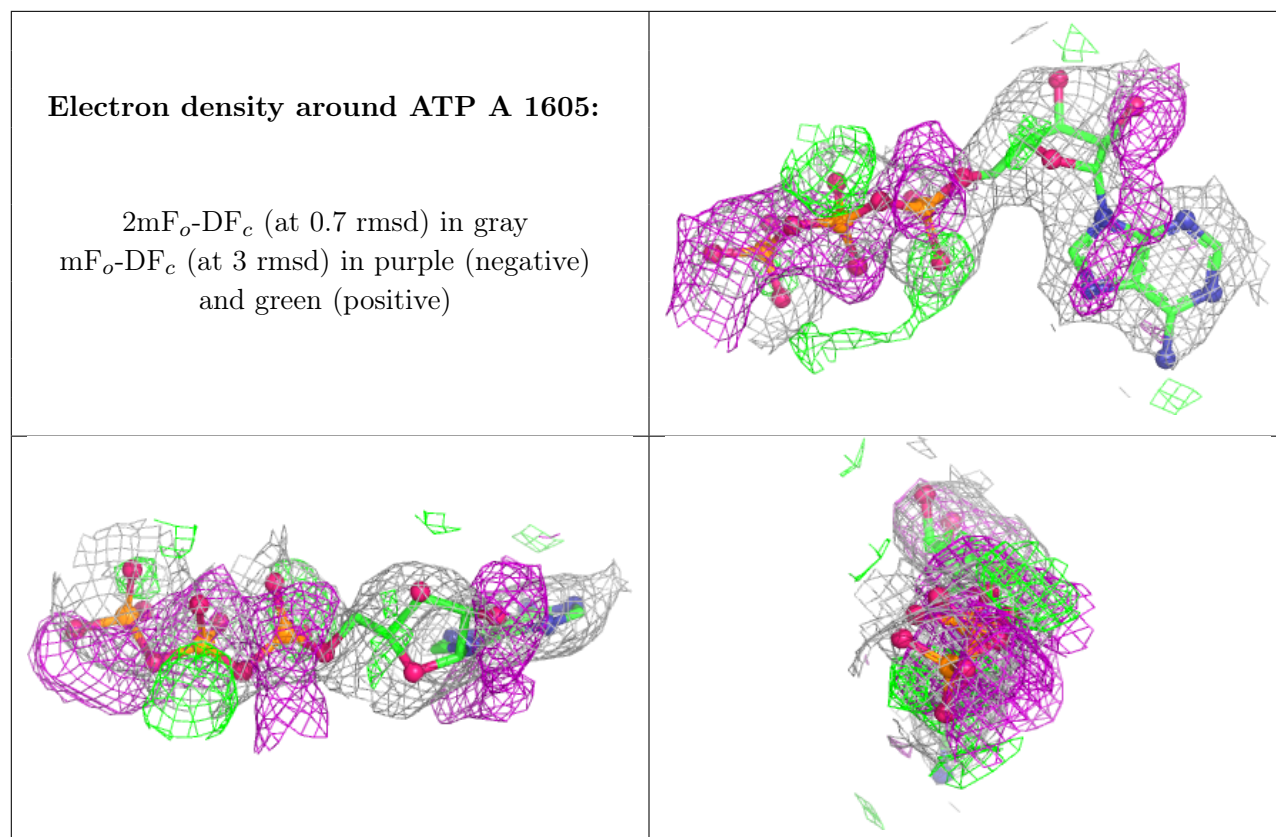
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ATP	B	1605	31/31	0.83	0.16	47,59,77,77	0
3	ATP	A	1605	31/31	0.88	0.15	43,51,77,77	0
2	AMP	B	1604	23/23	0.90	0.13	63,68,77,82	0
4	MG	B	1606	1/1	0.92	0.14	53,53,53,53	0
4	MG	A	1606	1/1	0.94	0.13	44,44,44,44	0
2	AMP	A	1604	23/23	0.94	0.10	49,55,57,61	0

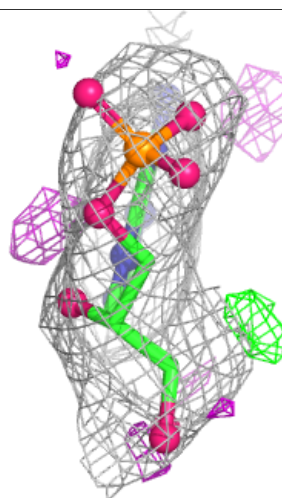
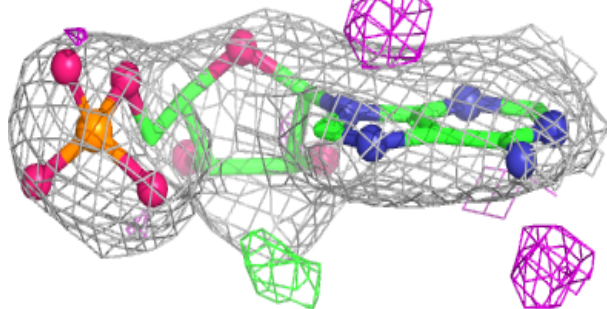
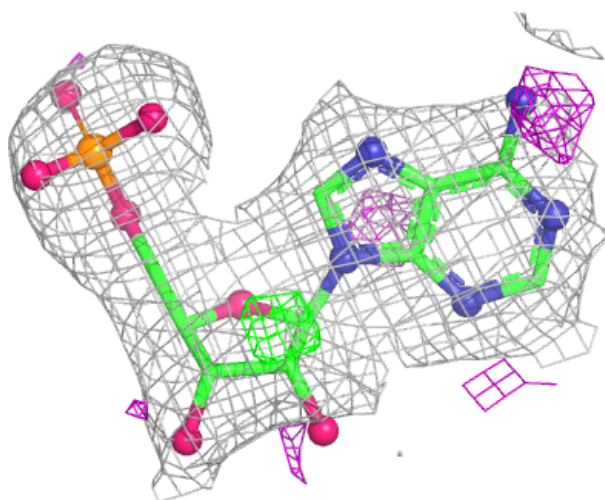
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

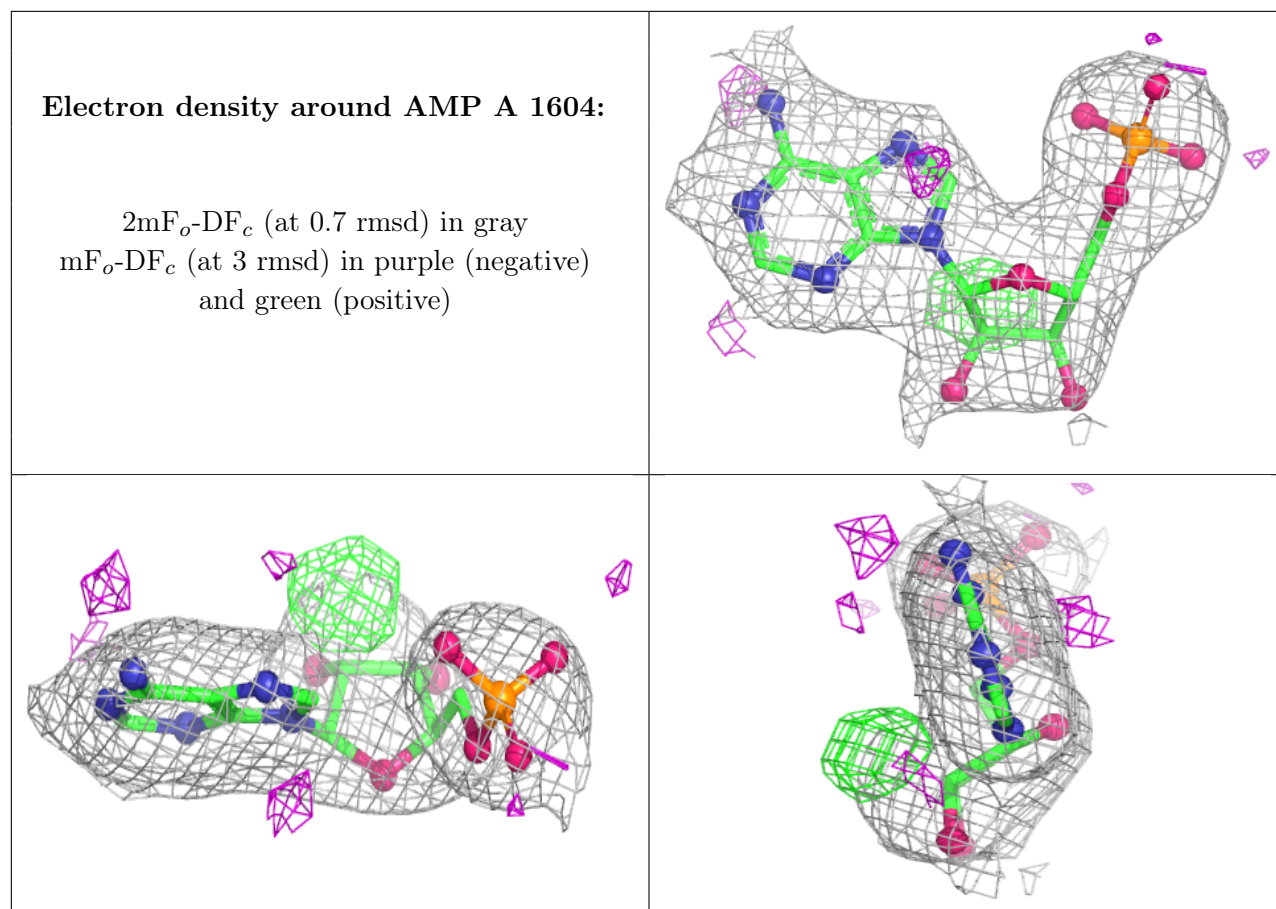




Electron density around AMP B 1604:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.