Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2023 – 02:17 PM EDT

PDB ID	:	3VNU
Title	:	Complex structure of viral RNA polymerase I
Authors	:	Takeshita, D.; Tomita, K.
Deposited on	:	2012-01-18
Resolution	:	3.20 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:

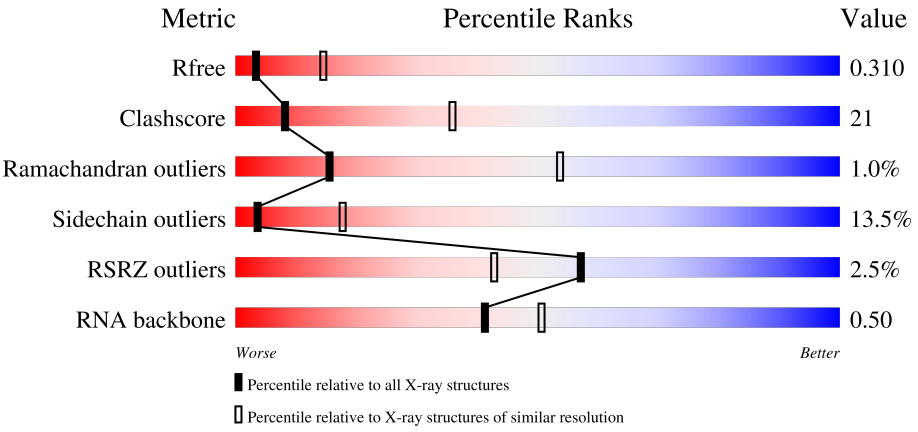
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	1289	2% 56% 31% 6% 7%
2	G	8	50% 25% 25%
3	T	8	25% 38% 12% 25%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ATP	A	2501	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9584 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 Elongation factor Ts, Elongation factor Tu, LINKER, Q beta replicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1203	9287	5865	1605	1772	45	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	284	HIS	-	linker	UNP P0A6P3
A	1284	HIS	-	expression tag	UNP Q8LTE0
A	1285	HIS	-	expression tag	UNP Q8LTE0
A	1286	HIS	-	expression tag	UNP Q8LTE0
A	1287	HIS	-	expression tag	UNP Q8LTE0
A	1288	HIS	-	expression tag	UNP Q8LTE0
A	1289	HIS	-	expression tag	UNP Q8LTE0

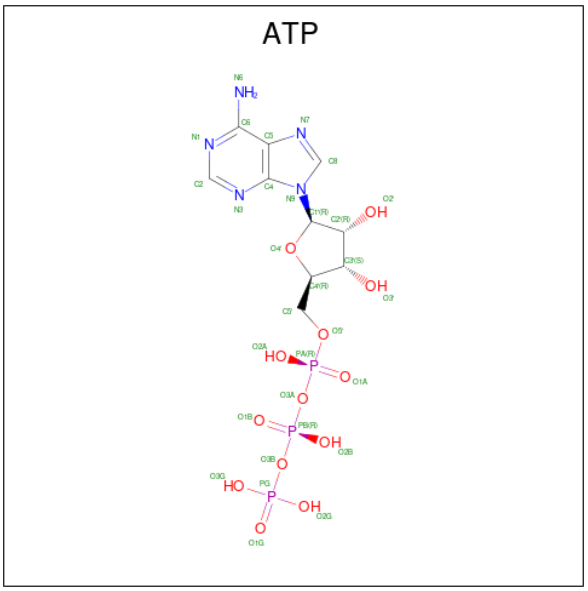
- Molecule 2 is a RNA chain called RNA (5'-R(*CP*CP*CP*UP*AP*CP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	G	6	121	55	19	41	6	0	0	0

- Molecule 3 is a RNA chain called RNA (5'-R(*GP*GP*GP*UP*AP*GP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	T	6	131	59	27	40	5	0	0	0

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Ca 2 2	0	0

- Molecule 6 is water.

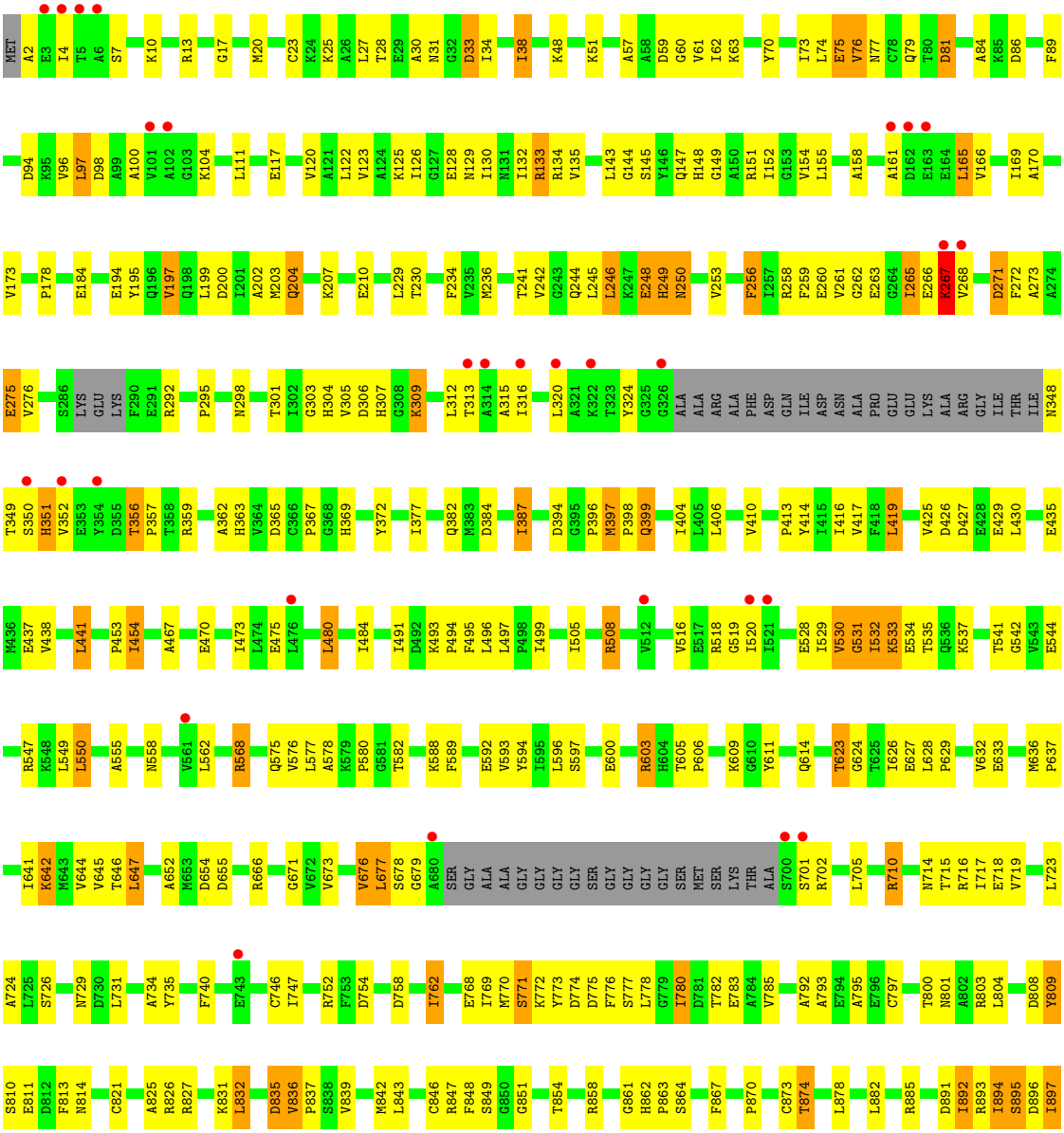
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	11	Total O 11 11	0	0
6	T	1	Total O 1 1	0	0

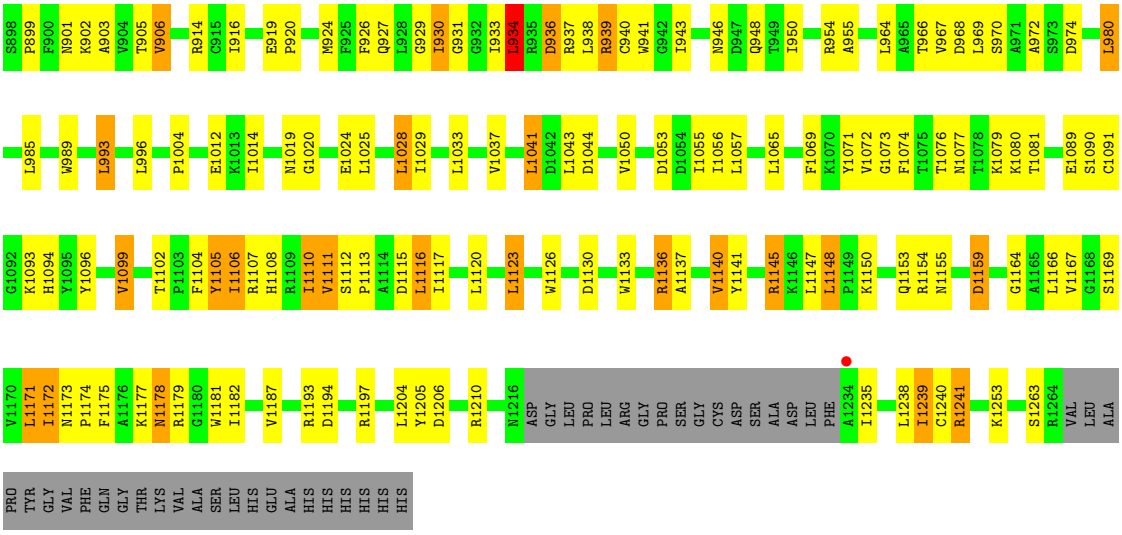
3 Residue-property plots (i)

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: Elongation factor Ts, Elongation factor Tu, LINKER, Q beta replicase

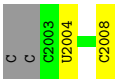
Chain A:





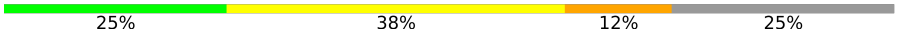
• Molecule 2: RNA (5'-R(*CP*CP*CP*UP*AP*CP*CP*C)-3')

Chain G:



• Molecule 3: RNA (5'-R(*GP*GP*GP*UP*AP*GP*GP*G)-3')

Chain T:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	139.00Å 255.51Å 101.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20 47.96 – 3.08	Depositor EDS
% Data completeness (in resolution range)	95.6 (20.00-3.20) 93.7 (47.96-3.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.274 , 0.316 0.272 , 0.310	Depositor DCC
R_{free} test set	1580 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	57.7	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.19 , 8.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.32$, $< L^2 > = 0.16$	Xtriage
Estimated twinning fraction	0.146 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.115 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	9584	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

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

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0.56	1/9456 (0.0%)	0.69	3/12787 (0.0%)
2	G	0.30	0/133	0.65	0/203
3	T	0.31	0/147	0.59	0/229
All	All	0.56	1/9736 (0.0%)	0.68	3/13219 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1133	TRP	CD2-CE2	5.02	1.47	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1159	ASP	CB-CG-OD1	6.76	124.39	118.30
1	A	934	LEU	CA-CB-CG	5.44	127.82	115.30
1	A	1041	LEU	CB-CG-CD2	-5.07	102.38	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	9287	0	9271	392	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	121	0	64	8	0
3	T	131	0	67	4	0
4	A	31	0	12	11	0
5	A	2	0	0	0	0
6	A	11	0	0	1	0
6	T	1	0	0	0	0
All	All	9584	0	9414	402	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 21.

All (402) 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:246:LEU:O	1:A:249:HIS:O	1.52	1.27
1:A:267:LYS:HD2	1:A:268:VAL:N	1.57	1.19
1:A:894:ILE:N	1:A:894:ILE:HD13	1.57	1.15
1:A:891:ASP:C	1:A:892:ILE:HD13	1.67	1.13
1:A:244:GLN:O	1:A:248:GLU:HG3	1.47	1.12
1:A:677:LEU:N	1:A:677:LEU:HD23	1.66	1.08
1:A:894:ILE:HD13	1:A:894:ILE:H	1.14	1.07
6:A:3111:HOH:O	3:T:2101:G:H5'	1.54	1.07
1:A:891:ASP:C	1:A:892:ILE:CD1	2.26	1.04
1:A:605:THR:HG22	1:A:606:PRO:HD2	1.38	1.04
1:A:244:GLN:O	1:A:248:GLU:CG	2.10	1.00
1:A:275:GLU:OE2	1:A:276:VAL:HA	1.62	0.99
1:A:897:ILE:HG22	1:A:897:ILE:O	1.61	0.98
1:A:1173:ASN:OD1	1:A:1174:PRO:HD2	1.63	0.98
1:A:531:GLY:C	1:A:532:ILE:CD1	2.33	0.96
1:A:529:ILE:O	1:A:529:ILE:HG23	1.65	0.96
1:A:892:ILE:HD13	1:A:892:ILE:N	1.74	0.95
1:A:267:LYS:CD	1:A:268:VAL:N	2.31	0.94
1:A:1240:CYS:C	1:A:1241:ARG:HE	1.70	0.93
1:A:530:VAL:HG22	1:A:652:ALA:HB2	1.51	0.92
1:A:531:GLY:C	1:A:532:ILE:HD13	1.91	0.92
1:A:894:ILE:N	1:A:894:ILE:CD1	2.32	0.91
1:A:133:ARG:NH1	1:A:265:ILE:HD11	1.85	0.91
1:A:272:PHE:CZ	1:A:313:THR:HG21	2.06	0.90
1:A:892:ILE:CD1	1:A:892:ILE:N	2.33	0.90
1:A:349:THR:O	1:A:350:SER:HB2	1.70	0.90
1:A:531:GLY:O	1:A:532:ILE:HD12	1.71	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:GLU:C	1:A:275:GLU:CD	2.31	0.88
1:A:968:ASP:H	1:A:1081:THR:HG22	1.39	0.87
1:A:267:LYS:HD2	1:A:268:VAL:H	1.38	0.86
1:A:261:VAL:C	1:A:263:GLU:OE1	2.12	0.86
1:A:891:ASP:O	1:A:892:ILE:HD12	1.76	0.86
1:A:676:VAL:C	1:A:677:LEU:HD23	1.97	0.85
1:A:152:ILE:CG1	1:A:260:GLU:HG3	2.07	0.84
1:A:352:VAL:HG22	1:A:363:HIS:HB3	1.59	0.84
1:A:531:GLY:HA3	1:A:575:GLN:HG2	1.60	0.84
1:A:532:ILE:CD1	1:A:532:ILE:N	2.41	0.84
1:A:267:LYS:HE3	1:A:268:VAL:O	1.77	0.84
1:A:677:LEU:N	1:A:677:LEU:CD2	2.41	0.83
1:A:272:PHE:HZ	1:A:313:THR:HG21	1.43	0.83
1:A:532:ILE:HD13	1:A:532:ILE:N	1.93	0.83
1:A:531:GLY:C	1:A:532:ILE:HD12	1.98	0.83
1:A:946:ASN:HA	3:T:2103:G:H4'	1.59	0.82
1:A:152:ILE:CD1	1:A:260:GLU:HG3	2.09	0.82
1:A:267:LYS:HD2	1:A:268:VAL:C	2.00	0.82
1:A:1240:CYS:C	1:A:1241:ARG:NE	2.32	0.82
1:A:629:PRO:HD2	1:A:632:VAL:CG1	2.09	0.81
1:A:267:LYS:CD	1:A:268:VAL:H	1.91	0.81
1:A:152:ILE:HD11	1:A:260:GLU:HG3	1.62	0.81
1:A:605:THR:CG2	1:A:606:PRO:HD2	2.09	0.80
1:A:267:LYS:HD2	1:A:268:VAL:CA	2.11	0.79
1:A:267:LYS:CE	1:A:268:VAL:O	2.31	0.79
1:A:348:ASN:O	1:A:351:HIS:CE1	2.36	0.78
1:A:1241:ARG:N	1:A:1241:ARG:CD	2.45	0.78
1:A:897:ILE:O	1:A:897:ILE:CG2	2.32	0.78
1:A:152:ILE:HG12	1:A:260:GLU:HG3	1.65	0.78
1:A:262:GLY:HA2	1:A:265:ILE:HG12	1.66	0.77
1:A:655:ASP:HA	1:A:673:VAL:HG23	1.66	0.76
1:A:267:LYS:HD2	1:A:268:VAL:O	1.85	0.76
1:A:275:GLU:OE2	1:A:276:VAL:CA	2.34	0.76
1:A:303:GLY:O	1:A:309:LYS:NZ	2.17	0.76
1:A:194:GLU:HA	1:A:197:VAL:HG12	1.68	0.75
1:A:234:PHE:CE1	1:A:236:MET:HB2	2.22	0.75
1:A:1206:ASP:OD1	1:A:1210:ARG:NH1	2.19	0.75
1:A:629:PRO:HD2	1:A:632:VAL:HG12	1.69	0.75
1:A:1050:VAL:HG13	1:A:1055:ILE:HG22	1.68	0.74
1:A:529:ILE:O	1:A:529:ILE:CG2	2.32	0.74
4:A:2501:ATP:H5'1	2:G:2008:C:C3'	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1241:ARG:N	1:A:1241:ARG:HD2	2.02	0.74
1:A:955:ALA:HB2	1:A:1090:SER:HB3	1.68	0.74
1:A:491:ILE:HG23	1:A:520:ILE:HD11	1.71	0.73
1:A:161:ALA:HB1	1:A:165:LEU:HB3	1.71	0.73
1:A:467:ALA:HA	1:A:470:GLU:HB2	1.71	0.73
1:A:800:THR:HG21	1:A:1073:GLY:HA2	1.71	0.73
1:A:304:HIS:HD2	1:A:306:ASP:H	1.37	0.72
1:A:499:ILE:HD11	1:A:577:LEU:HB2	1.71	0.72
1:A:530:VAL:CG2	1:A:652:ALA:HB2	2.20	0.72
4:A:2501:ATP:H5'1	2:G:2008:C:C2'	2.20	0.72
1:A:377:ILE:HG23	1:A:671:GLY:HA2	1.72	0.71
1:A:496:LEU:HD11	1:A:576:VAL:HB	1.72	0.71
1:A:273:ALA:HB2	1:A:350:SER:CA	2.21	0.71
1:A:267:LYS:CD	1:A:268:VAL:O	2.39	0.70
4:A:2501:ATP:H5'1	2:G:2008:C:H2'	1.74	0.70
1:A:416:ILE:HG23	1:A:453:PRO:HG2	1.74	0.70
1:A:891:ASP:O	1:A:892:ILE:CD1	2.38	0.70
1:A:1240:CYS:C	1:A:1241:ARG:CD	2.61	0.69
1:A:275:GLU:CD	1:A:275:GLU:O	2.31	0.69
1:A:772:LYS:HD2	1:A:1105:TYR:CD1	2.27	0.69
1:A:836:VAL:HG22	1:A:837:PRO:HD2	1.75	0.69
1:A:1240:CYS:HA	1:A:1241:ARG:HD2	1.74	0.68
1:A:550:LEU:HD13	1:A:550:LEU:H	1.58	0.68
1:A:271:ASP:OD1	1:A:271:ASP:C	2.31	0.68
1:A:846:CYS:SG	1:A:929:GLY:HA3	2.34	0.67
1:A:273:ALA:CB	1:A:350:SER:HA	2.24	0.67
1:A:1240:CYS:C	1:A:1241:ARG:HD2	2.14	0.67
1:A:533:LYS:O	1:A:534:GLU:C	2.32	0.67
1:A:717:ILE:HG13	1:A:718:GLU:H	1.59	0.67
1:A:1057:LEU:HD13	1:A:1065:LEU:HD22	1.75	0.67
1:A:894:ILE:H	1:A:894:ILE:CD1	1.93	0.67
1:A:628:LEU:HB3	1:A:632:VAL:HG13	1.76	0.67
1:A:826:ARG:HH21	1:A:827:ARG:HG2	1.59	0.67
1:A:158:ALA:HA	1:A:253:VAL:HA	1.74	0.67
1:A:261:VAL:O	1:A:263:GLU:OE1	2.12	0.66
1:A:768:GLU:O	1:A:771:SER:OG	2.13	0.66
1:A:762:ILE:HG12	1:A:1126:TRP:HH2	1.61	0.65
1:A:716:ARG:HG3	1:A:1111:VAL:HG22	1.76	0.65
1:A:20:MET:H	1:A:394:ASP:HA	1.61	0.65
1:A:301:THR:HA	1:A:387:ILE:HG22	1.78	0.65
1:A:568:ARG:HH12	1:A:1197:ARG:HH11	1.42	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:701:SER:HB2	1:A:1179:ARG:HD2	1.78	0.65
1:A:710:ARG:O	1:A:714:ASN:ND2	2.28	0.65
1:A:1104:PHE:HZ	1:A:1123:LEU:HD12	1.61	0.65
1:A:134:ARG:HG3	1:A:259:PHE:CE1	2.30	0.64
1:A:273:ALA:HB2	1:A:350:SER:HA	1.78	0.64
1:A:59:ASP:OD2	1:A:81:ASP:N	2.30	0.64
1:A:494:PRO:HB2	1:A:582:THR:HG21	1.79	0.64
1:A:13:ARG:HH22	1:A:396:PRO:HD2	1.62	0.64
1:A:250:ASN:OD1	1:A:250:ASN:N	2.31	0.64
1:A:399:GLN:H	1:A:399:GLN:HE21	1.44	0.64
1:A:1240:CYS:CA	1:A:1241:ARG:HD2	2.28	0.64
1:A:870:PRO:HA	1:A:893:ARG:HB2	1.81	0.63
1:A:895:SER:OG	1:A:896:ASP:N	2.31	0.63
2:G:2004:U:H3	3:T:2105:A:H61	1.47	0.63
1:A:1239:ILE:HG22	1:A:1239:ILE:O	1.99	0.63
1:A:62:ILE:O	1:A:147:GLN:NE2	2.32	0.62
1:A:348:ASN:O	1:A:351:HIS:ND1	2.32	0.62
1:A:906:VAL:HG13	1:A:914:ARG:HB2	1.81	0.62
4:A:2501:ATP:C4'	2:G:2008:C:H2'	2.30	0.62
1:A:832:LEU:HD21	1:A:940:CYS:HB2	1.80	0.62
1:A:260:GLU:HB3	1:A:263:GLU:CG	2.15	0.62
1:A:165:LEU:HD21	1:A:245:LEU:HD11	1.80	0.62
1:A:593:VAL:HG12	1:A:671:GLY:HA3	1.82	0.62
1:A:627:GLU:HG2	1:A:644:VAL:HB	1.82	0.62
1:A:244:GLN:O	1:A:248:GLU:HG2	1.97	0.62
1:A:351:HIS:ND1	1:A:351:HIS:O	2.32	0.61
1:A:1173:ASN:OD1	1:A:1174:PRO:CD	2.44	0.61
1:A:532:ILE:HB	1:A:533:LYS:HD3	1.81	0.61
1:A:304:HIS:HB3	1:A:307:HIS:CG	2.35	0.61
1:A:1050:VAL:HG22	1:A:1055:ILE:HB	1.81	0.61
1:A:839:VAL:HA	1:A:842:MET:HB3	1.83	0.61
1:A:265:ILE:HD13	1:A:265:ILE:N	2.16	0.61
1:A:614:GLN:HA	1:A:623:THR:HA	1.83	0.61
1:A:588:LYS:HB3	1:A:679:GLY:HA2	1.82	0.61
1:A:1159:ASP:HB2	1:A:1167:VAL:HG11	1.82	0.61
1:A:275:GLU:OE2	1:A:275:GLU:C	2.38	0.60
1:A:542:GLY:H	1:A:562:LEU:HB2	1.65	0.60
1:A:295:PRO:HG2	1:A:359:ARG:HG2	1.83	0.60
1:A:372:TYR:HE1	1:A:410:VAL:HG11	1.66	0.60
1:A:854:THR:HG22	1:A:920:PRO:HA	1.82	0.60
1:A:624:GLY:HA3	1:A:647:LEU:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:THR:HG22	1:A:359:ARG:H	1.67	0.59
1:A:592:GLU:HG2	1:A:642:LYS:HG2	1.84	0.59
1:A:885:ARG:NH1	1:A:892:ILE:H	2.00	0.59
1:A:558:ASN:HB3	1:A:1210:ARG:HD3	1.83	0.59
1:A:873:CYS:SG	1:A:874:THR:N	2.74	0.59
1:A:930:ILE:HG13	1:A:931:GLY:N	2.18	0.59
1:A:891:ASP:C	1:A:892:ILE:HD12	2.10	0.59
1:A:74:LEU:HD22	1:A:97:LEU:HD23	1.85	0.59
1:A:404:ILE:HD12	1:A:441:LEU:HD22	1.84	0.59
1:A:61:VAL:HG22	1:A:89:PHE:HE1	1.68	0.59
4:A:2501:ATP:C5'	2:G:2008:C:H2'	2.32	0.58
1:A:396:PRO:HG3	1:A:437:GLU:HB3	1.84	0.58
1:A:1171:LEU:N	1:A:1171:LEU:CD1	2.65	0.58
1:A:57:ALA:HA	1:A:79:GLN:HB3	1.86	0.58
1:A:59:ASP:OD2	1:A:81:ASP:OD1	2.20	0.58
1:A:878:LEU:HD13	1:A:897:ILE:HD11	1.86	0.58
1:A:133:ARG:HH11	1:A:265:ILE:HD11	1.67	0.58
1:A:265:ILE:N	1:A:265:ILE:CD1	2.67	0.57
1:A:266:GLU:O	1:A:267:LYS:CB	2.53	0.57
1:A:1154:ARG:HG2	1:A:1174:PRO:HG3	1.85	0.57
1:A:145:SER:HB2	1:A:155:LEU:HD13	1.86	0.57
1:A:304:HIS:CD2	1:A:306:ASP:H	2.22	0.56
1:A:1155:ASN:HB2	1:A:1175:PHE:HE1	1.68	0.56
1:A:2:ALA:N	1:A:426:ASP:O	2.38	0.56
1:A:611:TYR:HB3	1:A:626:ILE:HD11	1.88	0.56
1:A:938:LEU:HD13	1:A:1028:LEU:HD12	1.87	0.56
1:A:1116:LEU:HD12	1:A:1148:LEU:HD21	1.87	0.56
1:A:948:GLN:HB2	1:A:1091:CYS:SG	2.45	0.56
1:A:558:ASN:HB3	1:A:1210:ARG:HB3	1.87	0.56
1:A:1241:ARG:CZ	1:A:1241:ARG:HB3	2.35	0.56
1:A:491:ILE:HD13	1:A:555:ALA:HB3	1.87	0.55
1:A:916:ILE:HD12	4:A:2501:ATP:HN62	1.71	0.55
1:A:349:THR:O	1:A:350:SER:CB	2.47	0.55
1:A:793:ALA:HB1	1:A:974:ASP:HB3	1.88	0.55
1:A:934:LEU:HD13	1:A:1024:GLU:HB3	1.87	0.55
1:A:202:ALA:HB1	1:A:207:LYS:HD2	1.88	0.55
1:A:200:ASP:O	1:A:204:GLN:HB2	2.07	0.55
1:A:273:ALA:HB2	1:A:350:SER:C	2.27	0.55
1:A:702:ARG:H	1:A:1177:LYS:HE3	1.70	0.55
1:A:417:VAL:HB	1:A:454:ILE:HG23	1.89	0.55
1:A:245:LEU:O	1:A:249:HIS:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:GLU:OE1	1:A:133:ARG:NH2	2.39	0.55
1:A:63:LYS:HB2	1:A:97:LEU:HG	1.89	0.54
1:A:724:ALA:HB1	1:A:1106:ILE:HG21	1.88	0.54
1:A:1117:ILE:HD13	1:A:1166:LEU:HG	1.89	0.54
1:A:60:GLY:HA3	1:A:77:ASN:HB2	1.90	0.54
1:A:152:ILE:HG12	1:A:260:GLU:CG	2.35	0.54
1:A:272:PHE:CE1	1:A:313:THR:HG21	2.43	0.54
1:A:111:LEU:HD23	1:A:111:LEU:H	1.74	0.53
1:A:494:PRO:HB2	1:A:582:THR:CG2	2.38	0.53
1:A:1057:LEU:CD1	1:A:1065:LEU:HD22	2.39	0.53
1:A:13:ARG:O	1:A:17:GLY:N	2.41	0.53
1:A:972:ALA:HB3	4:A:2501:ATP:O3'	2.09	0.53
1:A:125:LYS:HE2	1:A:398:PRO:HG3	1.89	0.53
1:A:413:PRO:HB2	1:A:414:TYR:CD1	2.44	0.53
1:A:1178:ASN:OD1	1:A:1178:ASN:N	2.38	0.53
1:A:1164:GLY:HA3	1:A:1187:VAL:HB	1.91	0.53
1:A:723:LEU:HD23	1:A:1110:ILE:CG1	2.39	0.52
1:A:782:THR:OG1	1:A:783:GLU:N	2.42	0.52
1:A:1077:ASN:O	1:A:1081:THR:HG23	2.08	0.52
1:A:1171:LEU:HD13	1:A:1171:LEU:H	1.74	0.52
1:A:606:PRO:HB3	1:A:636:MET:HG2	1.91	0.52
1:A:372:TYR:CE1	1:A:410:VAL:HG21	2.45	0.52
1:A:1037:VAL:HG21	1:A:1065:LEU:HD12	1.90	0.52
1:A:773:TYR:HA	1:A:1107:ARG:O	2.10	0.52
1:A:954:ARG:HH12	1:A:1056:ILE:HG22	1.74	0.52
1:A:152:ILE:CG1	1:A:260:GLU:CG	2.86	0.52
1:A:747:ILE:HG22	1:A:771:SER:HA	1.91	0.52
1:A:919:GLU:HG3	1:A:1019:ASN:HA	1.91	0.51
1:A:1094:HIS:H	1:A:1102:THR:HG22	1.75	0.51
1:A:533:LYS:N	1:A:533:LYS:CD	2.74	0.51
1:A:236:MET:O	1:A:1181:TRP:HH2	1.93	0.51
1:A:348:ASN:O	1:A:351:HIS:CG	2.64	0.51
1:A:717:ILE:HG13	1:A:718:GLU:N	2.26	0.51
1:A:735:TYR:CE1	1:A:1136:ARG:HG3	2.45	0.51
1:A:985:LEU:HD13	1:A:993:LEU:HD13	1.92	0.51
1:A:266:GLU:O	1:A:267:LYS:HB3	2.09	0.51
1:A:133:ARG:HH21	1:A:134:ARG:NE	2.09	0.50
1:A:821:CYS:O	1:A:825:ALA:N	2.34	0.50
1:A:275:GLU:OE2	1:A:276:VAL:N	2.43	0.50
1:A:1033:LEU:O	1:A:1037:VAL:HG23	2.12	0.50
1:A:496:LEU:CD1	1:A:576:VAL:HB	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:782:THR:HG23	1:A:785:VAL:H	1.77	0.50
1:A:735:TYR:CG	1:A:762:ILE:HG13	2.46	0.50
1:A:133:ARG:HH12	1:A:265:ILE:HD11	1.73	0.50
1:A:399:GLN:HE21	1:A:399:GLN:N	2.08	0.50
1:A:746:CYS:HB3	1:A:770:MET:HG3	1.94	0.50
1:A:1116:LEU:HD12	1:A:1148:LEU:CD2	2.42	0.50
1:A:48:LYS:O	1:A:51:LYS:HB3	2.12	0.50
1:A:111:LEU:HD21	1:A:135:VAL:HG11	1.92	0.50
1:A:954:ARG:HH22	1:A:964:LEU:HD11	1.77	0.50
1:A:528:GLU:CD	1:A:580:PRO:HA	2.32	0.50
1:A:903:ALA:O	1:A:1004:PRO:HD3	2.12	0.50
1:A:1155:ASN:HB2	1:A:1175:PHE:CE1	2.46	0.49
1:A:723:LEU:HD23	1:A:1110:ILE:HG12	1.94	0.49
1:A:1043:LEU:HD12	1:A:1044:ASP:H	1.77	0.49
1:A:271:ASP:OD1	1:A:273:ALA:N	2.45	0.49
1:A:497:LEU:HD12	1:A:516:VAL:HB	1.94	0.49
1:A:809:TYR:CE1	1:A:814:ASN:O	2.66	0.49
1:A:769:ILE:HG23	1:A:770:MET:N	2.28	0.49
1:A:626:ILE:HG22	1:A:645:VAL:HA	1.95	0.49
1:A:847:ARG:NH1	3:T:2102:G:OP1	2.45	0.49
1:A:76:VAL:HA	1:A:132:ILE:HA	1.95	0.48
1:A:352:VAL:CG2	1:A:363:HIS:HB3	2.38	0.48
1:A:970:SER:O	4:A:2501:ATP:O3B	2.31	0.48
1:A:59:ASP:O	1:A:77:ASN:HB2	2.13	0.48
1:A:152:ILE:HD11	1:A:260:GLU:CG	2.40	0.48
1:A:849:SER:HA	1:A:863:PRO:HG3	1.94	0.48
1:A:303:GLY:H	1:A:309:LYS:HZ2	1.59	0.48
1:A:1116:LEU:HB3	1:A:1148:LEU:HD21	1.95	0.48
1:A:59:ASP:OD2	1:A:81:ASP:CA	2.61	0.48
1:A:301:THR:HB	1:A:363:HIS:NE2	2.28	0.48
1:A:605:THR:HG22	1:A:606:PRO:CD	2.26	0.48
1:A:792:ALA:HA	1:A:795:ALA:HB3	1.95	0.48
1:A:893:ARG:C	1:A:894:ILE:HD13	2.28	0.48
1:A:148:HIS:O	1:A:149:GLY:C	2.52	0.48
1:A:275:GLU:OE2	1:A:275:GLU:O	2.31	0.48
1:A:304:HIS:ND1	1:A:397:MET:HG2	2.28	0.48
1:A:891:ASP:CA	1:A:892:ILE:HD13	2.39	0.48
1:A:81:ASP:OD2	1:A:151:ARG:NH1	2.47	0.48
1:A:710:ARG:NH1	1:A:1253:LYS:HD3	2.28	0.48
1:A:17:GLY:O	1:A:125:LYS:HG3	2.13	0.48
1:A:596:LEU:HD12	1:A:600:GLU:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:LYS:CG	1:A:268:VAL:N	2.76	0.48
1:A:530:VAL:HG13	1:A:576:VAL:HG22	1.96	0.48
1:A:926:PHE:HB3	1:A:996:LEU:HD21	1.94	0.48
4:A:2501:ATP:C8	2:G:2008:C:C4	3.01	0.48
1:A:1240:CYS:O	1:A:1241:ARG:NE	2.32	0.48
1:A:435:GLU:HA	1:A:438:VAL:HG12	1.96	0.47
1:A:628:LEU:HB3	1:A:629:PRO:HD2	1.97	0.47
1:A:419:LEU:HD22	1:A:454:ILE:HG22	1.95	0.47
1:A:603:ARG:H	1:A:603:ARG:HG3	1.41	0.47
1:A:74:LEU:HD21	1:A:96:VAL:HG13	1.97	0.47
1:A:272:PHE:CD2	1:A:365:ASP:HB2	2.49	0.47
1:A:1145:ARG:HH11	1:A:1145:ARG:HB3	1.80	0.47
1:A:246:LEU:O	1:A:249:HIS:C	2.43	0.47
1:A:633:GLU:N	1:A:633:GLU:OE1	2.48	0.47
1:A:184:GLU:N	1:A:184:GLU:OE1	2.48	0.46
1:A:399:GLN:H	1:A:399:GLN:NE2	2.09	0.46
1:A:1025:LEU:O	1:A:1029:ILE:HG12	2.15	0.46
1:A:178:PRO:HG3	1:A:229:LEU:HD13	1.96	0.46
1:A:719:VAL:HG21	1:A:723:LEU:HD22	1.96	0.46
1:A:966:THR:HA	1:A:1056:ILE:HG13	1.97	0.46
1:A:544:GLU:HB3	1:A:549:LEU:HG	1.97	0.46
1:A:937:ARG:NH2	1:A:940:CYS:SG	2.88	0.46
1:A:154:VAL:HG21	1:A:170:ALA:O	2.16	0.46
1:A:878:LEU:O	1:A:882:LEU:HG	2.16	0.46
1:A:122:LEU:O	1:A:126:ILE:N	2.39	0.46
1:A:1145:ARG:HD2	1:A:1153:GLN:HE21	1.81	0.46
1:A:851:GLY:HA2	1:A:861:GLY:CA	2.46	0.45
1:A:74:LEU:HB2	1:A:97:LEU:HD23	1.98	0.45
1:A:304:HIS:HB3	1:A:307:HIS:CD2	2.51	0.45
1:A:752:ARG:NH1	1:A:754:ASP:OD1	2.49	0.45
1:A:641:ILE:HG13	1:A:642:LYS:O	2.16	0.45
1:A:862:HIS:CD2	1:A:864:SER:H	2.34	0.45
1:A:778:LEU:HA	1:A:778:LEU:HD23	1.59	0.45
1:A:810:SER:O	1:A:811:GLU:HG3	2.16	0.45
1:A:425:VAL:HG12	1:A:427:ASP:H	1.81	0.45
1:A:597:SER:HA	1:A:637:PRO:HB2	1.97	0.45
1:A:603:ARG:C	1:A:605:THR:H	2.20	0.45
1:A:655:ASP:N	1:A:655:ASP:OD1	2.49	0.45
1:A:980:LEU:HD13	1:A:1072:VAL:HB	1.99	0.45
1:A:1110:ILE:HD12	1:A:1115:ASP:HB2	1.99	0.45
1:A:397:MET:HB3	1:A:399:GLN:NE2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589:PHE:CE1	1:A:673:VAL:HG12	2.52	0.45
1:A:832:LEU:HG	1:A:941:TRP:NE1	2.32	0.45
1:A:967:VAL:HB	1:A:1055:ILE:HG12	1.99	0.45
1:A:533:LYS:HD3	1:A:533:LYS:N	2.32	0.44
1:A:128:GLU:O	1:A:130:ILE:N	2.49	0.44
1:A:735:TYR:OH	1:A:1137:ALA:HB2	2.16	0.44
1:A:919:GLU:HB2	1:A:924:MET:HG2	1.99	0.44
1:A:954:ARG:NH1	1:A:1056:ILE:HG22	2.32	0.44
1:A:7:SER:O	1:A:10:LYS:HG2	2.17	0.44
1:A:73:ILE:HD11	1:A:259:PHE:HB2	2.00	0.44
1:A:144:GLY:H	1:A:166:VAL:HG11	1.81	0.44
1:A:1079:LYS:HA	1:A:1079:LYS:HD3	1.82	0.44
1:A:316:ILE:HA	1:A:320:LEU:HD23	1.99	0.44
1:A:480:LEU:HD12	1:A:484:ILE:HD12	1.99	0.44
1:A:242:VAL:O	1:A:246:LEU:HD22	2.17	0.43
1:A:273:ALA:CB	1:A:350:SER:CA	2.89	0.43
1:A:803:ARG:NH1	1:A:1071:TYR:O	2.51	0.43
1:A:496:LEU:HD23	1:A:518:ARG:HH11	1.82	0.43
1:A:126:ILE:HG23	1:A:399:GLN:HE22	1.83	0.43
1:A:774:ASP:OD1	1:A:775:ASP:N	2.51	0.43
1:A:729:ASN:OD1	1:A:740:PHE:N	2.45	0.43
1:A:273:ALA:HB2	1:A:351:HIS:N	2.33	0.43
1:A:731:LEU:HD12	1:A:1140:VAL:HG21	2.00	0.43
4:A:2501:ATP:O3A	4:A:2501:ATP:O1G	2.36	0.43
1:A:377:ILE:HG21	1:A:594:TYR:H	1.83	0.43
1:A:528:GLU:HG3	1:A:580:PRO:HG3	2.01	0.43
1:A:70:TYR:OH	1:A:100:ALA:O	2.33	0.43
1:A:236:MET:O	1:A:1181:TRP:CH2	2.71	0.43
1:A:835:ASP:OD2	1:A:835:ASP:N	2.52	0.42
1:A:1093:LYS:HA	1:A:1102:THR:HG22	2.00	0.42
4:A:2501:ATP:O4'	2:G:2008:C:H2'	2.19	0.42
1:A:120:VAL:HA	1:A:123:VAL:HG12	2.00	0.42
1:A:30:ALA:HB1	1:A:33:ASP:OD2	2.19	0.42
1:A:303:GLY:H	1:A:309:LYS:NZ	2.18	0.42
1:A:531:GLY:O	1:A:532:ILE:CD1	2.49	0.42
1:A:609:LYS:HA	1:A:628:LEU:HD21	2.01	0.42
1:A:719:VAL:HG21	1:A:723:LEU:HB2	2.02	0.42
1:A:800:THR:O	1:A:804:LEU:HB2	2.18	0.42
1:A:826:ARG:NH2	1:A:827:ARG:HG2	2.32	0.42
1:A:298:ASN:HD22	1:A:362:ALA:HB3	1.85	0.42
1:A:60:GLY:HA3	1:A:77:ASN:CB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:715:THR:O	1:A:1113:PRO:HD3	2.20	0.42
1:A:1116:LEU:HD22	1:A:1116:LEU:HA	1.88	0.42
1:A:1171:LEU:CD1	1:A:1171:LEU:H	2.31	0.42
1:A:1173:ASN:HA	1:A:1174:PRO:HD3	1.83	0.42
1:A:126:ILE:HG23	1:A:399:GLN:NE2	2.35	0.42
1:A:531:GLY:CA	1:A:532:ILE:HD13	2.50	0.42
1:A:723:LEU:HD23	1:A:1110:ILE:HG13	2.01	0.42
1:A:780:ILE:HG13	1:A:780:ILE:O	2.20	0.42
1:A:1069:PHE:HA	1:A:1072:VAL:HG22	2.02	0.42
1:A:734:ALA:O	1:A:1136:ARG:HB2	2.20	0.42
1:A:1141:TYR:O	1:A:1145:ARG:HB2	2.20	0.42
1:A:851:GLY:HA2	1:A:861:GLY:HA3	2.02	0.41
1:A:969:LEU:HD13	1:A:1074:PHE:HB3	2.03	0.41
1:A:496:LEU:HD13	1:A:578:ALA:HB2	2.01	0.41
1:A:797:CYS:O	1:A:801:ASN:ND2	2.53	0.41
1:A:10:LYS:HB3	1:A:10:LYS:HE2	1.68	0.41
1:A:315:ALA:HB1	1:A:473:ILE:HG12	2.03	0.41
1:A:369:HIS:CD2	1:A:406:LEU:HD23	2.55	0.41
1:A:717:ILE:CG1	1:A:718:GLU:H	2.30	0.41
1:A:155:LEU:O	1:A:256:PHE:HA	2.20	0.41
1:A:324:TYR:CD1	1:A:357:PRO:HD3	2.55	0.41
1:A:731:LEU:O	1:A:734:ALA:HB3	2.21	0.41
1:A:936:ASP:O	1:A:939:ARG:HB3	2.21	0.41
1:A:1111:VAL:HG13	1:A:1112:SER:N	2.36	0.41
1:A:4:ILE:HD11	1:A:28:THR:HA	2.03	0.41
1:A:23:CYS:O	1:A:27:LEU:HB2	2.20	0.41
1:A:169:ILE:O	1:A:173:VAL:HG23	2.20	0.41
1:A:387:ILE:HD12	1:A:416:ILE:HB	2.02	0.41
1:A:1105:TYR:N	1:A:1105:TYR:CD2	2.89	0.41
1:A:495:PHE:HA	1:A:519:GLY:HA3	2.01	0.41
1:A:614:GLN:HG3	1:A:623:THR:HG23	2.03	0.41
1:A:34:ILE:O	1:A:38:ILE:HG23	2.21	0.40
1:A:493:LYS:HB3	1:A:493:LYS:HE2	1.78	0.40
1:A:505:ILE:HB	1:A:508:ARG:HB2	2.03	0.40
1:A:837:PRO:HD3	1:A:989:TRP:CD2	2.55	0.40
1:A:268:VAL:O	1:A:268:VAL:CG1	2.69	0.40
1:A:304:HIS:CD2	1:A:305:VAL:N	2.89	0.40
1:A:312:LEU:O	1:A:316:ILE:HG13	2.21	0.40
1:A:425:VAL:HG13	1:A:430:LEU:HD23	2.03	0.40
1:A:59:ASP:OD2	1:A:81:ASP:CG	2.59	0.40
1:A:589:PHE:CE1	1:A:645:VAL:HB	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:867:PHE:CD1	1:A:1205:TYR:HB2	2.57	0.40
1:A:61:VAL:HG13	1:A:84:ALA:HB1	2.04	0.40
1:A:927:GLN:OE1	1:A:1020:GLY:N	2.20	0.40
1:A:1096:TYR:O	1:A:1099:VAL:HG12	2.22	0.40
1:A:1120:LEU:HB2	1:A:1166:LEU:HD21	2.04	0.40
1:A:1169:SER:O	1:A:1172:ILE:HB	2.22	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	1193/1289 (93%)	1049 (88%)	132 (11%)	12 (1%)	15 54

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	531	GLY
1	A	777	SER
1	A	895	SER
1	A	104	LYS
1	A	267	LYS
1	A	1263	SER
1	A	129	ASN
1	A	230	THR
1	A	367	PRO
1	A	1111	VAL
1	A	950	ILE
1	A	899	PRO

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	995/1060 (94%)	861 (86%)	134 (14%)	4 18

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LYS
1	A	31	ASN
1	A	33	ASP
1	A	38	ILE
1	A	75	GLU
1	A	76	VAL
1	A	81	ASP
1	A	86	ASP
1	A	94	ASP
1	A	97	LEU
1	A	98	ASP
1	A	117	GLU
1	A	133	ARG
1	A	143	LEU
1	A	165	LEU
1	A	195	TYR
1	A	197	VAL
1	A	199	LEU
1	A	203	MET
1	A	204	GLN
1	A	210	GLU
1	A	241	THR
1	A	246	LEU
1	A	248	GLU
1	A	249	HIS
1	A	250	ASN
1	A	256	PHE
1	A	258	ARG
1	A	265	ILE
1	A	267	LYS

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Mol	Chain	Res	Type
1	A	271	ASP
1	A	275	GLU
1	A	292	ARG
1	A	309	LYS
1	A	351	HIS
1	A	356	THR
1	A	382	GLN
1	A	384	ASP
1	A	387	ILE
1	A	397	MET
1	A	399	GLN
1	A	419	LEU
1	A	429	GLU
1	A	441	LEU
1	A	454	ILE
1	A	475	GLU
1	A	480	LEU
1	A	508	ARG
1	A	530	VAL
1	A	532	ILE
1	A	533	LYS
1	A	535	THR
1	A	537	LYS
1	A	541	THR
1	A	547	ARG
1	A	550	LEU
1	A	568	ARG
1	A	603	ARG
1	A	623	THR
1	A	642	LYS
1	A	646	THR
1	A	647	LEU
1	A	654	ASP
1	A	666	ARG
1	A	676	VAL
1	A	677	LEU
1	A	678	SER
1	A	705	LEU
1	A	710	ARG
1	A	726	SER
1	A	758	ASP
1	A	762	ILE

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Mol	Chain	Res	Type
1	A	771	SER
1	A	776	PHE
1	A	780	ILE
1	A	808	ASP
1	A	809	TYR
1	A	813	PHE
1	A	831	LYS
1	A	832	LEU
1	A	835	ASP
1	A	836	VAL
1	A	843	LEU
1	A	848	PHE
1	A	858	ARG
1	A	874	THR
1	A	892	ILE
1	A	894	ILE
1	A	897	ILE
1	A	901	ASN
1	A	902	LYS
1	A	905	THR
1	A	906	VAL
1	A	930	ILE
1	A	933	ILE
1	A	934	LEU
1	A	936	ASP
1	A	939	ARG
1	A	943	ILE
1	A	980	LEU
1	A	993	LEU
1	A	1012	GLU
1	A	1014	ILE
1	A	1028	LEU
1	A	1041	LEU
1	A	1053	ASP
1	A	1076	THR
1	A	1080	LYS
1	A	1089	GLU
1	A	1099	VAL
1	A	1105	TYR
1	A	1106	ILE
1	A	1108	HIS
1	A	1110	ILE

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Mol	Chain	Res	Type
1	A	1116	LEU
1	A	1123	LEU
1	A	1130	ASP
1	A	1136	ARG
1	A	1140	VAL
1	A	1145	ARG
1	A	1147	LEU
1	A	1148	LEU
1	A	1150	LYS
1	A	1171	LEU
1	A	1172	ILE
1	A	1178	ASN
1	A	1182	ILE
1	A	1193	ARG
1	A	1194	ASP
1	A	1204	LEU
1	A	1235	ILE
1	A	1238	LEU
1	A	1239	ILE
1	A	1241	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	A	298	ASN
1	A	304	HIS
1	A	399	GLN
1	A	862	HIS
1	A	901	ASN
1	A	1153	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	G	4/8 (50%)	0	0
3	T	5/8 (62%)	1 (20%)	0
All	All	9/16 (56%)	1 (11%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	T	2105	A

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ATP	A	2501	5	26,33,33	1.13	2 (7%)	31,52,52	1.64	7 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	A	2501	5	-	8/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2501	ATP	C5-C4	2.72	1.48	1.40
4	A	2501	ATP	O4'-C1'	2.52	1.44	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2501	ATP	N3-C2-N1	-3.76	122.81	128.68
4	A	2501	ATP	PA-O3A-PB	-3.76	119.93	132.83
4	A	2501	ATP	C4-C5-N7	-3.16	106.11	109.40
4	A	2501	ATP	C3'-C2'-C1'	2.85	105.26	100.98
4	A	2501	ATP	O5'-C5'-C4'	-2.71	99.66	108.99
4	A	2501	ATP	PB-O3B-PG	-2.67	123.66	132.83
4	A	2501	ATP	O5'-PA-O1A	-2.09	100.91	109.07

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2501	ATP	C5'-O5'-PA-O1A
4	A	2501	ATP	C5'-O5'-PA-O2A
4	A	2501	ATP	PG-O3B-PB-O3A
4	A	2501	ATP	PB-O3B-PG-O3G
4	A	2501	ATP	PA-O3A-PB-O1B
4	A	2501	ATP	C5'-O5'-PA-O3A
4	A	2501	ATP	PG-O3B-PB-O1B
4	A	2501	ATP	PA-O3A-PB-O2B

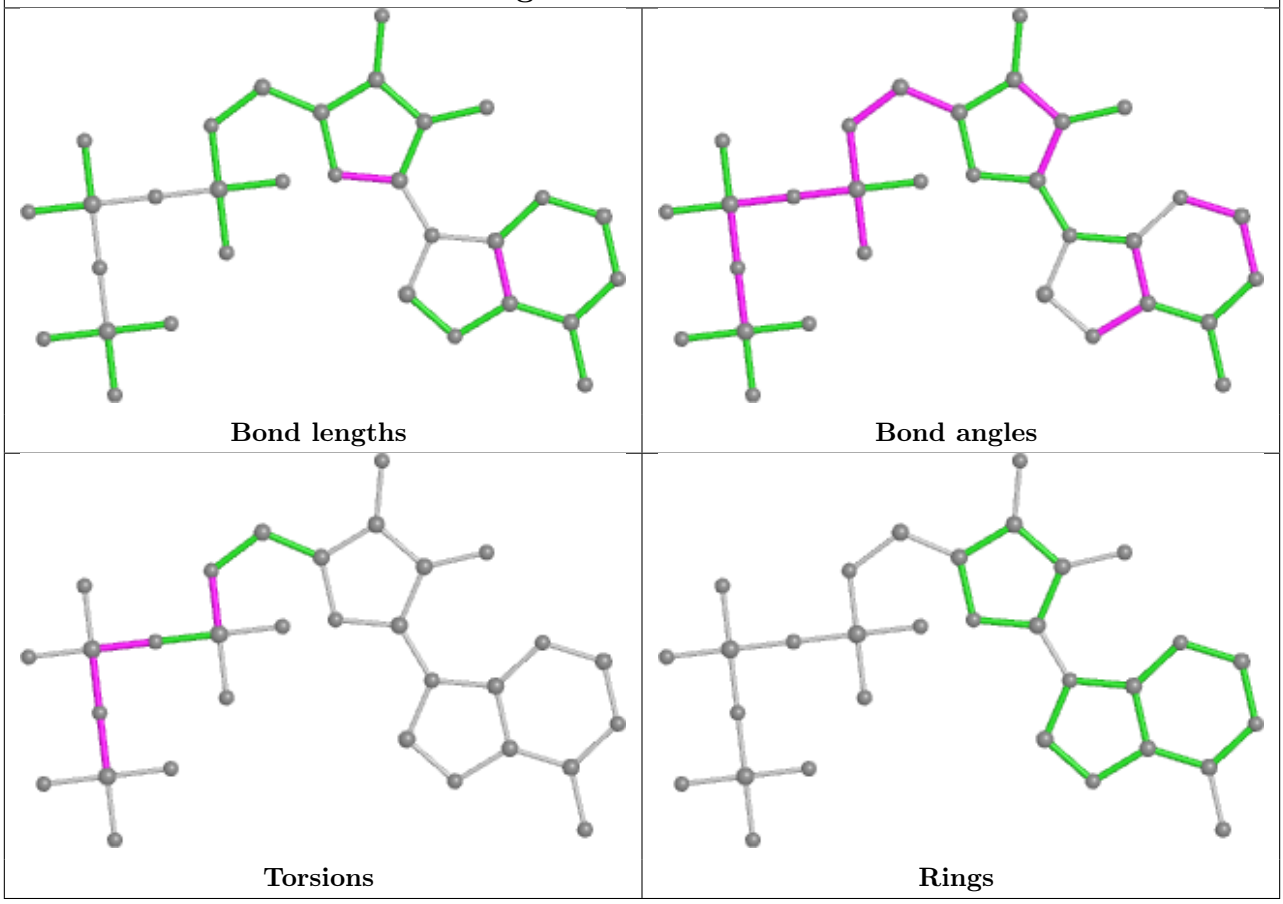
There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2501	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 A 2501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	1203/1289 (93%)	-0.14	30 (2%) 57 43	34, 80, 121, 166	0
2	G	6/8 (75%)	-0.04	0 100 100	111, 150, 174, 181	0
3	T	6/8 (75%)	-0.26	0 100 100	106, 129, 133, 157	0
All	All	1215/1305 (93%)	-0.14	30 (2%) 57 43	34, 80, 123, 181	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	326	GLY	6.0
1	A	701	SER	4.7
1	A	743	GLU	4.2
1	A	5	THR	4.2
1	A	161	ALA	3.9
1	A	163	GLU	3.7
1	A	162	ASP	3.7
1	A	101	VAL	3.7
1	A	6	ALA	3.4
1	A	268	VAL	3.1
1	A	700	SER	3.0
1	A	322	LYS	2.9
1	A	320	LEU	2.8
1	A	316	ILE	2.8
1	A	680	ALA	2.8
1	A	520	ILE	2.7
1	A	4	ILE	2.6
1	A	314	ALA	2.6
1	A	512	VAL	2.4
1	A	521	ILE	2.4
1	A	267	LYS	2.4
1	A	561	VAL	2.4
1	A	1234	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	313	THR	2.3
1	A	350	SER	2.2
1	A	476	LEU	2.2
1	A	352	VAL	2.1
1	A	3	GLU	2.0
1	A	102	ALA	2.0
1	A	354	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

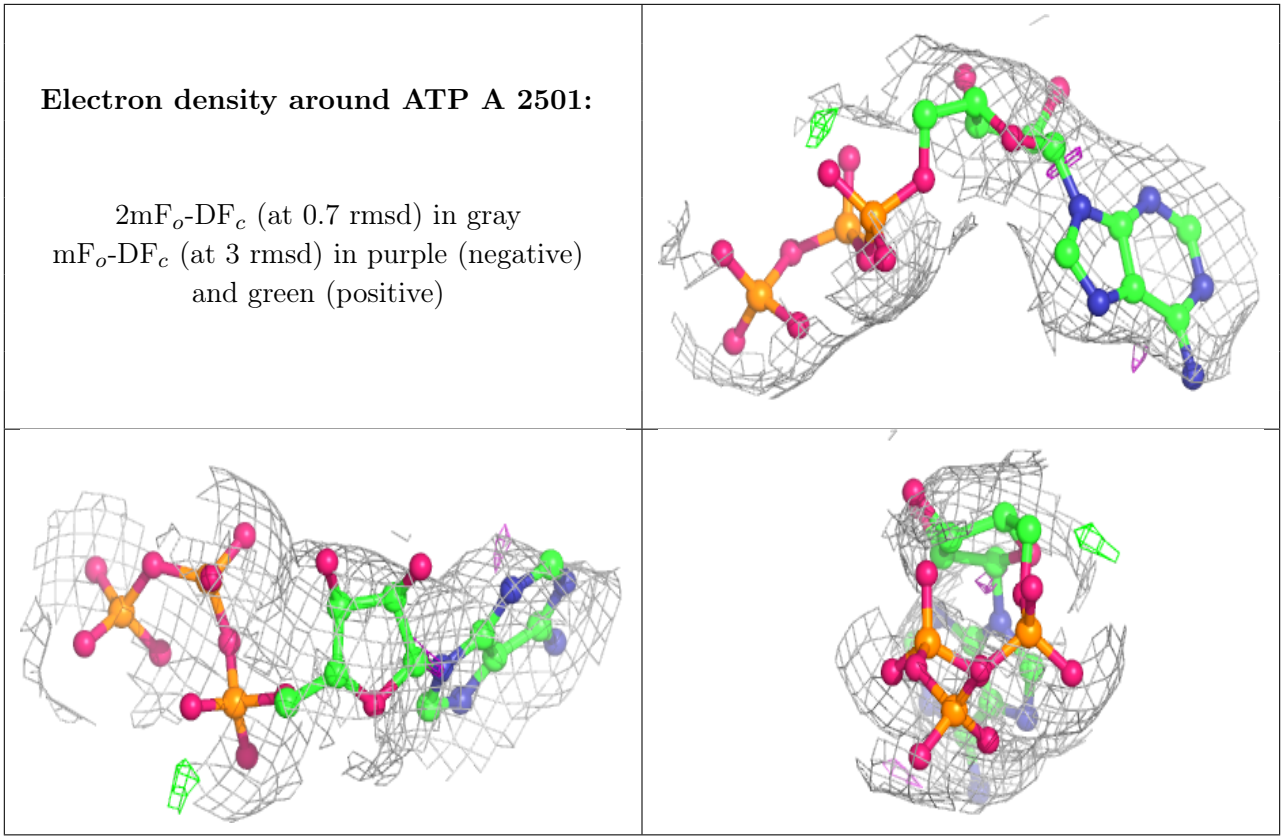
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ATP	A	2501	31/31	0.94	0.19	63,79,96,105	0
5	CA	A	2502	1/1	0.98	0.20	52,52,52,52	0
5	CA	A	2503	1/1	0.98	0.20	33,33,33,33	0

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

Electron density around ATP A 2501:

$2mF_o$-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.