Full wwPDB X-ray Structure Validation Report (i)

Nov 6, 2023 – 04:27 PM EST

PDB ID	:	1KMN
Title	:	HISTIDYL-TRNA SYNTHETASE COMPLEXED WITH HISTIDINOL AND ATP
Authors	:	Arnez, J.G.; Francklyn, C.S.; Moras, D.
Deposited on	:	1997-05-09
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 (i) 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 (i)) were used in the production of this report:

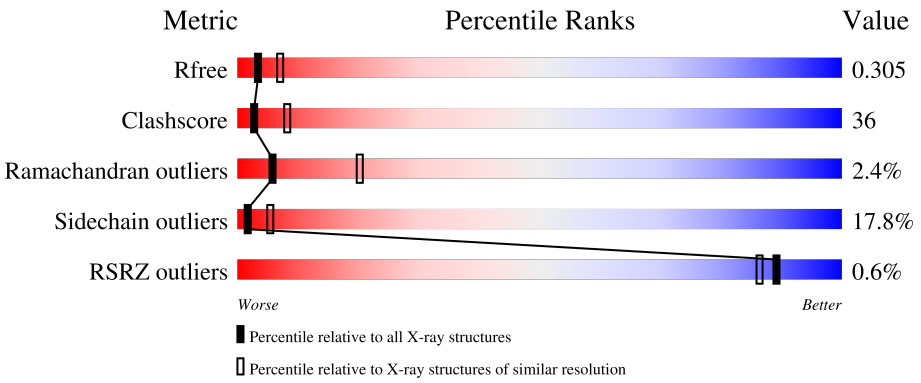
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	424	36% 45% 7% • 11%
1	B	424	% 37% 39% 9% 14%
1	C	424	42% 41% 9% 9%
1	D	424	% 39% 38% 8% 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ATP	B	452	-	-	X	-
3	ATP	D	452	-	-	X	-

2 Entry composition (i)

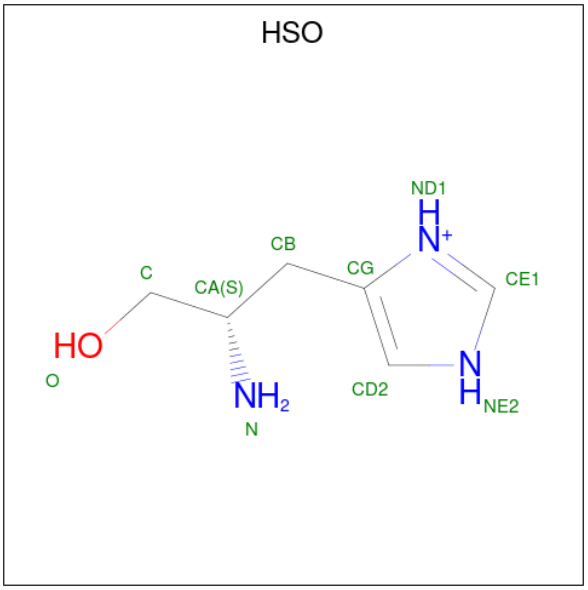
There are 4 unique types of molecules in this entry. The entry contains 14397 atoms, of which 2666 are hydrogens and 0 are deuteriums.

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 HISTIDYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	379	3612	1848	674	528	551	11	0	0	0
1	B	364	3455	1768	643	505	528	11	0	0	0
1	C	387	3666	1876	682	536	561	11	0	0	0
1	D	364	3452	1765	643	505	528	11	0	0	0

- Molecule 2 is L-histidinol (three-letter code: HSO) (formula: $C_6H_{12}N_3O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
2	A	1	13	6	3	3	1	0	0
2	B	1	13	6	3	3	1	0	0

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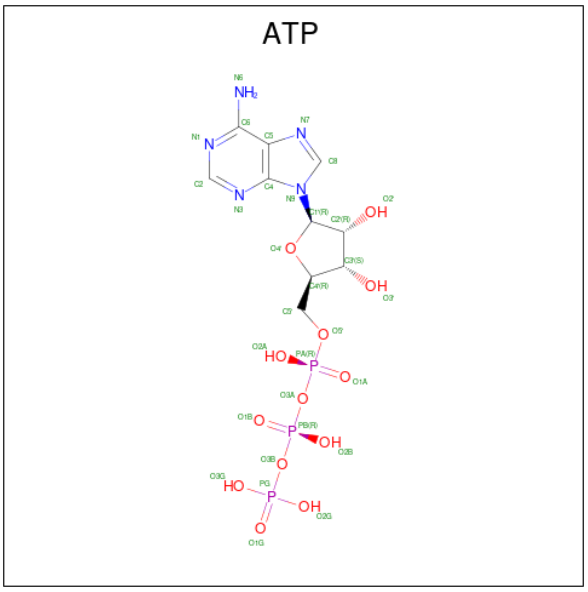
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
2	C	1	13	6	3	3	1	0	0
			Total	C	H	N	O		
2	D	1	13	6	3	3	1	0	0

- 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
			Total	C	H	N	O	P		
3	A	1	34	10	3	5	13	3	0	0
			Total	C	H	N	O	P		
3	B	1	34	10	3	5	13	3	0	0
			Total	C	H	N	O	P		
3	C	1	34	10	3	5	13	3	0	0
			Total	C	H	N	O	P		
3	D	1	34	10	3	5	13	3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	13	13	13	0	0
			Total	O		
4	B	5	5	5	0	0
			Total	O		
4	C	4	4	4	0	0

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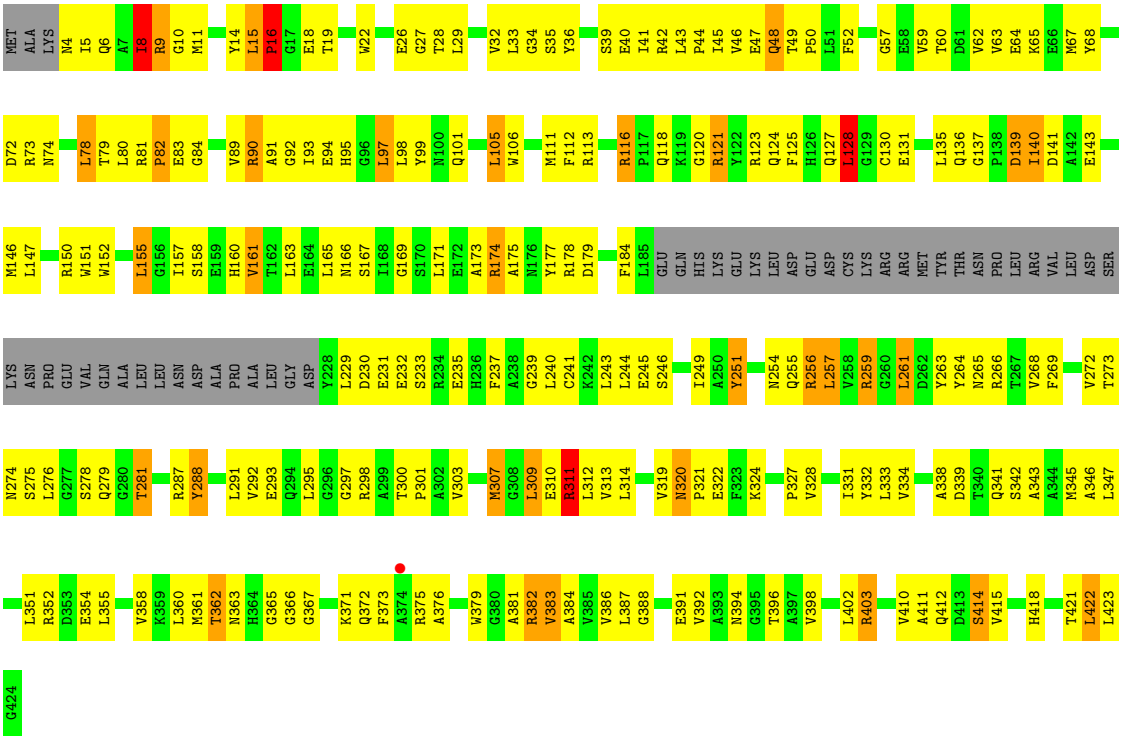
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	D	2	2	2	0	0

3 Residue-property plots (i)

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.

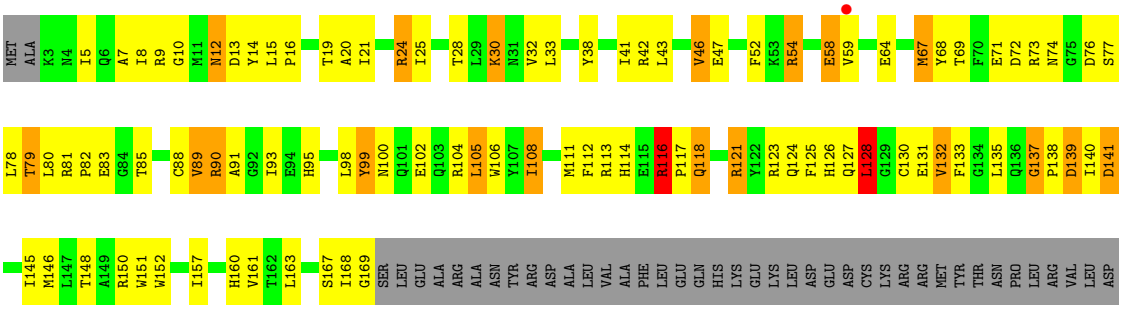
• Molecule 1: HISTIDYL-TRNA SYNTHETASE

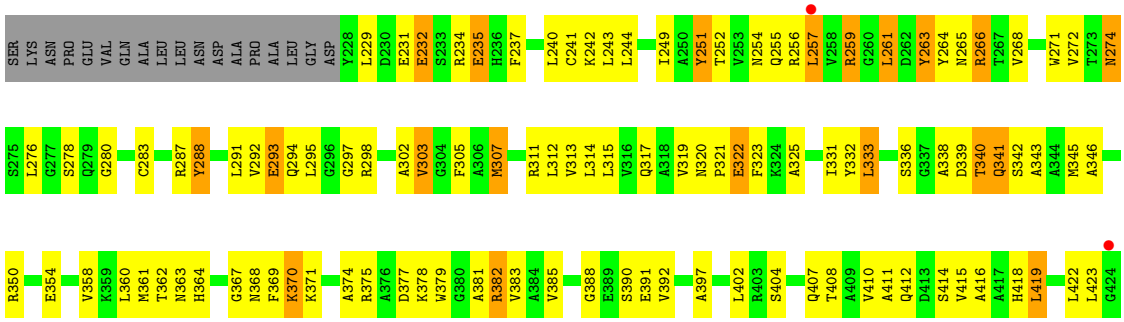
Chain A: 36% 45% 7% • 11%



• Molecule 1: HISTIDYL-TRNA SYNTHETASE

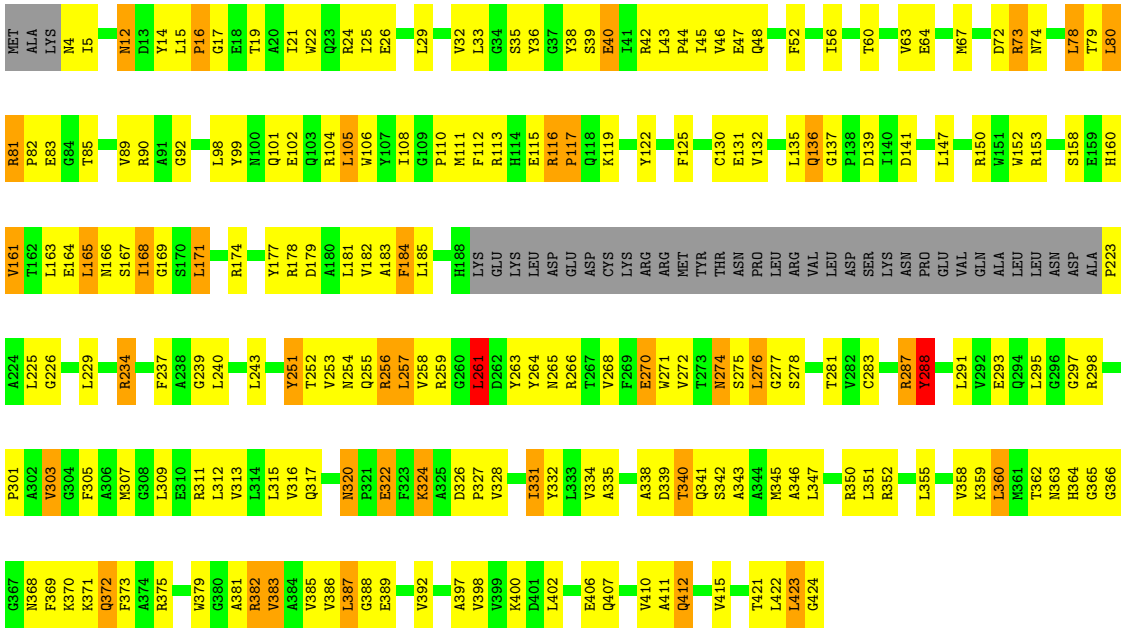
Chain B: % 37% 39% 9% 14%





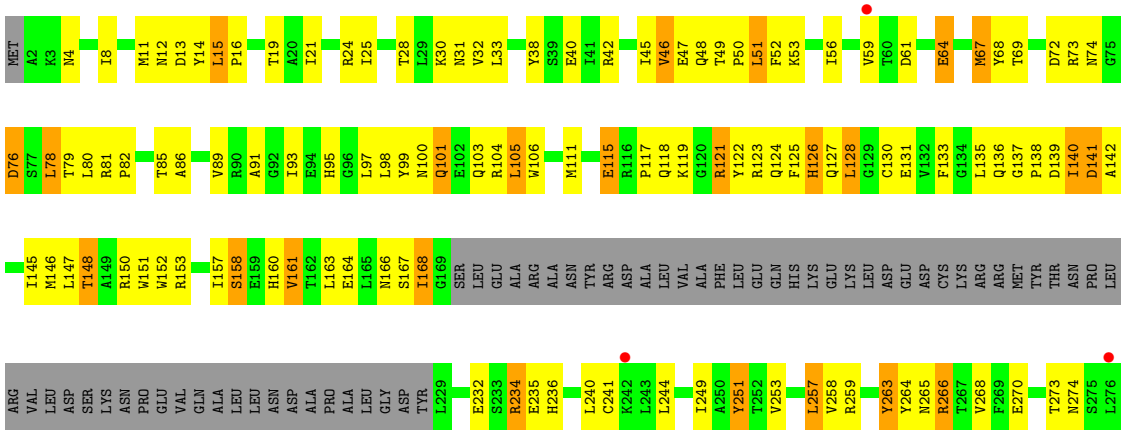
• Molecule 1: HISTIDYL-TRNA SYNTHETASE

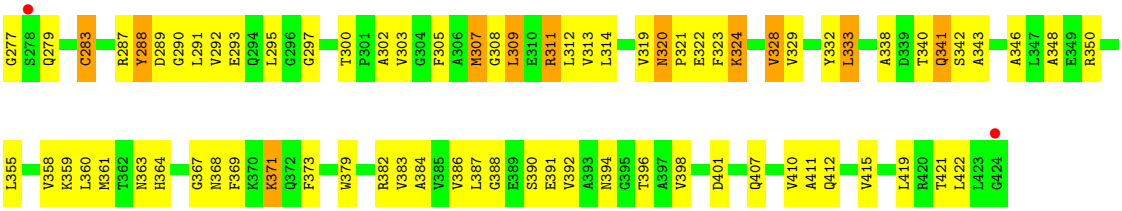
Chain C:



• Molecule 1: HISTIDYL-TRNA SYNTHETASE

Chain D:




G277
S278
Q279
C283
R287
Y288
D289
G290
L291
V292
E293
Q294
L295
G296
G297
T300
P301
A302
V303
G304
F305
A306
M307
G308
L309
E310
R311
L312
V313
L314
V319
N320
P321
E322
F323
K324
V328
V329
Y332
L333
A338
D339
T340
Q341
S342
A343
A346
L347
A348
E349
R350
L355
V358
K359
L360
M361
T362
N363
H364
G367
N368
F369
K370
K371
Q372
F373
W379
R382
V383
A384
V385
V386
L387
G388
E389
S390
E391
V392
A393
N394
G395
T396
A397
V398
D401
Q407
V410
A411
Q412
V415
L419
R420
T421
L422
L423
G424

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	60.90Å 107.30Å 107.20Å 114.10° 97.40° 90.00°	Depositor
Resolution (Å)	13.00 – 2.80 13.94 – 2.60	Depositor EDS
% Data completeness (in resolution range)	64.0 (13.00-2.80) 67.3 (13.94-2.60)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.35 (at 2.61Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.249 , 0.348 0.269 , 0.305	Depositor DCC
R_{free} test set	1585 reflections (2.50%)	wwPDB-VP
Wilson B-factor (Å^2)	26.7	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 17.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	14397	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.78	3/2991 (0.1%)	0.96	8/4046 (0.2%)
1	B	0.79	0/2863	0.92	5/3873 (0.1%)
1	C	0.74	0/3037	0.91	3/4109 (0.1%)
1	D	0.76	0/2860	0.90	2/3869 (0.1%)
All	All	0.77	3/11751 (0.0%)	0.92	18/15897 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	2
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	131	GLU	CD-OE2	6.02	1.32	1.25
1	A	131	GLU	CD-OE1	-5.22	1.20	1.25
1	A	143	GLU	CB-CG	5.05	1.61	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	116	ARG	C-N-CD	-10.59	97.30	120.60
1	A	320	ASN	C-N-CD	-8.14	102.68	120.60
1	A	311	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	A	309	LEU	CA-CB-CG	-7.15	98.85	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	311	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	C	261	LEU	CA-CB-CG	6.62	130.53	115.30
1	B	360	LEU	CA-CB-CG	6.60	130.49	115.30
1	D	360	LEU	CA-CB-CG	6.25	129.68	115.30
1	A	128	LEU	N-CA-C	-5.95	94.95	111.00
1	A	155	LEU	CA-CB-CG	5.84	128.73	115.30
1	B	128	LEU	N-CA-C	-5.64	95.78	111.00
1	C	223	PRO	N-CA-CB	5.51	109.91	103.30
1	D	128	LEU	N-CA-C	-5.44	96.32	111.00
1	C	298	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	B	419	LEU	CA-CB-CG	-5.19	103.37	115.30
1	B	128	LEU	CA-CB-CG	-5.11	103.54	115.30
1	A	422	LEU	CB-CG-CD1	-5.10	102.33	111.00
1	A	90	ARG	NE-CZ-NH1	5.07	122.84	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	99	TYR	Sidechain
1	C	122	TYR	Sidechain
1	C	288	TYR	Sidechain

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	2938	674	2899	212	0
1	B	2812	643	2768	220	0
1	C	2984	682	2932	210	0
1	D	2809	643	2762	224	0
2	A	10	3	11	0	0
2	B	10	3	11	1	0
2	C	10	3	11	2	0
2	D	10	3	11	0	0
3	A	31	3	12	3	0
3	B	31	3	12	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	31	3	12	8	0
3	D	31	3	12	11	0
4	A	13	0	0	0	0
4	B	5	0	0	1	0
4	C	4	0	0	0	0
4	D	2	0	0	0	0
All	All	11731	2666	11453	827	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 36.

All (827) 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:C:67:MET:HE3	1:C:79:THR:HG21	1.27	1.08
1:A:136:GLN:HG2	1:A:301:PRO:HG2	1.34	1.05
1:A:120:GLY:HA3	1:A:279:GLN:HG2	1.38	1.03
1:C:350:ARG:HH22	1:C:412:GLN:HG2	1.19	1.02
1:B:311:ARG:NH1	3:B:452:ATP:H2'	1.76	1.00
1:C:370:LYS:HE2	1:C:370:LYS:HA	1.43	1.00
1:B:311:ARG:CZ	3:B:452:ATP:H2'	1.93	0.98
1:A:382:ARG:HG2	1:A:403:ARG:HH21	1.30	0.96
1:C:311:ARG:NH2	3:C:452:ATP:H2'	1.78	0.96
1:C:15:LEU:HD22	1:D:97:LEU:HD11	1.45	0.95
1:C:46:VAL:HG23	1:D:8:ILE:HD12	1.51	0.92
1:D:33:LEU:HD23	1:D:147:LEU:HD11	1.53	0.91
1:D:46:VAL:HG13	1:D:80:LEU:HD12	1.53	0.90
1:C:46:VAL:HG12	1:C:80:LEU:HD12	1.53	0.90
1:D:293:GLU:HA	1:D:297:GLY:O	1.71	0.90
1:A:32:VAL:HG13	1:A:150:ARG:HD2	1.50	0.90
1:B:67:MET:HE3	1:B:79:THR:HG21	1.54	0.90
1:A:97:LEU:HD11	1:B:15:LEU:HD12	1.52	0.89
1:C:259:ARG:HG3	1:C:259:ARG:HH11	1.37	0.89
1:C:14:TYR:HB2	1:D:42:ARG:HB2	1.55	0.89
1:A:178:ARG:HG3	1:A:178:ARG:HH11	1.37	0.87
1:D:15:LEU:HD22	1:D:15:LEU:H	1.36	0.87
1:C:331:ILE:HB	1:C:360:LEU:HD12	1.57	0.86
1:C:400:LYS:HG2	1:C:407:GLN:HB3	1.55	0.86
1:A:371:LYS:HE2	1:A:375:ARG:HH21	1.41	0.85
1:B:265:ASN:ND2	1:B:266:ARG:HE	1.73	0.85
1:A:22:TRP:O	1:A:26:GLU:HG3	1.77	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:ARG:HH21	3:C:452:ATP:C2'	1.89	0.85
1:C:105:LEU:HD23	1:C:131:GLU:O	1.78	0.84
1:B:141:ASP:HB2	1:B:240:LEU:HD13	1.60	0.84
1:B:382:ARG:HG3	1:B:382:ARG:HH11	1.40	0.84
1:B:46:VAL:HG13	1:B:80:LEU:HD12	1.60	0.83
1:B:67:MET:CE	1:B:79:THR:HG21	2.09	0.83
1:D:130:CYS:SG	1:D:305:PHE:CE2	2.72	0.83
1:A:388:GLY:O	1:A:392:VAL:HG23	1.79	0.82
1:A:14:TYR:HB2	1:B:42:ARG:HB2	1.58	0.82
1:D:234:ARG:HG2	1:D:234:ARG:HH11	1.42	0.82
1:C:256:ARG:HD2	1:C:256:ARG:O	1.80	0.82
1:A:261:LEU:HD23	1:A:264:TYR:HE2	1.43	0.81
1:C:42:ARG:HB2	1:D:14:TYR:HB2	1.62	0.81
1:A:382:ARG:HG2	1:A:403:ARG:NH2	1.94	0.81
1:C:322:GLU:HG3	1:C:324:LYS:HE3	1.63	0.81
1:B:167:SER:HA	1:B:266:ARG:O	1.80	0.81
1:C:104:ARG:HG2	1:C:132:VAL:HG13	1.61	0.81
1:B:382:ARG:HG3	1:B:382:ARG:NH1	1.93	0.80
1:D:332:TYR:CE1	1:D:363:ASN:HB2	2.17	0.80
1:D:121:ARG:HH22	3:D:452:ATP:PG	2.05	0.79
1:B:278:SER:CA	1:B:311:ARG:HB3	2.12	0.79
1:A:259:ARG:HG3	1:A:259:ARG:HH11	1.49	0.78
1:C:168:ILE:HG22	1:C:265:ASN:O	1.84	0.78
1:D:412:GLN:HA	1:D:415:VAL:HG23	1.66	0.78
1:C:311:ARG:NH2	3:C:452:ATP:C2'	2.46	0.78
1:D:383:VAL:HG11	1:D:419:LEU:CD2	2.14	0.78
1:B:21:ILE:O	1:B:25:ILE:HG13	1.83	0.77
1:C:334:VAL:HG11	1:C:373:PHE:HE1	1.48	0.77
1:D:142:ALA:HA	1:D:145:ILE:HD12	1.65	0.77
1:C:350:ARG:NH2	1:C:412:GLN:HG2	1.98	0.77
1:C:287:ARG:HA	1:C:303:VAL:HG12	1.67	0.77
1:D:241:CYS:SG	1:D:251:TYR:CZ	2.76	0.77
1:A:52:PHE:CE1	1:A:82:PRO:HD2	2.20	0.76
1:C:25:ILE:HD13	1:C:316:VAL:HG21	1.66	0.76
1:A:345:MET:HG3	1:A:362:THR:HG21	1.67	0.75
1:C:169:GLY:HA3	1:C:229:LEU:CD2	2.16	0.75
1:A:310:GLU:O	1:A:314:LEU:HD13	1.86	0.75
1:D:328:VAL:HG22	1:D:329:VAL:HG23	1.69	0.75
1:A:352:ARG:HB2	1:B:150:ARG:HH12	1.49	0.75
1:C:168:ILE:HD11	1:C:258:VAL:HG22	1.70	0.74
1:C:334:VAL:HG21	1:C:373:PHE:CE1	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:LEU:HD23	1:C:271:TRP:CE2	2.22	0.74
1:C:423:LEU:HD12	1:C:424:GLY:O	1.87	0.74
1:A:9:ARG:H	1:A:9:ARG:NE	1.85	0.74
1:C:115:GLU:O	1:C:117:PRO:HD3	1.88	0.73
1:A:105:LEU:HD23	1:A:105:LEU:N	2.03	0.73
1:C:397:ALA:HB2	1:C:412:GLN:NE2	2.04	0.73
2:C:451:HSO:H1	3:C:452:ATP:O1A	1.89	0.73
1:C:383:VAL:HG11	1:C:422:LEU:HD13	1.70	0.73
1:B:311:ARG:NH1	3:B:452:ATP:C2'	2.52	0.73
1:B:234:ARG:HH21	1:B:237:PHE:HD2	1.36	0.73
1:C:167:SER:HA	1:C:266:ARG:O	1.88	0.73
1:B:38:TYR:CE1	1:B:104:ARG:HD3	2.25	0.72
1:C:178:ARG:HA	1:C:181:LEU:HB3	1.71	0.72
1:C:136:GLN:HG3	1:C:301:PRO:HG2	1.72	0.72
1:D:141:ASP:HB2	1:D:240:LEU:HD13	1.71	0.72
1:B:24:ARG:HD3	1:B:325:ALA:HB1	1.70	0.72
1:C:254:ASN:OD1	1:C:256:ARG:HG3	1.89	0.72
1:D:265:ASN:ND2	1:D:289:ASP:H	1.88	0.72
1:C:67:MET:CE	1:C:79:THR:HG21	2.13	0.72
1:A:414:SER:O	1:A:418:HIS:HD2	1.73	0.71
1:B:255:GLN:HA	1:B:255:GLN:OE1	1.89	0.71
1:C:169:GLY:HA3	1:C:229:LEU:HD21	1.72	0.71
1:A:160:HIS:O	1:A:161:VAL:HG13	1.90	0.71
1:B:293:GLU:HA	1:B:297:GLY:O	1.91	0.71
1:D:73:ARG:HH11	1:D:73:ARG:HG3	1.56	0.71
1:B:114:HIS:CE1	1:B:123:ARG:HH21	2.08	0.71
1:C:371:LYS:HD2	1:C:375:ARG:HE	1.56	0.71
1:D:244:LEU:HD12	1:D:251:TYR:HD2	1.55	0.71
1:A:256:ARG:HD2	1:A:256:ARG:O	1.91	0.70
1:C:364:HIS:HD2	1:D:104:ARG:NH2	1.89	0.70
1:C:12:ASN:H	1:C:12:ASN:ND2	1.86	0.70
1:C:388:GLY:O	1:C:392:VAL:HG23	1.90	0.70
1:D:333:LEU:HD13	1:D:348:ALA:HB2	1.74	0.70
1:B:28:THR:O	1:B:32:VAL:HG23	1.92	0.70
1:D:28:THR:O	1:D:32:VAL:HG23	1.92	0.70
1:A:9:ARG:H	1:A:9:ARG:HE	1.40	0.70
1:C:324:LYS:H	1:C:324:LYS:HD2	1.57	0.69
1:C:352:ARG:HB2	1:D:150:ARG:HH12	1.56	0.69
1:D:264:TYR:HA	1:D:287:ARG:O	1.92	0.69
1:D:104:ARG:C	1:D:105:LEU:HG	2.11	0.69
1:A:42:ARG:HB2	1:B:14:TYR:HB2	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:VAL:HG21	1:C:291:LEU:HD22	1.73	0.69
1:A:92:GLY:HA3	1:A:98:LEU:HD11	1.74	0.69
1:D:257:LEU:HD23	1:D:268:VAL:HG12	1.73	0.69
1:A:244:LEU:HD12	1:A:249:ILE:HB	1.74	0.68
1:B:332:TYR:CE1	1:B:363:ASN:HB2	2.28	0.68
1:B:331:ILE:HD11	1:B:423:LEU:HD11	1.74	0.68
1:A:178:ARG:HG3	1:A:179:ASP:N	2.08	0.68
1:A:239:GLY:O	1:A:243:LEU:HD13	1.93	0.68
1:C:5:ILE:HD12	1:D:51:LEU:HG	1.75	0.68
1:B:264:TYR:HA	1:B:287:ARG:O	1.92	0.68
1:B:121:ARG:HH12	3:B:452:ATP:PG	2.16	0.68
1:D:307:MET:SD	1:D:312:LEU:HD22	2.33	0.68
1:D:308:GLY:O	1:D:311:ARG:HG2	1.92	0.68
1:D:257:LEU:HD11	1:D:270:GLU:OE2	1.93	0.68
1:C:52:PHE:CE2	1:C:82:PRO:HD2	2.28	0.68
1:C:234:ARG:NH1	1:C:237:PHE:HD2	1.92	0.68
1:A:60:THR:O	1:A:64:GLU:HG3	1.94	0.68
1:D:111:MET:HB2	1:D:125:PHE:CE1	2.29	0.67
1:D:235:GLU:HG2	1:D:236:HIS:N	2.09	0.67
1:B:52:PHE:CE1	1:B:82:PRO:HD2	2.28	0.67
1:C:105:LEU:O	1:C:130:CYS:HB2	1.94	0.67
1:D:167:SER:HA	1:D:266:ARG:O	1.95	0.67
1:A:332:TYR:HD2	1:A:376:ALA:HB2	1.59	0.67
1:C:111:MET:HB2	1:C:125:PHE:CE1	2.29	0.67
1:C:272:VAL:HG12	1:C:281:THR:HG22	1.76	0.66
1:B:382:ARG:HH11	1:B:382:ARG:CG	2.09	0.66
1:C:311:ARG:HH21	3:C:452:ATP:C1'	2.09	0.66
1:C:44:PRO:HA	1:D:124:GLN:HE22	1.61	0.66
1:B:388:GLY:O	1:B:392:VAL:HG23	1.96	0.65
1:B:91:ALA:O	1:B:95:HIS:HD2	1.79	0.65
1:D:259:ARG:HB2	1:D:264:TYR:CD2	2.31	0.65
1:A:171:LEU:HD13	1:A:174:ARG:HH12	1.60	0.65
1:B:383:VAL:HG11	1:B:419:LEU:HD21	1.79	0.65
1:D:47:GLU:HB2	1:D:52:PHE:CE2	2.32	0.65
1:D:121:ARG:NH2	3:D:452:ATP:PG	2.70	0.65
1:A:373:PHE:O	1:A:376:ALA:HB3	1.97	0.65
1:C:22:TRP:O	1:C:26:GLU:HG3	1.97	0.65
1:A:97:LEU:N	1:A:97:LEU:HD23	2.12	0.65
1:D:168:ILE:HG22	1:D:265:ASN:O	1.96	0.65
1:A:60:THR:HG22	1:A:62:VAL:H	1.61	0.65
1:C:160:HIS:O	1:C:161:VAL:HG13	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:LEU:O	1:A:313:VAL:HG23	1.97	0.64
1:B:9:ARG:HE	1:B:116:ARG:HH22	1.45	0.64
1:B:38:TYR:N	1:B:38:TYR:HD1	1.96	0.64
1:B:237:PHE:O	1:B:241:CYS:SG	2.53	0.64
1:B:105:LEU:O	1:B:130:CYS:HB2	1.97	0.64
1:A:113:ARG:HG3	1:A:125:PHE:HE2	1.62	0.64
1:C:347:LEU:HG	1:C:351:LEU:CD1	2.28	0.64
1:C:271:TRP:HB2	1:C:283:CYS:HB3	1.80	0.64
1:C:36:TYR:HE1	1:C:150:ARG:HD2	1.62	0.64
1:D:263:TYR:HD2	1:D:291:LEU:HD13	1.63	0.64
1:D:311:ARG:HG3	1:D:311:ARG:HH11	1.63	0.64
1:C:92:GLY:HA3	1:C:98:LEU:HD11	1.80	0.64
1:C:309:LEU:O	1:C:313:VAL:HG23	1.97	0.64
1:B:74:ASN:HB3	1:B:76:ASP:OD1	1.97	0.63
1:B:383:VAL:HG11	1:B:419:LEU:CD2	2.28	0.63
1:C:116:ARG:HH11	1:C:116:ARG:HG3	1.62	0.63
1:A:165:LEU:HD12	1:A:166:ASN:H	1.63	0.63
1:C:40:GLU:HB2	1:C:106:TRP:CZ2	2.34	0.63
1:A:141:ASP:HB2	1:A:240:LEU:HD13	1.80	0.63
1:D:135:LEU:O	1:D:287:ARG:NH2	2.32	0.63
1:B:89:VAL:HG21	1:B:291:LEU:HD21	1.80	0.63
1:B:152:TRP:CD1	1:B:161:VAL:HG21	2.34	0.63
1:A:33:LEU:HD23	1:A:147:LEU:HD11	1.80	0.62
1:B:135:LEU:HD23	1:B:140:ILE:HD13	1.81	0.62
1:C:352:ARG:CB	1:D:150:ARG:HH12	2.11	0.62
1:D:127:GLN:NE2	3:D:452:ATP:H5'1	2.14	0.62
1:C:52:PHE:HB3	1:C:56:ILE:HD12	1.80	0.62
1:A:45:ILE:HG12	1:B:124:GLN:HE22	1.63	0.62
1:A:175:ALA:O	1:A:178:ARG:HG2	1.99	0.62
1:B:21:ILE:H	1:B:21:ILE:HD12	1.64	0.62
1:B:265:ASN:ND2	1:B:266:ARG:NE	2.46	0.62
1:D:15:LEU:H	1:D:15:LEU:CD2	2.11	0.62
1:B:10:GLY:HA3	1:B:123:ARG:HG2	1.80	0.62
1:D:105:LEU:O	1:D:130:CYS:HB2	1.99	0.62
1:D:49:THR:O	1:D:53:LYS:HG3	2.00	0.62
1:A:178:ARG:HG3	1:A:179:ASP:H	1.63	0.62
1:B:343:ALA:O	1:B:346:ALA:HB3	2.00	0.62
1:D:259:ARG:NH2	3:D:452:ATP:O1A	2.33	0.62
1:A:163:LEU:HD21	1:A:165:LEU:HD22	1.81	0.62
1:A:381:ALA:O	1:A:402:LEU:HD12	1.99	0.62
1:D:72:ASP:HB2	1:D:78:LEU:CD2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:ARG:NH2	3:C:452:ATP:O1A	2.32	0.61
1:D:157:ILE:HG22	1:D:319:VAL:CG1	2.30	0.61
1:D:259:ARG:HG2	1:D:268:VAL:HG13	1.82	0.61
1:B:38:TYR:N	1:B:38:TYR:CD1	2.68	0.61
1:D:412:GLN:HA	1:D:415:VAL:CG2	2.31	0.61
1:A:383:VAL:HG11	1:A:422:LEU:HD13	1.83	0.61
1:C:287:ARG:O	1:C:288:TYR:HB3	1.98	0.61
1:B:125:PHE:HE1	1:B:127:GLN:HG3	1.66	0.61
1:C:347:LEU:HG	1:C:351:LEU:HD12	1.83	0.61
1:B:68:TYR:HB2	1:B:80:LEU:HB2	1.82	0.60
1:C:29:LEU:HD11	1:C:312:LEU:CD2	2.31	0.60
1:B:141:ASP:O	1:B:145:ILE:HD12	2.01	0.60
1:B:251:TYR:H	1:B:251:TYR:HD1	1.47	0.60
1:B:418:HIS:O	1:B:422:LEU:HD23	2.01	0.60
1:D:45:ILE:O	1:D:81:ARG:HG2	2.01	0.60
1:B:168:ILE:HG13	1:B:265:ASN:O	2.02	0.60
1:A:259:ARG:HH11	1:A:259:ARG:CG	2.14	0.60
1:A:259:ARG:NH2	3:A:452:ATP:O1A	2.34	0.60
1:B:106:TRP:HA	1:B:130:CYS:HA	1.82	0.60
1:C:259:ARG:HH11	1:C:259:ARG:CG	2.11	0.60
1:C:334:VAL:HG11	1:C:373:PHE:CE1	2.32	0.60
1:A:251:TYR:HD1	1:A:251:TYR:H	1.50	0.60
1:C:340:THR:HG23	1:C:387:LEU:HD13	1.83	0.60
1:A:165:LEU:HD13	1:A:269:PHE:HB3	1.83	0.60
1:C:277:GLY:O	1:C:311:ARG:HG2	2.02	0.60
1:A:298:ARG:HG3	1:A:298:ARG:HH11	1.66	0.59
1:A:29:LEU:HD13	1:A:128:LEU:HD23	1.83	0.59
1:C:38:TYR:CE2	1:C:104:ARG:HB3	2.37	0.59
1:C:293:GLU:HA	1:C:297:GLY:O	2.03	0.59
1:D:279:GLN:H	1:D:311:ARG:NH2	1.99	0.59
1:B:333:LEU:HD13	1:B:385:VAL:O	2.03	0.59
1:C:226:GLY:O	1:C:229:LEU:HB2	2.02	0.59
1:D:141:ASP:HB2	1:D:240:LEU:CD1	2.32	0.59
1:B:12:ASN:H	1:B:12:ASN:ND2	1.99	0.59
1:C:368:ASN:OD1	1:C:370:LYS:HB2	2.03	0.59
1:B:15:LEU:O	1:B:19:THR:HG23	2.02	0.59
1:C:72:ASP:HB2	1:C:78:LEU:CD2	2.32	0.59
1:C:72:ASP:HB2	1:C:78:LEU:HD22	1.84	0.59
1:A:165:LEU:HD23	1:A:251:TYR:HD2	1.68	0.59
1:A:83:GLU:HG3	1:A:84:GLY:N	2.13	0.59
1:B:118:GLN:HA	1:B:118:GLN:NE2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:345:MET:HG3	1:C:362:THR:HG21	1.84	0.59
1:D:136:GLN:HE22	1:D:266:ARG:HH12	1.50	0.59
1:A:22:TRP:HH2	1:A:310:GLU:HG3	1.68	0.59
1:C:105:LEU:N	1:C:105:LEU:CD2	2.66	0.59
1:D:67:MET:CE	1:D:79:THR:HG21	2.33	0.59
1:D:157:ILE:HG22	1:D:319:VAL:HG11	1.84	0.59
1:B:58:GLU:CD	1:B:58:GLU:H	2.06	0.59
1:D:67:MET:HE2	1:D:79:THR:HG21	1.85	0.59
1:A:293:GLU:HA	1:A:297:GLY:O	2.02	0.59
1:A:355:LEU:O	1:A:358:VAL:HG22	2.03	0.58
1:D:141:ASP:O	1:D:145:ILE:HG13	2.02	0.58
1:A:163:LEU:HD23	1:A:251:TYR:HB3	1.85	0.58
1:C:104:ARG:HG2	1:C:132:VAL:CG1	2.33	0.58
1:D:99:TYR:O	1:D:101:GLN:HG2	2.02	0.58
1:A:167:SER:HA	1:A:266:ARG:O	2.02	0.58
1:C:313:VAL:HG12	1:C:317:GLN:NE2	2.17	0.58
1:D:21:ILE:O	1:D:25:ILE:HG13	2.03	0.58
1:D:332:TYR:CZ	1:D:363:ASN:HB2	2.38	0.58
1:B:21:ILE:HD12	1:B:21:ILE:N	2.19	0.58
1:C:291:LEU:HD21	1:C:295:LEU:HD22	1.84	0.58
1:D:30:LYS:HZ3	1:D:30:LYS:HB2	1.68	0.58
1:B:234:ARG:NH2	1:B:237:PHE:HD2	2.01	0.58
1:A:254:ASN:OD1	1:A:256:ARG:HG3	2.03	0.58
1:B:331:ILE:HD12	1:B:331:ILE:N	2.19	0.58
1:A:147:LEU:HD23	1:A:147:LEU:O	2.04	0.58
1:A:173:ALA:O	1:A:177:TYR:HB2	2.04	0.58
1:D:38:TYR:N	1:D:38:TYR:CD1	2.72	0.58
1:B:112:PHE:HA	1:B:123:ARG:O	2.04	0.58
1:D:234:ARG:HH11	1:D:234:ARG:CG	2.14	0.58
1:A:307:MET:SD	1:A:312:LEU:HD22	2.43	0.58
1:C:259:ARG:HG3	1:C:259:ARG:NH1	2.15	0.57
1:D:106:TRP:HA	1:D:130:CYS:HA	1.85	0.57
1:C:311:ARG:NH2	3:C:452:ATP:C4	2.72	0.57
1:C:382:ARG:HH11	1:C:382:ARG:HB2	1.69	0.57
1:D:38:TYR:N	1:D:38:TYR:HD1	2.01	0.57
1:C:22:TRP:CE2	1:C:313:VAL:HG21	2.40	0.57
1:D:52:PHE:HB2	1:D:67:MET:HE1	1.86	0.57
1:B:43:LEU:HD11	1:B:88:CYS:HA	1.86	0.57
1:B:130:CYS:SG	1:B:305:PHE:CE1	2.96	0.57
1:C:174:ARG:HG3	1:C:174:ARG:HH11	1.69	0.57
1:D:265:ASN:HD21	1:D:289:ASP:H	1.50	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:ARG:HE	1:C:111:MET:HE2	1.69	0.57
1:C:105:LEU:HD23	1:C:105:LEU:N	2.20	0.57
1:C:254:ASN:HD21	1:C:256:ARG:NE	2.02	0.57
1:C:381:ALA:O	1:C:402:LEU:HD12	2.03	0.57
1:C:257:LEU:HD11	1:C:270:GLU:HG2	1.87	0.57
1:B:46:VAL:CG1	1:B:80:LEU:HD12	2.32	0.57
1:C:181:LEU:HG	1:C:182:VAL:N	2.19	0.57
1:A:331:ILE:O	1:A:360:LEU:HA	2.05	0.56
1:B:47:GLU:HB2	1:B:52:PHE:HE2	1.70	0.56
1:A:72:ASP:HB2	1:A:78:LEU:HD22	1.86	0.56
1:A:384:ALA:HB2	1:A:402:LEU:HD21	1.85	0.56
1:C:47:GLU:OE2	1:C:90:ARG:HD3	2.05	0.56
1:B:265:ASN:HD21	1:B:266:ARG:HE	1.52	0.56
1:C:182:VAL:HA	1:C:185:LEU:HB2	1.86	0.56
1:C:234:ARG:HH12	1:C:237:PHE:HD2	1.53	0.56
1:B:72:ASP:HB2	1:B:78:LEU:HD11	1.87	0.56
1:B:283:CYS:SG	1:B:305:PHE:HD2	2.29	0.56
1:B:311:ARG:CZ	3:B:452:ATP:C2'	2.77	0.56
1:A:264:TYR:HA	1:A:287:ARG:O	2.06	0.56
1:B:137:GLY:O	1:B:140:ILE:HG22	2.06	0.56
1:B:259:ARG:HG2	1:B:268:VAL:HG13	1.88	0.56
1:D:311:ARG:HD3	3:D:452:ATP:N3	2.20	0.56
1:A:178:ARG:HH11	1:A:178:ARG:CG	2.15	0.56
1:B:89:VAL:HG21	1:B:291:LEU:CD2	2.36	0.56
1:B:141:ASP:HB2	1:B:240:LEU:CD1	2.32	0.56
1:D:164:GLU:HB2	1:D:270:GLU:HG3	1.87	0.56
1:A:163:LEU:HD23	1:A:251:TYR:CB	2.35	0.56
1:A:254:ASN:HD21	1:A:256:ARG:NH2	2.04	0.56
1:C:147:LEU:HD23	1:C:147:LEU:O	2.06	0.56
1:B:261:LEU:HD12	1:B:263:TYR:CZ	2.42	0.55
1:B:287:ARG:O	1:B:288:TYR:HB3	2.06	0.55
1:C:147:LEU:HD23	1:C:147:LEU:C	2.26	0.55
1:D:72:ASP:HB2	1:D:78:LEU:HD22	1.88	0.55
1:A:394:ASN:O	1:A:396:THR:HG23	2.07	0.55
1:B:14:TYR:HE2	1:B:126:HIS:HE1	1.54	0.55
1:C:113:ARG:HD2	1:C:125:PHE:CE1	2.41	0.55
1:A:8:ILE:H	1:A:8:ILE:CD1	2.19	0.55
1:C:81:ARG:HD2	1:C:111:MET:SD	2.45	0.55
1:C:166:ASN:HB3	1:C:268:VAL:HG23	1.87	0.55
1:C:313:VAL:HG12	1:C:317:GLN:HE21	1.72	0.55
1:A:382:ARG:HG3	1:A:403:ARG:HE	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:355:LEU:O	1:C:358:VAL:HG22	2.06	0.55
1:D:121:ARG:NH2	3:D:452:ATP:O2G	2.40	0.55
1:B:283:CYS:SG	1:B:305:PHE:CD2	3.00	0.55
1:D:103:GLN:HG3	1:D:105:LEU:HD21	1.88	0.55
1:A:273:THR:OG1	1:A:275:SER:HB3	2.07	0.55
1:C:99:TYR:O	1:C:101:GLN:HG3	2.07	0.55
1:C:345:MET:SD	1:C:364:HIS:HE1	2.29	0.55
1:A:95:HIS:HB2	1:A:97:LEU:HD21	1.89	0.54
1:A:361:MET:SD	1:B:104:ARG:NH1	2.80	0.54
1:D:368:ASN:ND2	1:D:371:LYS:HE3	2.22	0.54
1:B:47:GLU:HB2	1:B:52:PHE:CE2	2.42	0.54
1:B:274:ASN:OD1	1:B:274:ASN:N	2.40	0.54
1:A:171:LEU:H	1:A:171:LEU:HD22	1.72	0.54
1:D:383:VAL:HG12	1:D:384:ALA:N	2.22	0.54
1:A:292:VAL:HG21	1:A:300:THR:HG22	1.89	0.54
1:D:49:THR:HG23	1:D:79:THR:OG1	2.08	0.54
1:D:147:LEU:HD23	1:D:147:LEU:O	2.07	0.54
1:A:178:ARG:HG3	1:A:178:ARG:NH1	2.09	0.54
1:C:33:LEU:HD23	1:C:147:LEU:HD11	1.89	0.54
1:C:225:LEU:O	1:C:229:LEU:HG	2.08	0.54
1:B:278:SER:C	1:B:280:GLY:H	2.10	0.54
1:D:166:ASN:HD22	1:D:168:ILE:HD13	1.73	0.53
1:B:69:THR:HA	1:B:78:LEU:O	2.07	0.53
1:D:133:PHE:HE1	1:D:288:TYR:OH	1.91	0.53
1:D:136:GLN:HE22	1:D:266:ARG:NH1	2.05	0.53
1:D:148:THR:O	1:D:151:TRP:HB2	2.08	0.53
1:A:105:LEU:N	1:A:105:LEU:CD2	2.72	0.53
1:A:382:ARG:CG	1:A:403:ARG:HE	2.21	0.53
1:C:46:VAL:HG23	1:D:8:ILE:CD1	2.32	0.53
1:B:320:ASN:C	1:B:322:GLU:H	2.11	0.53
1:D:141:ASP:CB	1:D:240:LEU:HD13	2.39	0.53
1:D:319:VAL:C	1:D:321:PRO:HD3	2.28	0.53
1:D:321:PRO:O	1:D:324:LYS:NZ	2.42	0.53
1:C:169:GLY:HA3	1:C:229:LEU:HD22	1.89	0.53
1:B:288:TYR:O	1:B:288:TYR:CD1	2.62	0.53
1:D:125:PHE:CD2	3:D:452:ATP:C6	2.96	0.53
1:C:234:ARG:NH1	1:C:237:PHE:CD2	2.76	0.53
1:C:335:ALA:HB1	1:C:340:THR:HG21	1.90	0.53
1:D:311:ARG:HG3	1:D:311:ARG:NH1	2.24	0.53
3:B:452:ATP:H8	3:B:452:ATP:O2B	1.92	0.53
1:A:89:VAL:O	1:A:93:ILE:HG13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:LEU:HD23	1:A:105:LEU:H	1.74	0.52
1:A:174:ARG:HB2	1:A:174:ARG:HH11	1.73	0.52
1:D:168:ILE:HD11	1:D:258:VAL:HG12	1.89	0.52
1:A:45:ILE:HD13	1:A:81:ARG:NH2	2.24	0.52
1:C:328:VAL:HG21	1:C:379:TRP:HE3	1.74	0.52
1:A:382:ARG:NH2	1:A:423:LEU:HD22	2.24	0.52
1:B:278:SER:CA	1:B:311:ARG:HD3	2.40	0.52
1:B:312:LEU:HD23	1:B:313:VAL:N	2.24	0.52
1:C:22:TRP:NE1	1:C:313:VAL:HG11	2.24	0.52
1:B:74:ASN:ND2	1:B:74:ASN:O	2.42	0.52
1:C:106:TRP:HA	1:C:130:CYS:HA	1.92	0.52
1:C:370:LYS:HA	1:C:370:LYS:CE	2.27	0.52
1:A:45:ILE:H	1:B:124:GLN:HE22	1.58	0.52
1:A:375:ARG:O	1:A:379:TRP:CD1	2.62	0.52
1:B:259:ARG:CG	1:B:268:VAL:HG13	2.39	0.52
1:D:21:ILE:HD12	1:D:21:ILE:H	1.74	0.52
1:D:119:LYS:HG3	1:D:122:TYR:OH	2.10	0.52
1:A:174:ARG:HH21	1:A:265:ASN:HA	1.75	0.52
1:A:298:ARG:HG3	1:A:298:ARG:NH1	2.25	0.52
1:D:328:VAL:O	1:D:359:LYS:HD3	2.09	0.52
1:B:412:GLN:HA	1:B:415:VAL:HG23	1.92	0.52
1:C:412:GLN:HA	1:C:415:VAL:HG23	1.91	0.52
1:D:139:ASP:O	1:D:142:ALA:HB3	2.09	0.52
1:A:261:LEU:HD23	1:A:264:TYR:CE2	2.32	0.52
1:A:345:MET:CE	1:B:146:MET:SD	2.98	0.52
1:B:354:GLU:OE1	1:B:416:ALA:HB2	2.09	0.52
1:C:283:CYS:SG	1:C:305:PHE:CD1	3.02	0.52
1:D:91:ALA:O	1:D:95:HIS:HD2	1.92	0.52
1:B:415:VAL:HG12	1:B:419:LEU:HD12	1.91	0.52
1:C:331:ILE:O	1:C:360:LEU:HA	2.10	0.52
1:D:73:ARG:HH11	1:D:73:ARG:CG	2.22	0.52
1:A:345:MET:HE3	1:B:146:MET:SD	2.50	0.51
1:A:410:VAL:HG12	1:A:411:ALA:N	2.24	0.51
1:D:130:CYS:SG	1:D:305:PHE:HE2	2.32	0.51
1:A:273:THR:C	1:A:275:SER:H	2.13	0.51
1:A:422:LEU:O	1:A:422:LEU:HD23	2.10	0.51
1:A:5:ILE:HD12	1:B:54:ARG:NH2	2.25	0.51
1:B:111:MET:HB2	1:B:125:PHE:CE1	2.44	0.51
1:B:332:TYR:CZ	1:B:363:ASN:HB2	2.45	0.51
1:D:133:PHE:HE1	1:D:288:TYR:HH	1.57	0.51
1:A:136:GLN:HG2	1:A:301:PRO:CG	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:ARG:CB	1:B:150:ARG:HH12	2.22	0.51
1:D:93:ILE:HG12	1:D:297:GLY:HA3	1.92	0.51
1:A:11:MET:HG2	1:A:124:GLN:HB2	1.93	0.51
1:A:332:TYR:CD2	1:A:376:ALA:HB2	2.43	0.51
1:B:89:VAL:HG12	1:B:292:VAL:HG12	1.93	0.51
1:B:410:VAL:HG12	1:B:411:ALA:N	2.24	0.51
1:B:133:PHE:HE1	1:B:288:TYR:OH	1.92	0.51
1:B:240:LEU:O	1:B:244:LEU:HD23	2.10	0.51
1:B:370:LYS:CD	1:B:370:LYS:H	2.24	0.51
1:B:371:LYS:O	1:B:375:ARG:HG3	2.11	0.51
1:B:132:VAL:HG21	1:B:140:ILE:HD11	1.93	0.51
1:B:311:ARG:HD2	3:B:452:ATP:O2'	2.10	0.51
1:A:28:THR:O	1:A:32:VAL:HG23	2.11	0.51
1:B:369:PHE:HB2	1:B:370:LYS:HZ1	1.76	0.51
1:D:311:ARG:NH1	3:D:452:ATP:O2'	2.43	0.51
1:A:241:CYS:O	1:A:245:GLU:HG3	2.11	0.51
1:D:136:GLN:NE2	1:D:266:ARG:HH12	2.08	0.51
1:A:232:GLU:HB2	1:A:266:ARG:NH2	2.26	0.50
1:B:244:LEU:HD12	1:B:249:ILE:HB	1.92	0.50
1:B:287:ARG:HA	1:B:303:VAL:HG13	1.92	0.50
1:D:259:ARG:CB	1:D:264:TYR:CE2	2.94	0.50
1:C:259:ARG:NH1	1:C:264:TYR:CZ	2.79	0.50
1:B:375:ARG:HA	1:B:378:LYS:HG3	1.92	0.50
1:C:165:LEU:O	1:C:253:VAL:HA	2.12	0.50
1:D:93:ILE:HD11	1:D:292:VAL:O	2.11	0.50
1:D:288:TYR:CE1	1:D:302:ALA:HB1	2.46	0.50
1:A:178:ARG:CG	1:A:178:ARG:NH1	2.72	0.50
1:D:130:CYS:SG	1:D:305:PHE:CZ	3.01	0.50
1:D:263:TYR:HB3	1:D:291:LEU:HD12	1.93	0.50
1:A:135:LEU:HD12	1:A:140:ILE:HG12	1.94	0.50
1:A:136:GLN:CG	1:A:301:PRO:HG2	2.24	0.50
1:A:386:VAL:HB	1:A:398:VAL:HB	1.94	0.50
1:D:388:GLY:O	1:D:392:VAL:HG23	2.12	0.50
1:A:127:GLN:HE21	3:A:452:ATP:H5'1	1.76	0.50
1:A:287:ARG:HG2	1:A:288:TYR:H	1.76	0.50
1:A:383:VAL:HG22	1:A:422:LEU:HD22	1.94	0.50
1:C:152:TRP:HB3	1:C:158:SER:HA	1.92	0.50
1:C:332:TYR:CZ	1:C:363:ASN:HB2	2.46	0.50
1:A:74:ASN:HA	1:D:73:ARG:O	2.12	0.50
1:A:384:ALA:CB	1:A:402:LEU:HD21	2.42	0.50
1:B:169:GLY:H	1:B:229:LEU:HD11	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:MET:HG3	1:D:249:ILE:HD11	1.93	0.50
1:A:343:ALA:O	1:A:346:ALA:HB3	2.12	0.50
1:A:347:LEU:HD13	1:A:412:GLN:HG2	1.93	0.50
1:B:381:ALA:O	1:B:402:LEU:HD12	2.10	0.50
1:C:89:VAL:HG21	1:C:291:LEU:CD2	2.38	0.50
1:D:383:VAL:HG11	1:D:419:LEU:HD21	1.94	0.50
1:A:40:GLU:HB2	1:A:106:TRP:CZ2	2.46	0.50
1:B:369:PHE:HB2	1:B:370:LYS:NZ	2.27	0.50
1:A:157:ILE:HD12	1:A:157:ILE:O	2.12	0.49
1:A:171:LEU:HA	1:A:174:ARG:HH12	1.77	0.49
1:A:332:TYR:CZ	1:A:363:ASN:HB2	2.47	0.49
1:B:125:PHE:CE1	1:B:127:GLN:HG3	2.47	0.49
1:B:151:TRP:CZ3	1:B:307:MET:HE2	2.47	0.49
1:B:390:SER:HB2	1:B:391:GLU:OE1	2.12	0.49
1:D:265:ASN:OD1	1:D:266:ARG:N	2.45	0.49
1:A:165:LEU:HD12	1:A:166:ASN:N	2.27	0.49
1:B:320:ASN:O	1:B:322:GLU:N	2.45	0.49
1:D:85:THR:O	1:D:89:VAL:HG23	2.12	0.49
1:B:278:SER:C	1:B:280:GLY:N	2.64	0.49
1:C:315:LEU:O	1:C:315:LEU:HD12	2.12	0.49
1:D:244:LEU:HD12	1:D:251:TYR:CD2	2.43	0.49
1:D:369:PHE:O	1:D:373:PHE:CD2	2.65	0.49
1:B:121:ARG:NH1	1:B:311:ARG:HH22	2.10	0.49
1:C:350:ARG:HH22	1:C:412:GLN:CG	2.08	0.49
1:C:371:LYS:HD2	1:C:375:ARG:NE	2.27	0.49
1:D:259:ARG:NH1	1:D:264:TYR:OH	2.45	0.49
1:A:367:GLY:O	1:A:372:GLN:NE2	2.45	0.49
1:B:85:THR:OG1	2:B:451:HSO:N	2.45	0.49
1:B:254:ASN:HB3	1:B:257:LEU:HB2	1.95	0.49
1:C:287:ARG:HA	1:C:303:VAL:CG1	2.41	0.49
1:C:259:ARG:CG	1:C:259:ARG:NH1	2.72	0.49
1:C:410:VAL:HG12	1:C:411:ALA:N	2.27	0.49
1:D:52:PHE:O	1:D:56:ILE:HB	2.11	0.49
1:A:146:MET:CE	1:B:345:MET:SD	3.00	0.49
1:A:241:CYS:SG	1:A:251:TYR:HE2	2.36	0.49
1:C:343:ALA:O	1:C:346:ALA:HB3	2.12	0.49
1:B:15:LEU:N	1:B:15:LEU:HD22	2.28	0.49
1:D:135:LEU:CD1	1:D:140:ILE:HG12	2.42	0.49
1:D:288:TYR:CE1	1:D:302:ALA:CB	2.96	0.49
1:A:8:ILE:H	1:A:8:ILE:HD13	1.78	0.49
1:A:287:ARG:NH1	1:A:303:VAL:CG2	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:ASN:HB3	1:D:76:ASP:OD1	2.13	0.49
1:D:152:TRP:HB3	1:D:158:SER:HA	1.95	0.49
1:A:279:GLN:HB2	1:A:311:ARG:NH1	2.29	0.48
1:B:261:LEU:HD12	1:B:263:TYR:CE2	2.48	0.48
1:D:265:ASN:OD1	1:D:266:ARG:HD3	2.13	0.48
1:A:8:ILE:CD1	1:A:8:ILE:N	2.75	0.48
1:A:43:LEU:HB3	1:A:44:PRO:HD2	1.95	0.48
1:B:69:THR:HG23	1:B:78:LEU:O	2.14	0.48
1:D:138:PRO:HB2	1:D:240:LEU:HB2	1.95	0.48
1:A:232:GLU:HB2	1:A:266:ARG:HH21	1.78	0.48
1:C:104:ARG:HH22	1:D:364:HIS:HD2	1.60	0.48
1:C:182:VAL:O	1:C:185:LEU:N	2.46	0.48
1:C:335:ALA:HB1	1:C:340:THR:CG2	2.43	0.48
1:D:136:GLN:NE2	1:D:266:ARG:NH1	2.62	0.48
1:A:5:ILE:HG22	1:A:6:GLN:N	2.29	0.48
1:B:9:ARG:HG2	1:B:9:ARG:HH11	1.77	0.48
3:B:452:ATP:O2B	3:B:452:ATP:C8	2.67	0.48
1:C:36:TYR:HB3	1:C:38:TYR:CE1	2.47	0.48
1:D:291:LEU:HD21	1:D:295:LEU:CD1	2.43	0.48
1:B:99:TYR:O	1:B:100:ASN:ND2	2.47	0.48
1:D:115:GLU:O	1:D:117:PRO:HD3	2.12	0.48
1:D:126:HIS:ND1	1:D:126:HIS:N	2.61	0.48
1:B:67:MET:HE2	1:B:79:THR:HG21	1.91	0.48
1:C:110:PRO:O	1:C:111:MET:HE2	2.13	0.48
1:C:239:GLY:O	1:C:243:LEU:HG	2.13	0.48
1:D:383:VAL:HG22	1:D:422:LEU:HD13	1.95	0.48
1:A:41:ILE:HG22	1:A:106:TRP:O	2.13	0.48
1:A:89:VAL:HG13	1:A:292:VAL:HG12	1.96	0.48
1:C:152:TRP:CD1	1:C:161:VAL:HG21	2.49	0.48
1:D:106:TRP:HB3	1:D:130:CYS:HB3	1.95	0.48
1:B:369:PHE:N	1:B:370:LYS:HZ2	2.12	0.48
1:C:47:GLU:HB2	1:C:52:PHE:CE1	2.49	0.48
1:B:368:ASN:OD1	1:B:370:LYS:HD2	2.14	0.48
1:C:316:VAL:O	1:C:320:ASN:HB2	2.13	0.48
1:D:93:ILE:HG23	1:D:99:TYR:OH	2.14	0.48
1:D:259:ARG:HG3	1:D:259:ARG:HH11	1.79	0.48
1:D:386:VAL:HG12	1:D:387:LEU:N	2.29	0.48
1:D:410:VAL:HG12	1:D:411:ALA:N	2.29	0.48
1:A:72:ASP:HB2	1:A:78:LEU:CD2	2.44	0.47
1:A:171:LEU:HA	1:A:174:ARG:NH1	2.29	0.47
1:B:283:CYS:SG	1:B:307:MET:HG3	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:THR:HA	1:D:78:LEU:O	2.14	0.47
1:D:251:TYR:C	1:D:251:TYR:HD1	2.18	0.47
1:C:111:MET:HB2	1:C:125:PHE:CZ	2.49	0.47
1:D:136:GLN:O	1:D:287:ARG:NH2	2.47	0.47
1:D:379:TRP:HA	1:D:379:TRP:CE3	2.47	0.47
1:A:45:ILE:HD13	1:A:81:ARG:CZ	2.44	0.47
1:A:72:ASP:C	1:A:74:ASN:H	2.17	0.47
1:B:21:ILE:H	1:B:21:ILE:CD1	2.26	0.47
1:D:263:TYR:CD2	1:D:291:LEU:HD13	2.46	0.47
1:A:116:ARG:O	1:A:118:GLN:HG3	2.15	0.47
1:C:364:HIS:HD2	1:D:104:ARG:HH22	1.58	0.47
1:D:51:LEU:HD21	1:D:295:LEU:HD13	1.96	0.47
1:A:111:MET:HB2	1:A:125:PHE:CZ	2.49	0.47
1:C:234:ARG:HA	1:C:234:ARG:HD3	1.74	0.47
1:D:73:ARG:CG	1:D:73:ARG:NH1	2.78	0.47
1:D:259:ARG:HG2	1:D:268:VAL:CG1	2.45	0.47
1:D:367:GLY:HA2	1:D:371:LYS:HD2	1.95	0.47
1:A:32:VAL:CG1	1:A:150:ARG:HD2	2.36	0.47
1:A:411:ALA:O	1:A:415:VAL:HG13	2.14	0.47
1:A:414:SER:O	1:A:418:HIS:CD2	2.60	0.47
1:B:148:THR:HB	1:B:152:TRP:CZ2	2.49	0.47
1:C:334:VAL:HG21	1:C:373:PHE:HE1	1.75	0.47
1:D:361:MET:HE2	1:D:379:TRP:HE1	1.80	0.47
1:D:383:VAL:CG2	1:D:422:LEU:HD13	2.44	0.47
1:A:333:LEU:HD23	1:A:334:VAL:O	2.15	0.47
1:B:231:GLU:O	1:B:235:GLU:HG3	2.15	0.47
1:B:367:GLY:HA2	1:B:371:LYS:HD2	1.96	0.47
1:C:44:PRO:O	1:C:81:ARG:NH1	2.48	0.47
1:C:179:ASP:O	1:C:183:ALA:HB2	2.15	0.47
1:D:51:LEU:HD22	1:D:86:ALA:HB1	1.97	0.47
1:B:89:VAL:HG11	1:B:291:LEU:CD2	2.45	0.47
1:C:311:ARG:NH2	3:C:452:ATP:N3	2.62	0.47
1:C:369:PHE:HA	1:C:372:GLN:HG3	1.97	0.47
1:B:241:CYS:HB2	1:B:242:LYS:HE2	1.97	0.47
1:D:251:TYR:C	1:D:251:TYR:CD1	2.88	0.47
1:B:112:PHE:N	1:B:112:PHE:CD1	2.82	0.46
1:D:72:ASP:HB2	1:D:78:LEU:HD21	1.97	0.46
1:A:171:LEU:O	1:A:175:ALA:N	2.47	0.46
1:C:46:VAL:HG22	1:D:11:MET:SD	2.55	0.46
1:C:60:THR:O	1:C:64:GLU:HG3	2.15	0.46
1:A:272:VAL:HG12	1:A:281:THR:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:TYR:HB3	1:C:38:TYR:CD1	2.50	0.46
1:C:139:ASP:HA	1:C:243:LEU:CD1	2.45	0.46
1:C:385:VAL:HG12	1:C:385:VAL:O	2.15	0.46
1:D:81:ARG:HA	1:D:82:PRO:HD2	1.75	0.46
1:A:146:MET:HE1	1:B:345:MET:SD	2.56	0.46
1:A:351:LEU:HD21	1:A:415:VAL:CG2	2.45	0.46
1:C:185:LEU:HD23	1:C:185:LEU:HA	1.75	0.46
1:D:135:LEU:HD13	1:D:140:ILE:HG12	1.97	0.46
1:A:46:VAL:HG23	1:B:8:ILE:HD12	1.98	0.46
1:A:47:GLU:OE2	1:A:90:ARG:HD3	2.15	0.46
1:B:113:ARG:O	1:B:123:ARG:HA	2.15	0.46
1:B:341:GLN:NE2	1:B:364:HIS:ND1	2.64	0.46
1:C:169:GLY:CA	1:C:229:LEU:HD21	2.43	0.46
1:D:33:LEU:HD13	1:D:106:TRP:CG	2.51	0.46
1:D:235:GLU:CG	1:D:236:HIS:N	2.79	0.46
1:B:121:ARG:NH1	3:B:452:ATP:O2G	2.48	0.46
1:C:345:MET:SD	1:C:364:HIS:CE1	3.09	0.46
1:D:291:LEU:HD21	1:D:295:LEU:HD11	1.98	0.46
1:B:121:ARG:NH1	3:B:452:ATP:O1G	2.45	0.46
1:B:157:ILE:HG22	1:B:319:VAL:CG1	2.46	0.46
1:D:122:TYR:H	3:D:452:ATP:HN62	1.64	0.46
1:A:22:TRP:CH2	1:A:310:GLU:HG3	2.49	0.46
1:B:89:VAL:HG11	1:B:291:LEU:HD23	1.97	0.46
1:B:138:PRO:HB3	1:B:240:LEU:HB2	1.96	0.46
1:B:160:HIS:ND1	1:B:319:VAL:HG21	2.31	0.46
1:B:287:ARG:NH2	1:B:303:VAL:HG21	2.31	0.46
1:C:85:THR:OG1	2:C:451:HSO:CD2	2.64	0.46
1:D:152:TRP:HB3	1:D:157:ILE:HD12	1.98	0.46
1:A:150:ARG:HG3	1:A:150:ARG:HH11	1.81	0.46
1:A:382:ARG:HH21	1:A:423:LEU:HD22	1.81	0.46
1:B:25:ILE:HG21	1:B:312:LEU:HD21	1.98	0.46
1:C:332:TYR:OH	1:C:363:ASN:HB2	2.16	0.46
1:C:397:ALA:HB2	1:C:412:GLN:HE21	1.80	0.46
1:A:99:TYR:O	1:A:101:GLN:HG3	2.15	0.45
1:A:135:LEU:CD1	1:A:140:ILE:HG12	2.46	0.45
1:A:391:GLU:HA	1:A:396:THR:OG1	2.16	0.45
1:B:54:ARG:O	1:B:294:GLN:NE2	2.49	0.45
1:B:67:MET:HB3	1:B:79:THR:HG21	1.98	0.45
1:A:287:ARG:NH1	1:A:303:VAL:HG21	2.31	0.45
1:A:46:VAL:HG12	1:A:80:LEU:HA	1.99	0.45
1:D:343:ALA:O	1:D:346:ALA:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:LEU:CD1	1:A:269:PHE:HB3	2.47	0.45
1:B:157:ILE:HD13	1:B:315:LEU:HD23	1.99	0.45
1:A:48:GLN:HB3	1:A:50:PRO:HD2	1.97	0.45
1:A:59:VAL:HG22	1:A:59:VAL:O	2.17	0.45
1:A:259:ARG:CG	1:A:259:ARG:NH1	2.77	0.45
1:B:288:TYR:CE1	1:B:302:ALA:CB	2.99	0.45
1:B:361:MET:HE1	1:B:379:TRP:CE2	2.51	0.45
1:A:261:LEU:N	1:A:261:LEU:HD22	2.31	0.45
1:A:412:GLN:HA	1:A:415:VAL:HG13	1.99	0.45
1:B:291:LEU:HD23	1:B:291:LEU:C	2.37	0.45
1:C:17:GLY:O	1:C:21:ILE:HD12	2.17	0.45
1:D:259:ARG:HB2	1:D:264:TYR:HD2	1.80	0.45
1:A:5:ILE:CG2	1:A:6:GLN:N	2.79	0.45
1:A:60:THR:HG22	1:A:62:VAL:HG23	1.99	0.45
1:B:89:VAL:O	1:B:93:ILE:HG13	2.17	0.45
1:D:127:GLN:HE22	3:D:452:ATP:H5'1	1.81	0.45
1:D:152:TRP:CE3	1:D:157:ILE:HD11	2.52	0.45
1:D:160:HIS:O	1:D:161:VAL:HG13	2.16	0.45
1:B:14:TYR:HE2	1:B:126:HIS:CE1	2.32	0.45
1:B:331:ILE:HD13	1:B:358:VAL:CG1	2.47	0.45
1:C:32:VAL:HG13	1:C:150:ARG:CD	2.47	0.45
1:C:45:ILE:HG12	1:D:124:GLN:OE1	2.17	0.45
1:C:334:VAL:HG12	1:C:369:PHE:HE1	1.81	0.45
1:C:368:ASN:ND2	1:C:371:LYS:HB2	2.32	0.45
1:A:151:TRP:O	1:A:155:LEU:HD22	2.17	0.45
1:B:419:LEU:HA	1:B:419:LEU:HD23	1.67	0.45
1:C:4:ASN:HD21	1:D:93:ILE:HG21	1.82	0.45
1:D:241:CYS:SG	1:D:251:TYR:OH	2.54	0.45
1:A:254:ASN:HD21	1:A:256:ARG:CZ	2.29	0.44
1:D:25:ILE:HD12	1:D:313:VAL:HG22	1.99	0.44
1:A:57:GLY:O	1:A:63:VAL:HG21	2.16	0.44
1:A:127:GLN:NE2	3:A:452:ATP:H5'1	2.32	0.44
1:A:309:LEU:HD23	1:A:309:LEU:HA	1.66	0.44
1:B:125:PHE:CD2	3:B:452:ATP:C6	3.05	0.44
1:B:341:GLN:NE2	1:B:364:HIS:HA	2.33	0.44
1:B:350:ARG:NH1	1:B:412:GLN:HB3	2.31	0.44
1:A:120:GLY:C	1:A:311:ARG:HH21	2.21	0.44
1:C:163:LEU:HD12	1:C:165:LEU:HD12	1.99	0.44
1:A:49:THR:HG23	1:A:79:THR:OG1	2.17	0.44
1:B:20:ALA:HB3	1:B:21:ILE:HD12	1.99	0.44
1:B:244:LEU:HD13	1:B:244:LEU:HA	1.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:PHE:HZ	1:D:45:ILE:HG13	1.83	0.44
1:B:15:LEU:HD22	1:B:15:LEU:H	1.82	0.44
1:C:116:ARG:HG3	1:C:116:ARG:NH1	2.28	0.44
1:D:98:LEU:CD2	1:D:133:PHE:HD2	2.30	0.44
1:D:290:GLY:O	1:D:293:GLU:HG2	2.17	0.44
1:D:312:LEU:O	1:D:313:VAL:C	2.55	0.44
1:A:274:ASN:N	1:A:274:ASN:HD22	2.15	0.44
1:C:174:ARG:HA	1:C:177:TYR:HB3	1.99	0.44
1:D:151:TRP:CZ3	1:D:307:MET:HE2	2.52	0.44
1:D:163:LEU:HD23	1:D:251:TYR:HB3	1.98	0.44
1:A:97:LEU:N	1:A:97:LEU:CD2	2.81	0.44
1:B:291:LEU:O	1:B:295:LEU:HG	2.18	0.44
1:D:148:THR:HG22	1:D:152:TRP:CZ2	2.53	0.44
1:D:234:ARG:CG	1:D:234:ARG:NH1	2.77	0.44
1:D:369:PHE:HB3	1:D:373:PHE:HE2	1.83	0.44
1:B:73:ARG:HG3	4:B:512:HOH:O	2.18	0.44
1:C:40:GLU:HG2	1:D:19:THR:HB	2.00	0.44
1:C:45:ILE:O	1:C:81:ARG:HG2	2.18	0.44
1:C:386:VAL:HB	1:C:398:VAL:HB	1.99	0.44
1:D:253:VAL:O	1:D:253:VAL:HG13	2.18	0.44
1:D:332:TYR:OH	1:D:363:ASN:OD1	2.33	0.44
1:C:52:PHE:CD2	1:C:82:PRO:HD2	2.52	0.44
1:C:326:ASP:HB2	1:C:359:LYS:NZ	2.33	0.44
1:A:16:PRO:HG3	1:B:105:LEU:CD2	2.48	0.43
1:B:148:THR:O	1:B:151:TRP:HB2	2.18	0.43
1:C:5:ILE:HD12	1:D:51:LEU:CG	2.45	0.43
1:C:12:ASN:H	1:C:12:ASN:HD22	1.62	0.43
1:C:38:TYR:CD2	1:C:104:ARG:HB3	2.53	0.43
1:C:166:ASN:O	1:C:268:VAL:HG22	2.18	0.43
1:C:274:ASN:OD1	1:C:275:SER:N	2.50	0.43
1:A:233:SER:OG	1:A:266:ARG:HG2	2.19	0.43
1:D:288:TYR:O	1:D:288:TYR:CD1	2.70	0.43
1:A:257:LEU:HD13	1:A:268:VAL:HG12	2.00	0.43
1:A:291:LEU:HD12	1:A:291:LEU:O	2.17	0.43
1:B:333:LEU:HB3	1:B:362:THR:HA	2.01	0.43
1:B:336:SER:O	1:B:340:THR:HG21	2.18	0.43
1:B:85:THR:O	1:B:89:VAL:CG2	2.66	0.43
1:C:43:LEU:HA	1:C:44:PRO:HD3	1.86	0.43
1:A:27:GLY:O	1:A:28:THR:C	2.57	0.43
1:D:47:GLU:HB2	1:D:52:PHE:CZ	2.53	0.43
1:D:145:ILE:HG13	1:D:145:ILE:H	1.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:320:ASN:N	1:D:321:PRO:HD3	2.33	0.43
1:D:383:VAL:HG11	1:D:419:LEU:HD23	1.98	0.43
1:A:45:ILE:HG12	1:B:124:GLN:NE2	2.31	0.43
1:A:90:ARG:NH2	1:B:13:ASP:OD2	2.49	0.43
1:B:288:TYR:O	1:B:288:TYR:HD1	2.01	0.43
1:B:391:GLU:OE1	1:B:391:GLU:N	2.51	0.43
1:C:251:TYR:HD1	1:C:251:TYR:H	1.66	0.43
1:C:331:ILE:N	1:C:331:ILE:HD12	2.33	0.43
1:D:49:THR:N	1:D:50:PRO:HD2	2.32	0.43
1:A:15:LEU:O	1:A:16:PRO:C	2.57	0.43
1:A:147:LEU:HD23	1:A:147:LEU:C	2.38	0.43
1:C:141:ASP:OD1	1:C:287:ARG:NH2	2.51	0.43
1:C:312:LEU:HA	1:C:312:LEU:HD12	1.77	0.43
1:A:167:SER:HB2	1:A:237:PHE:CD1	2.54	0.43
1:A:169:GLY:HA3	1:A:229:LEU:CD2	2.48	0.43
1:B:98:LEU:HD22	1:B:133:PHE:CD2	2.52	0.43
1:B:161:VAL:HG23	1:B:271:TRP:CE3	2.54	0.43
1:C:40:GLU:O	1:D:19:THR:HG21	2.19	0.43
1:D:329:VAL:HB	1:D:379:TRP:HB3	2.01	0.43
1:D:340:THR:O	1:D:343:ALA:N	2.51	0.43
1:D:383:VAL:CG1	1:D:384:ALA:N	2.81	0.43
1:A:386:VAL:HG12	1:A:387:LEU:N	2.34	0.43
1:B:41:ILE:O	1:B:41:ILE:HG23	2.19	0.43
1:B:108:ILE:HB	1:B:128:LEU:HD12	1.99	0.43
1:B:314:LEU:HA	1:B:317:GLN:OE1	2.19	0.43
1:C:163:LEU:HD23	1:C:271:TRP:NE1	2.33	0.43
1:C:164:GLU:HA	1:C:252:THR:O	2.19	0.43
1:D:128:LEU:HB3	1:D:309:LEU:HD11	2.00	0.43
1:D:133:PHE:CE1	1:D:288:TYR:OH	2.71	0.43
1:A:49:THR:N	1:A:50:PRO:CD	2.81	0.43
1:A:152:TRP:HB3	1:A:158:SER:HA	2.01	0.43
1:B:81:ARG:HA	1:B:82:PRO:HD2	1.98	0.43
1:C:19:THR:O	1:C:22:TRP:N	2.52	0.43
1:D:166:ASN:ND2	1:D:168:ILE:HD13	2.34	0.43
1:D:287:ARG:O	1:D:288:TYR:HB3	2.19	0.43
1:D:292:VAL:HG21	1:D:300:THR:HG22	2.01	0.43
1:D:324:LYS:HD2	1:D:324:LYS:N	2.34	0.43
1:D:386:VAL:HB	1:D:398:VAL:HB	2.01	0.43
1:A:91:ALA:HA	1:A:94:GLU:HB3	2.01	0.42
1:B:30:LYS:O	1:B:33:LEU:HB2	2.19	0.42
1:D:314:LEU:HD23	1:D:314:LEU:HA	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:GLU:HB2	1:C:52:PHE:HE1	1.84	0.42
1:C:331:ILE:HD12	1:C:331:ILE:H	1.84	0.42
1:A:278:SER:CA	1:A:311:ARG:HD3	2.49	0.42
1:A:319:VAL:HG12	1:A:320:ASN:HD22	1.82	0.42
1:B:5:ILE:N	1:B:5:ILE:HD12	2.33	0.42
1:B:83:GLU:OE2	1:B:85:THR:HB	2.19	0.42
1:B:232:GLU:OE1	1:B:266:ARG:NH1	2.51	0.42
1:B:370:LYS:H	1:B:370:LYS:CE	2.31	0.42
1:C:181:LEU:O	1:C:184:PHE:HB3	2.19	0.42
1:C:334:VAL:CG1	1:C:373:PHE:HE1	2.26	0.42
1:D:40:GLU:HG3	1:D:106:TRP:CH2	2.55	0.42
1:D:168:ILE:O	1:D:168:ILE:HG23	2.20	0.42
1:C:347:LEU:HG	1:C:351:LEU:HD11	2.00	0.42
1:D:68:TYR:OH	1:D:123:ARG:NE	2.52	0.42
1:A:139:ASP:HA	1:A:243:LEU:HD23	2.01	0.42
1:B:72:ASP:HB2	1:B:78:LEU:CD1	2.48	0.42
1:B:242:LYS:O	1:B:243:LEU:C	2.56	0.42
1:B:288:TYR:CE1	1:B:302:ALA:HB1	2.55	0.42
1:C:63:VAL:HA	1:C:67:MET:SD	2.60	0.42
1:A:165:LEU:HD13	1:A:269:PHE:CB	2.49	0.42
1:A:166:ASN:O	1:A:268:VAL:N	2.50	0.42
1:D:46:VAL:CG1	1:D:80:LEU:HD12	2.35	0.42
1:B:157:ILE:HG22	1:B:319:VAL:HG11	2.01	0.42
1:B:259:ARG:HB2	1:B:264:TYR:CD2	2.55	0.42
1:C:347:LEU:HD12	1:C:347:LEU:HA	1.80	0.42
1:D:125:PHE:CE1	1:D:127:GLN:HG3	2.55	0.42
1:A:184:PHE:CD1	1:A:184:PHE:C	2.93	0.42
1:B:361:MET:CE	1:B:379:TRP:NE1	2.83	0.42
1:C:163:LEU:CD1	1:C:165:LEU:HD12	2.50	0.42
1:D:259:ARG:CG	1:D:268:VAL:HG13	2.48	0.42
1:A:10:GLY:O	1:A:123:ARG:N	2.51	0.42
1:A:287:ARG:NH1	1:A:303:VAL:HG22	2.35	0.42
1:C:45:ILE:CD1	1:C:81:ARG:NH2	2.83	0.42
1:C:256:ARG:HD2	1:C:256:ARG:C	2.39	0.42
1:D:235:GLU:HG2	1:D:236:HIS:H	1.81	0.42
1:A:34:GLY:O	1:A:36:TYR:N	2.52	0.41
1:A:80:LEU:HD23	1:A:112:PHE:CD2	2.55	0.41
1:A:112:PHE:CD1	1:A:112:PHE:N	2.88	0.41
1:B:8:ILE:O	1:B:9:ARG:C	2.58	0.41
1:B:361:MET:HE2	1:B:379:TRP:NE1	2.35	0.41
1:C:307:MET:SD	1:C:312:LEU:HD22	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:361:MET:HE2	1:D:379:TRP:NE1	2.35	0.41
1:A:410:VAL:HG12	1:A:411:ALA:O	2.20	0.41
1:B:161:VAL:HA	1:B:272:VAL:O	2.20	0.41
1:C:334:VAL:HG21	1:C:373:PHE:CD1	2.53	0.41
1:A:231:GLU:OE1	1:A:231:GLU:HA	2.21	0.41
1:A:383:VAL:HG11	1:A:422:LEU:CD1	2.49	0.41
1:A:44:PRO:HA	1:B:124:GLN:OE1	2.19	0.41
1:A:68:TYR:HB2	1:A:80:LEU:HB2	2.03	0.41
1:B:139:ASP:HA	1:B:243:LEU:HD13	2.02	0.41
1:B:33:LEU:HD11	1:B:128:LEU:HD21	2.00	0.41
1:D:391:GLU:HG2	1:D:398:VAL:HG23	2.02	0.41
1:D:394:ASN:O	1:D:396:THR:HG23	2.20	0.41
1:A:105:LEU:O	1:A:130:CYS:HB2	2.20	0.41
1:A:230:ASP:OD2	1:A:233:SER:HB2	2.21	0.41
1:B:9:ARG:HE	1:B:116:ARG:NH2	2.15	0.41
1:D:257:LEU:HD21	1:D:270:GLU:HG2	2.03	0.41
1:A:90:ARG:NH2	1:B:7:ALA:HB2	2.36	0.41
1:B:102:GLU:OE2	1:B:135:LEU:HD21	2.20	0.41
1:B:312:LEU:HD23	1:B:312:LEU:C	2.41	0.41
1:D:89:VAL:HG21	1:D:291:LEU:HD22	2.03	0.41
1:D:265:ASN:HD22	1:D:288:TYR:HA	1.85	0.41
1:D:283:CYS:SG	1:D:307:MET:HB2	2.60	0.41
1:A:8:ILE:O	1:A:9:ARG:C	2.58	0.41
1:A:383:VAL:CG2	1:A:422:LEU:HD22	2.51	0.41
1:B:244:LEU:HD12	1:B:249:ILE:CG2	2.51	0.41
1:B:265:ASN:HD22	1:B:266:ARG:NE	2.15	0.41
1:C:106:TRP:HB3	1:C:130:CYS:HB3	2.03	0.41
1:D:103:GLN:OE1	1:D:103:GLN:HA	2.21	0.41
1:B:287:ARG:HG3	1:B:302:ALA:O	2.21	0.41
1:C:105:LEU:HD23	1:C:105:LEU:H	1.84	0.41
1:D:322:GLU:HA	1:D:324:LYS:NZ	2.36	0.41
1:D:415:VAL:HG12	1:D:419:LEU:CD1	2.51	0.41
1:A:410:VAL:CG1	1:A:411:ALA:N	2.84	0.41
1:B:130:CYS:SG	1:B:305:PHE:HE1	2.44	0.41
1:C:44:PRO:HA	1:D:124:GLN:NE2	2.32	0.41
1:C:102:GLU:OE1	1:C:135:LEU:HD21	2.21	0.41
1:C:171:LEU:N	1:C:171:LEU:HD13	2.36	0.41
1:A:4:ASN:N	1:B:54:ARG:HH22	2.18	0.40
1:B:91:ALA:O	1:B:95:HIS:CD2	2.68	0.40
1:B:235:GLU:HG3	1:B:235:GLU:H	1.75	0.40
1:B:341:GLN:HE22	1:B:364:HIS:HA	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:ILE:HG23	1:C:261:LEU:HD13	2.03	0.40
1:D:128:LEU:CB	1:D:309:LEU:HD11	2.51	0.40
1:D:263:TYR:HB3	1:D:291:LEU:CD1	2.51	0.40
1:D:259:ARG:NH1	1:D:264:TYR:CZ	2.89	0.40
1:B:397:ALA:HB3	1:B:415:VAL:HG21	2.03	0.40
1:C:5:ILE:HG21	1:D:48:GLN:HB2	2.04	0.40
1:C:73:ARG:HA	1:C:73:ARG:HD3	1.65	0.40
1:C:174:ARG:O	1:C:177:TYR:N	2.54	0.40
1:C:254:ASN:HD21	1:C:256:ARG:CZ	2.35	0.40
1:D:273:THR:CG2	1:D:277:GLY:H	2.35	0.40
1:D:311:ARG:HD3	3:D:452:ATP:C2	2.56	0.40
1:D:368:ASN:HD21	1:D:371:LYS:HE3	1.84	0.40
1:B:368:ASN:CG	1:B:370:LYS:HD2	2.41	0.40
1:D:355:LEU:HB3	1:D:358:VAL:HG21	2.03	0.40
1:A:41:ILE:O	1:A:41:ILE:HG23	2.21	0.40
1:A:121:ARG:H	1:A:121:ARG:HG2	1.59	0.40
1:B:47:GLU:OE2	1:B:90:ARG:HD3	2.21	0.40
1:B:163:LEU:HD23	1:B:251:TYR:HB3	2.03	0.40
1:B:374:ALA:O	1:B:377:ASP:HB2	2.21	0.40
1:C:56:ILE:HG12	1:C:261:LEU:HD12	2.04	0.40
1:D:133:PHE:CE1	1:D:302:ALA:HB1	2.57	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	375/424 (88%)	326 (87%)	38 (10%)	11 (3%)	4 15
1	B	360/424 (85%)	317 (88%)	35 (10%)	8 (2%)	6 22
1	C	383/424 (90%)	331 (86%)	41 (11%)	11 (3%)	4 15
1	D	360/424 (85%)	317 (88%)	38 (11%)	5 (1%)	11 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1478/1696 (87%)	1291 (87%)	152 (10%)	35 (2%)	6 20

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	288	TYR
1	A	338	ALA
1	B	64	GLU
1	B	288	TYR
1	B	338	ALA
1	C	137	GLY
1	C	276	LEU
1	C	278	SER
1	C	288	TYR
1	C	338	ALA
1	D	288	TYR
1	A	8	ILE
1	A	73	ARG
1	A	137	GLY
1	A	321	PRO
1	B	117	PRO
1	B	137	GLY
1	C	136	GLN
1	C	341	GLN
1	C	366	GLY
1	D	137	GLY
1	D	338	ALA
1	A	341	GLN
1	A	366	GLY
1	B	276	LEU
1	D	64	GLU
1	D	341	GLN
1	A	16	PRO
1	B	321	PRO
1	C	16	PRO
1	C	340	THR
1	B	341	GLN
1	A	82	PRO
1	A	365	GLY
1	C	365	GLY

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	299/342 (87%)	251 (84%)	48 (16%)	2 7
1	B	286/342 (84%)	235 (82%)	51 (18%)	2 5
1	C	301/342 (88%)	247 (82%)	54 (18%)	2 5
1	D	285/342 (83%)	229 (80%)	56 (20%)	1 4
All	All	1171/1368 (86%)	962 (82%)	209 (18%)	2 5

All (209) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ILE
1	A	9	ARG
1	A	15	LEU
1	A	16	PRO
1	A	18	GLU
1	A	19	THR
1	A	35	SER
1	A	39	SER
1	A	48	GLN
1	A	65	LYS
1	A	67	MET
1	A	78	LEU
1	A	97	LEU
1	A	105	LEU
1	A	116	ARG
1	A	121	ARG
1	A	128	LEU
1	A	139	ASP
1	A	140	ILE
1	A	161	VAL
1	A	174	ARG
1	A	235	GLU
1	A	246	SER
1	A	251	TYR

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Mol	Chain	Res	Type
1	A	255	GLN
1	A	256	ARG
1	A	257	LEU
1	A	259	ARG
1	A	261	LEU
1	A	263	TYR
1	A	276	LEU
1	A	281	THR
1	A	295	LEU
1	A	307	MET
1	A	311	ARG
1	A	322	GLU
1	A	324	LYS
1	A	327	PRO
1	A	328	VAL
1	A	339	ASP
1	A	342	SER
1	A	354	GLU
1	A	362	THR
1	A	382	ARG
1	A	383	VAL
1	A	403	ARG
1	A	414	SER
1	A	421	THR
1	B	12	ASN
1	B	16	PRO
1	B	24	ARG
1	B	30	LYS
1	B	46	VAL
1	B	54	ARG
1	B	58	GLU
1	B	59	VAL
1	B	67	MET
1	B	71	GLU
1	B	77	SER
1	B	79	THR
1	B	89	VAL
1	B	90	ARG
1	B	105	LEU
1	B	108	ILE
1	B	116	ARG
1	B	118	GLN

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Mol	Chain	Res	Type
1	B	121	ARG
1	B	128	LEU
1	B	131	GLU
1	B	132	VAL
1	B	139	ASP
1	B	141	ASP
1	B	232	GLU
1	B	235	GLU
1	B	251	TYR
1	B	252	THR
1	B	256	ARG
1	B	257	LEU
1	B	259	ARG
1	B	261	LEU
1	B	263	TYR
1	B	266	ARG
1	B	274	ASN
1	B	293	GLU
1	B	298	ARG
1	B	303	VAL
1	B	307	MET
1	B	322	GLU
1	B	323	PHE
1	B	333	LEU
1	B	339	ASP
1	B	340	THR
1	B	342	SER
1	B	370	LYS
1	B	382	ARG
1	B	404	SER
1	B	407	GLN
1	B	408	THR
1	B	414	SER
1	C	12	ASN
1	C	16	PRO
1	C	24	ARG
1	C	35	SER
1	C	39	SER
1	C	40	GLU
1	C	48	GLN
1	C	73	ARG
1	C	74	ASN

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Mol	Chain	Res	Type
1	C	78	LEU
1	C	80	LEU
1	C	81	ARG
1	C	83	GLU
1	C	105	LEU
1	C	108	ILE
1	C	116	ARG
1	C	117	PRO
1	C	119	LYS
1	C	153	ARG
1	C	161	VAL
1	C	165	LEU
1	C	168	ILE
1	C	171	LEU
1	C	184	PHE
1	C	234	ARG
1	C	240	LEU
1	C	251	TYR
1	C	255	GLN
1	C	256	ARG
1	C	257	LEU
1	C	261	LEU
1	C	263	TYR
1	C	270	GLU
1	C	274	ASN
1	C	276	LEU
1	C	287	ARG
1	C	303	VAL
1	C	320	ASN
1	C	322	GLU
1	C	324	LYS
1	C	327	PRO
1	C	331	ILE
1	C	339	ASP
1	C	342	SER
1	C	360	LEU
1	C	372	GLN
1	C	382	ARG
1	C	383	VAL
1	C	387	LEU
1	C	389	GLU
1	C	406	GLU

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Mol	Chain	Res	Type
1	C	412	GLN
1	C	421	THR
1	C	423	LEU
1	D	4	ASN
1	D	12	ASN
1	D	13	ASP
1	D	15	LEU
1	D	16	PRO
1	D	24	ARG
1	D	31	ASN
1	D	46	VAL
1	D	51	LEU
1	D	59	VAL
1	D	61	ASP
1	D	64	GLU
1	D	67	MET
1	D	76	ASP
1	D	78	LEU
1	D	100	ASN
1	D	101	GLN
1	D	105	LEU
1	D	115	GLU
1	D	118	GLN
1	D	121	ARG
1	D	126	HIS
1	D	131	GLU
1	D	140	ILE
1	D	141	ASP
1	D	148	THR
1	D	153	ARG
1	D	158	SER
1	D	161	VAL
1	D	168	ILE
1	D	232	GLU
1	D	234	ARG
1	D	251	TYR
1	D	257	LEU
1	D	263	TYR
1	D	266	ARG
1	D	274	ASN
1	D	283	CYS
1	D	303	VAL

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Mol	Chain	Res	Type
1	D	307	MET
1	D	309	LEU
1	D	311	ARG
1	D	320	ASN
1	D	323	PHE
1	D	324	LYS
1	D	328	VAL
1	D	333	LEU
1	D	341	GLN
1	D	342	SER
1	D	350	ARG
1	D	371	LYS
1	D	382	ARG
1	D	390	SER
1	D	401	ASP
1	D	407	GLN
1	D	421	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	255	GLN
1	A	274	ASN
1	A	317	GLN
1	A	320	ASN
1	A	363	ASN
1	A	372	GLN
1	A	418	HIS
1	B	12	ASN
1	B	95	HIS
1	B	114	HIS
1	B	118	GLN
1	B	124	GLN
1	B	166	ASN
1	B	341	GLN
1	C	4	ASN
1	C	12	ASN
1	C	100	ASN
1	C	118	GLN
1	C	255	GLN
1	C	294	GLN

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Mol	Chain	Res	Type
1	C	317	GLN
1	C	320	ASN
1	C	363	ASN
1	C	364	HIS
1	C	412	GLN
1	C	418	HIS
1	D	12	ASN
1	D	48	GLN
1	D	136	GLN
1	D	166	ASN
1	D	320	ASN
1	D	364	HIS
1	D	407	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

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	C	452	-	26,33,33	0.80	1 (3%)	31,52,52	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HSO	B	451	-	6,10,10	1.70	1 (16%)	4,12,12	1.66	2 (50%)
3	ATP	A	452	-	26,33,33	0.78	1 (3%)	31,52,52	1.00	1 (3%)
2	HSO	A	451	-	6,10,10	1.86	1 (16%)	4,12,12	1.67	2 (50%)
2	HSO	C	451	-	6,10,10	1.77	1 (16%)	4,12,12	1.75	1 (25%)
3	ATP	B	452	-	26,33,33	0.76	1 (3%)	31,52,52	0.78	0
3	ATP	D	452	-	26,33,33	0.73	0	31,52,52	0.94	2 (6%)
2	HSO	D	451	-	6,10,10	1.73	1 (16%)	4,12,12	1.84	2 (50%)

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	C	452	-	-	2/18/38/38	0/3/3/3
2	HSO	B	451	-	-	4/6/6/6	0/1/1/1
3	ATP	A	452	-	-	7/18/38/38	0/3/3/3
2	HSO	A	451	-	-	4/6/6/6	0/1/1/1
2	HSO	C	451	-	-	0/6/6/6	0/1/1/1
3	ATP	B	452	-	-	5/18/38/38	0/3/3/3
3	ATP	D	452	-	-	6/18/38/38	0/3/3/3
2	HSO	D	451	-	-	2/6/6/6	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	451	HSO	O-C	-4.44	1.23	1.42
2	C	451	HSO	O-C	-4.19	1.24	1.42
2	D	451	HSO	O-C	-4.15	1.24	1.42
2	B	451	HSO	O-C	-3.96	1.25	1.42
3	C	452	ATP	C2-N3	2.22	1.35	1.32
3	A	452	ATP	C2-N3	2.19	1.35	1.32
3	B	452	ATP	C2-N3	2.15	1.35	1.32

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	452	ATP	C5-C6-N6	2.82	124.63	120.35
2	D	451	HSO	O-C-CA	2.48	121.33	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	451	HSO	O-C-CA	2.33	120.74	111.52
2	B	451	HSO	CD2-NE2-CE1	2.31	109.39	105.78
2	D	451	HSO	CD2-NE2-CE1	2.30	109.37	105.78
2	A	451	HSO	CD2-NE2-CE1	2.24	109.28	105.78
2	A	451	HSO	O-C-CA	2.24	120.36	111.52
3	D	452	ATP	C5-C6-N6	2.20	123.69	120.35
2	B	451	HSO	O-C-CA	2.17	120.11	111.52
3	D	452	ATP	O3G-PG-O2G	2.01	115.31	107.64

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	451	HSO	O-C-CA-N
2	A	451	HSO	O-C-CA-CB
2	A	451	HSO	CA-CB-CG-ND1
2	B	451	HSO	N-CA-CB-CG
2	B	451	HSO	C-CA-CB-CG
2	B	451	HSO	O-C-CA-CB
2	D	451	HSO	O-C-CA-CB
3	A	452	ATP	C5'-O5'-PA-O1A
3	B	452	ATP	PB-O3A-PA-O5'
3	B	452	ATP	C5'-O5'-PA-O1A
3	B	452	ATP	C5'-O5'-PA-O2A
3	D	452	ATP	C5'-O5'-PA-O1A
3	C	452	ATP	PB-O3A-PA-O1A
3	D	452	ATP	PB-O3A-PA-O1A
3	D	452	ATP	C5'-O5'-PA-O3A
2	B	451	HSO	O-C-CA-N
2	D	451	HSO	O-C-CA-N
3	A	452	ATP	C5'-O5'-PA-O2A
3	D	452	ATP	C5'-O5'-PA-O2A
3	A	452	ATP	C4'-C5'-O5'-PA
3	D	452	ATP	PG-O3B-PB-O1B
3	D	452	ATP	PB-O3A-PA-O2A
3	A	452	ATP	PG-O3B-PB-O2B
3	A	452	ATP	C5'-O5'-PA-O3A
3	B	452	ATP	C5'-O5'-PA-O3A
3	A	452	ATP	PG-O3B-PB-O1B
3	A	452	ATP	PA-O3A-PB-O2B
3	B	452	ATP	PA-O3A-PB-O2B
3	C	452	ATP	PB-O3A-PA-O2A

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Mol	Chain	Res	Type	Atoms
2	A	451	HSO	CA-CB-CG-CD2

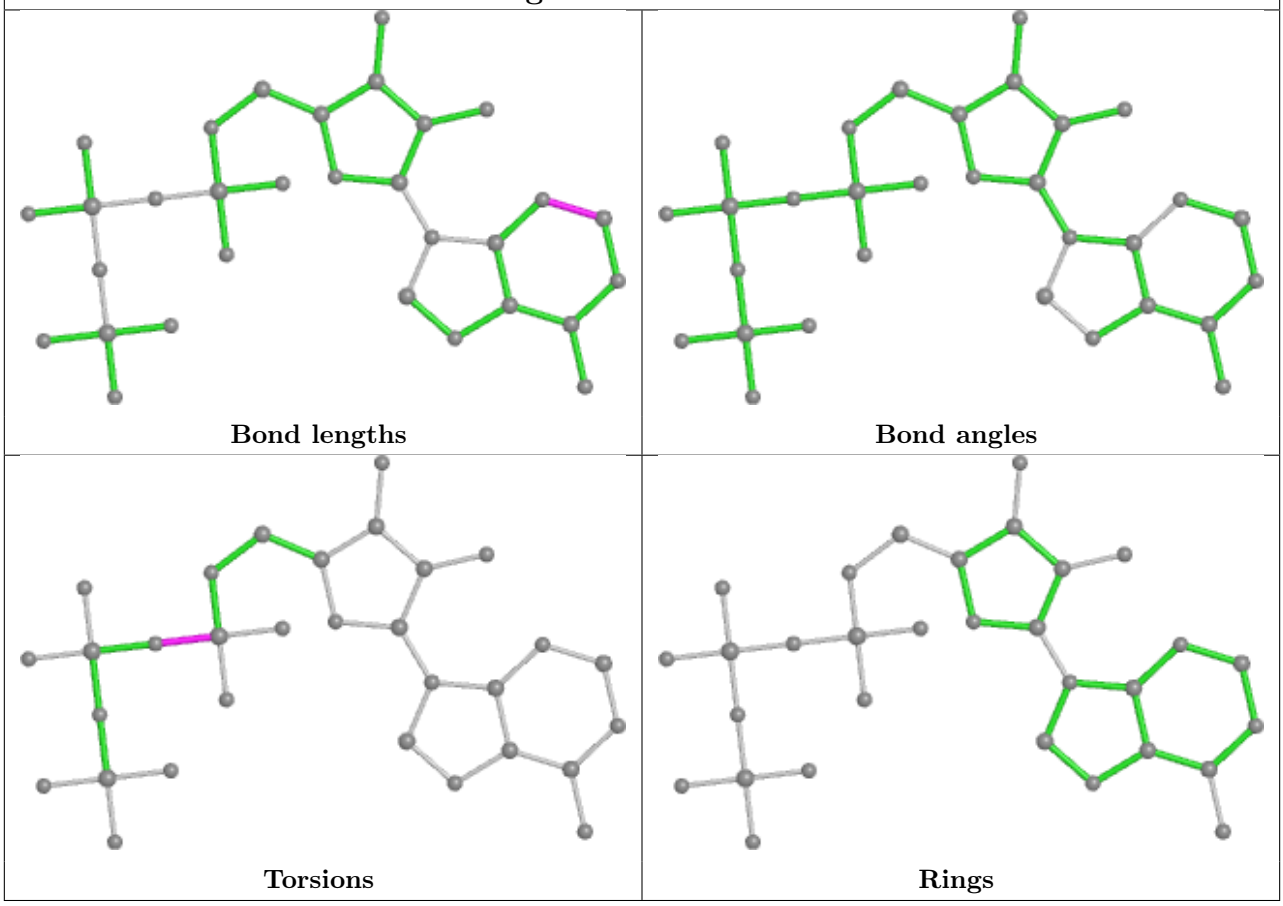
There are no ring outliers.

6 monomers are involved in 35 short contacts:

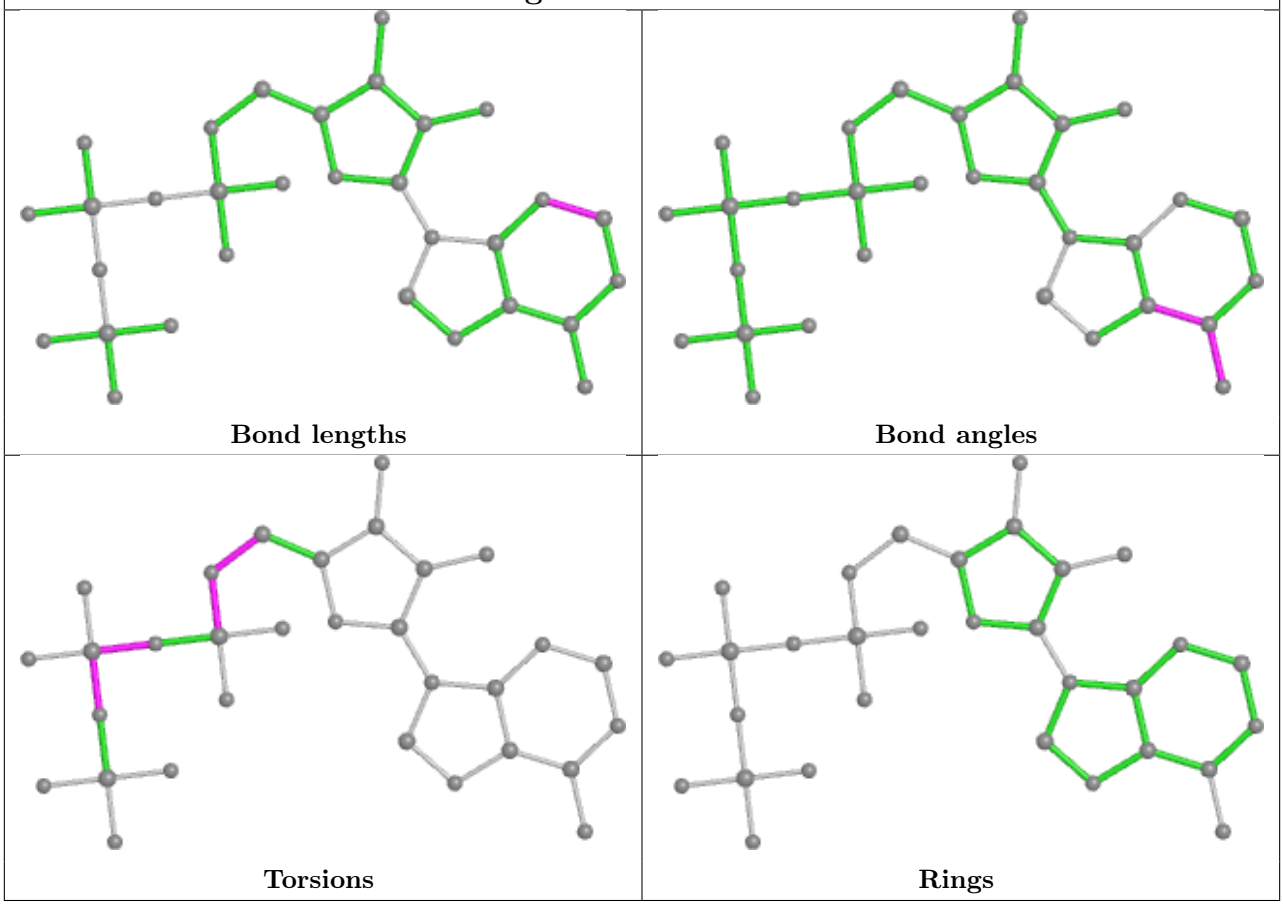
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	452	ATP	8	0
2	B	451	HSO	1	0
3	A	452	ATP	3	0
2	C	451	HSO	2	0
3	B	452	ATP	11	0
3	D	452	ATP	11	0

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

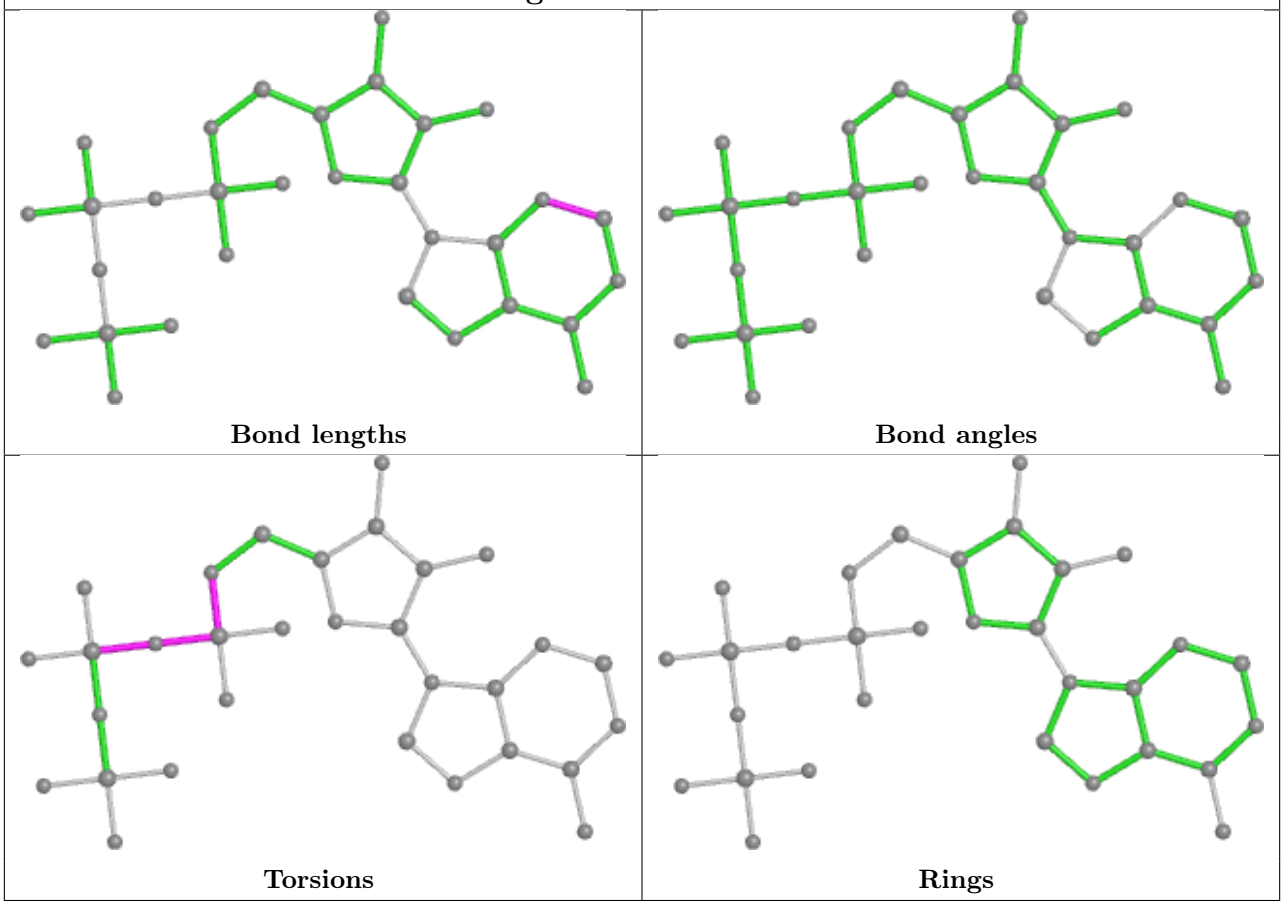
Ligand ATP C 452



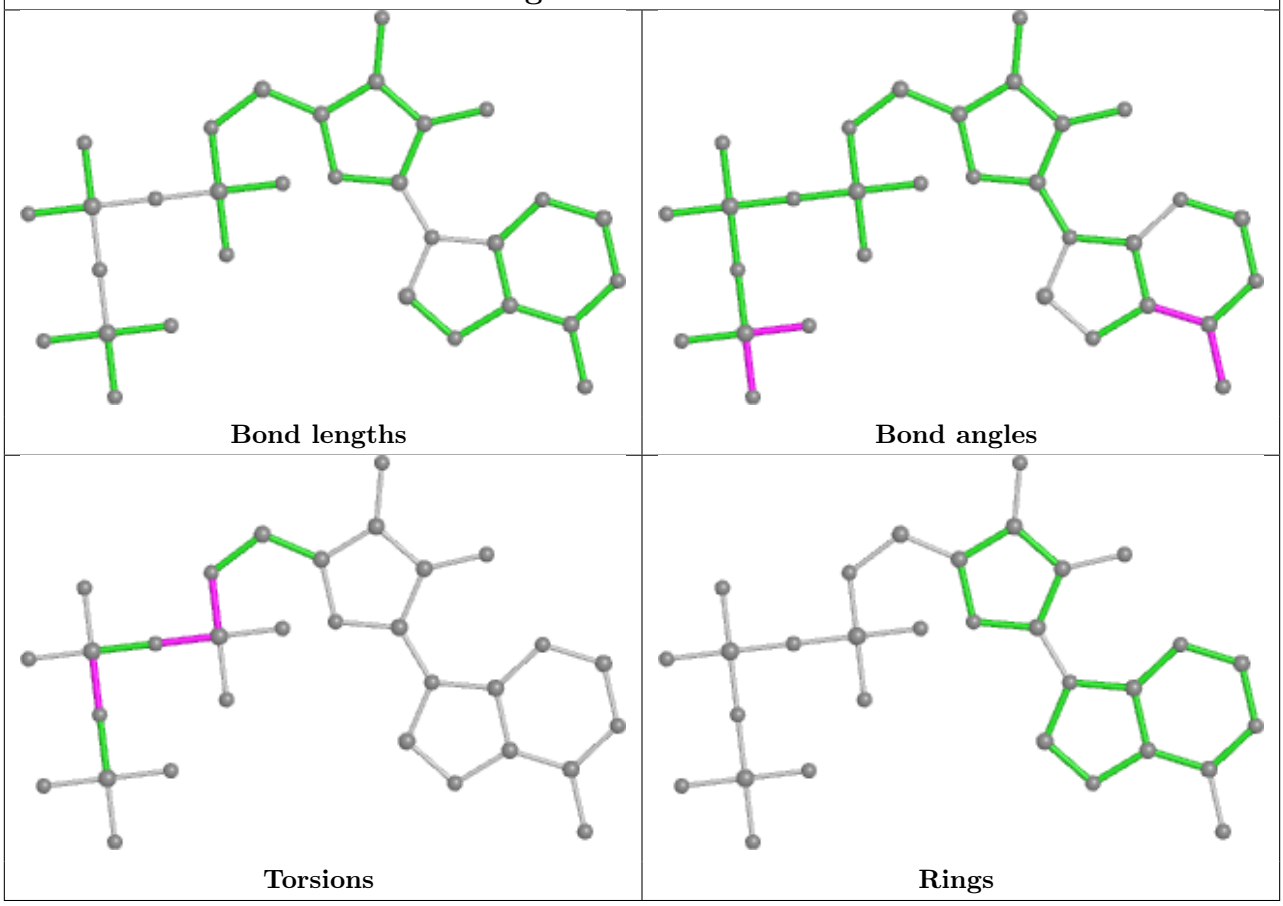
Ligand ATP A 452



Ligand ATP B 452



Ligand ATP D 452



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	379/424 (89%)	-0.45	1 (0%)	94	93	13, 41, 69, 81	0
1	B	364/424 (85%)	-0.39	3 (0%)	86	81	16, 44, 75, 96	0
1	C	387/424 (91%)	-0.45	0	100	100	14, 43, 69, 77	0
1	D	364/424 (85%)	-0.42	5 (1%)	75	70	16, 44, 76, 99	0
All	All	1494/1696 (88%)	-0.43	9 (0%)	89	86	13, 43, 72, 99	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	278	SER	4.4
1	D	424	GLY	3.3
1	B	424	GLY	3.0
1	B	59	VAL	3.0
1	B	257	LEU	2.9
1	D	59	VAL	2.5
1	D	276	LEU	2.5
1	A	374	ALA	2.2
1	D	242	LYS	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 monosaccharides in this entry.

6.4 Ligands (i)

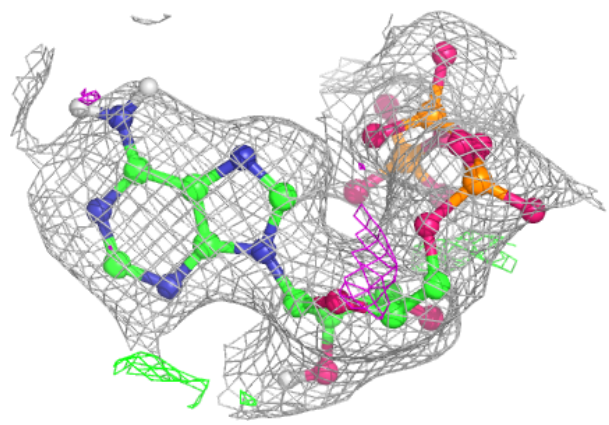
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

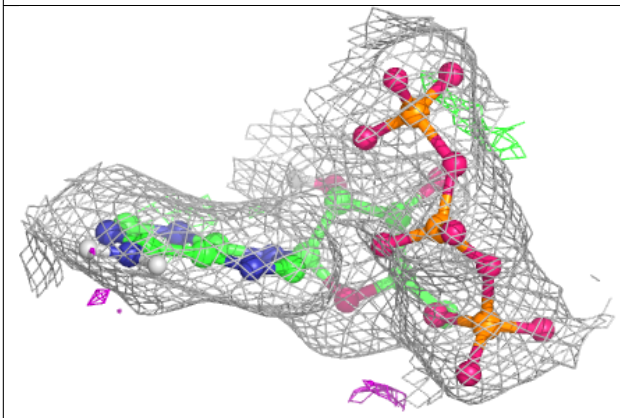
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ATP	B	452	31/31	0.90	0.15	0,45,78,79	0
3	ATP	D	452	31/31	0.91	0.16	0,57,69,70	0
2	HSO	C	451	10/10	0.92	0.18	0,31,35,41	0
2	HSO	A	451	10/10	0.92	0.18	0,28,34,37	0
2	HSO	B	451	10/10	0.92	0.17	0,26,32,32	0
2	HSO	D	451	10/10	0.93	0.15	0,35,38,40	0
3	ATP	C	452	31/31	0.94	0.13	0,35,55,58	0
3	ATP	A	452	31/31	0.94	0.13	0,35,47,52	0

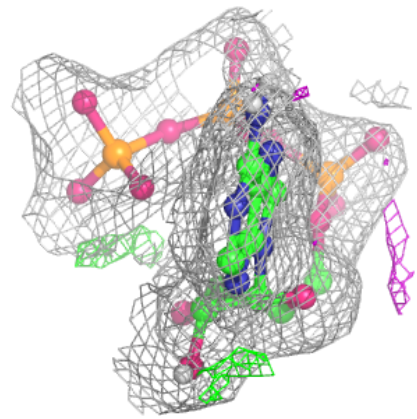
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP B 452:

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

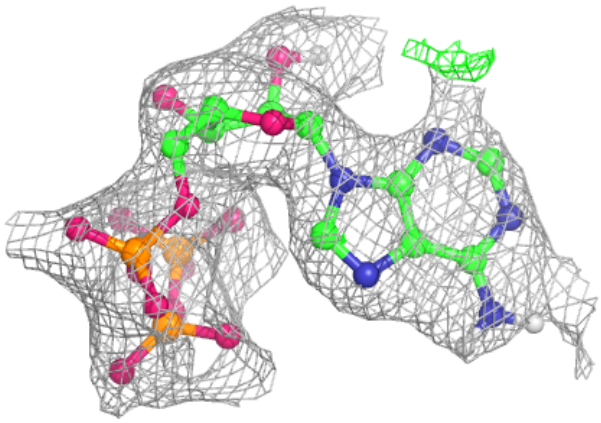


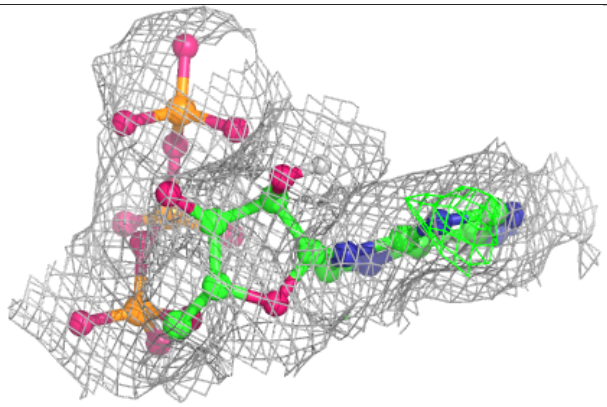


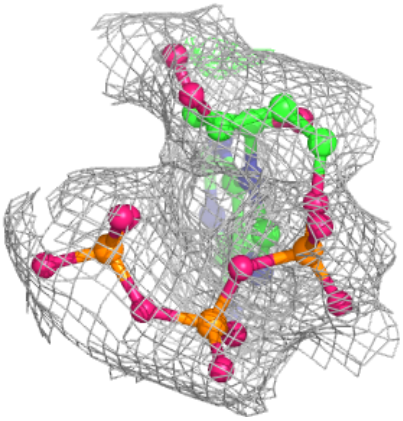


Electron density around ATP D 452:

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

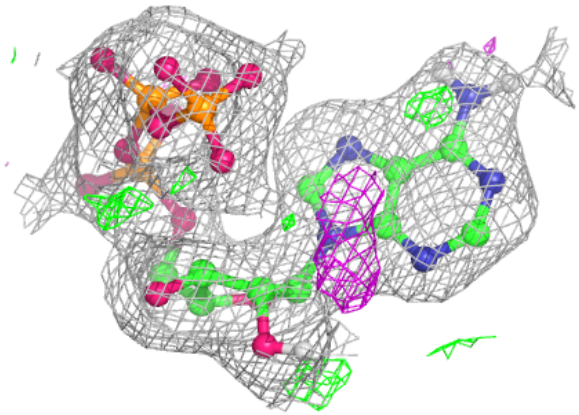


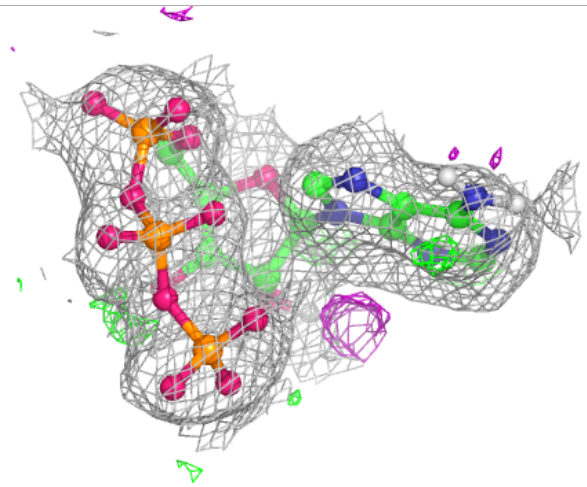


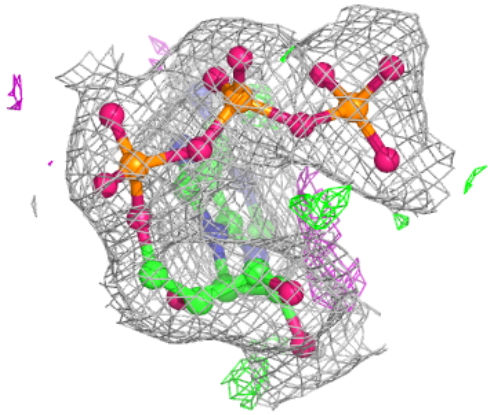


Electron density around ATP C 452:

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

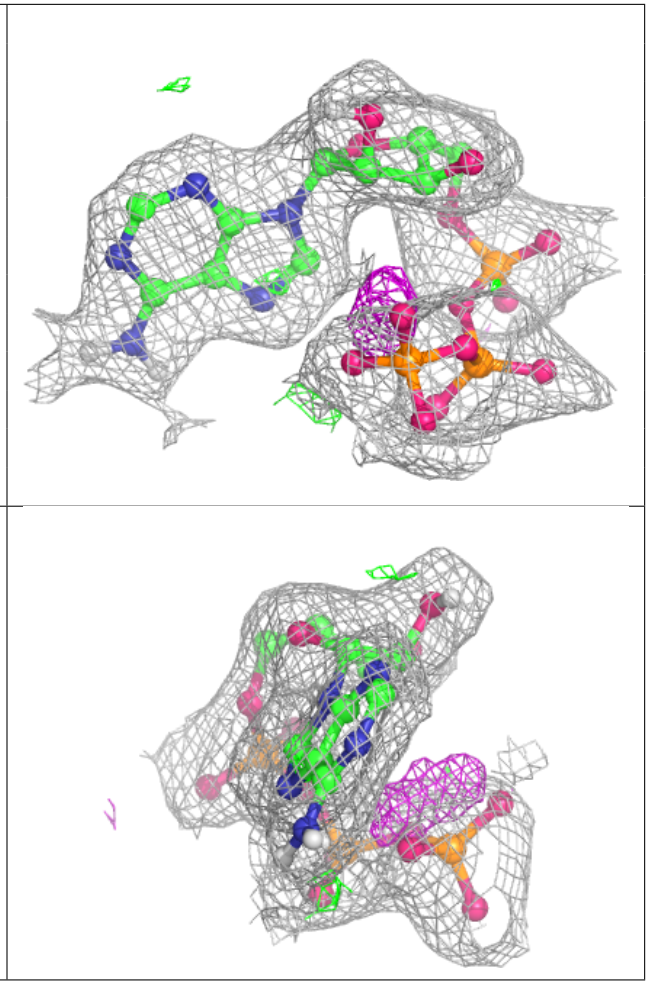






Electron density around ATP A 452:

$2mF_o$-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.