



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:22 PM UTC

PDB ID : 4Q5S / pdb_00004q5s
Title : Thermus thermophilus RNA polymerase initially transcribing complex containing 6-mer RNA
Authors : Murakami, K.S.
Deposited on : 2014-04-17
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

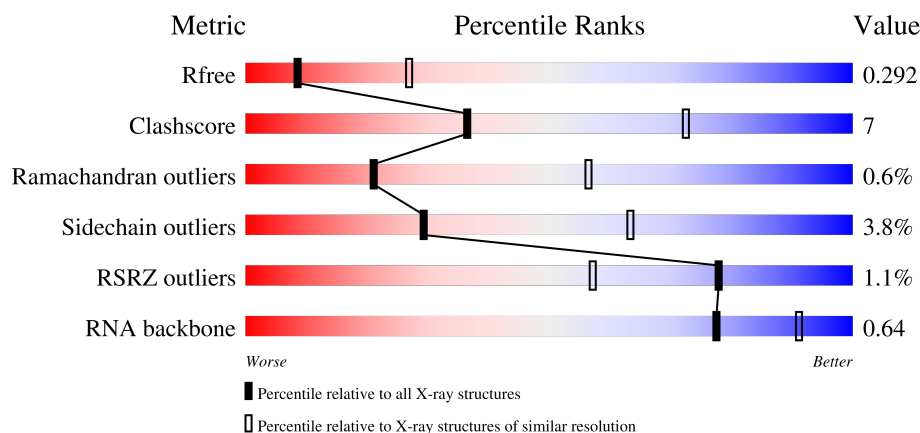
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	315	2% 58% 13% 28%
1	B	315	59% 10% 30%
2	C	1119	2% 77% 21% ..
3	D	1524	77% 19% ..

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Mol	Chain	Length	Quality of chain
4	E	99	% 81%13%5%
5	F	423	2% 62%16%20%
6	G	22	5% 32%27%5%36%
7	H	27	37%22%41%
8	I	5	60%40%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 28290 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1782	1138	310	332	2			
1	B	222	Total	C	N	O	S	0	0	0
			1750	1118	304	326	2			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1111	Total	C	N	O	S	0	0	0
			8770	5548	1564	1634	24			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1484	Total	C	N	O	S	0	0	0
			11722	7430	2064	2192	36			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	94	Total	C	N	O	S	0	0	0
			761	486	132	139	4			

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	338	Total	C	N	O	S	0	0	0
			2747	1736	500	507	4			

- Molecule 6 is a DNA chain called DNA (5'-D(*CP*CP*TP*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*GP*CP*AP*GP*CP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	14	Total	C	N	O	P	0	0	0
			289	137	52	86	14			

- Molecule 7 is a DNA chain called DNA (5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	16	Total	C	N	O	P	0	0	0
			333	159	66	93	15			

- Molecule 8 is a RNA chain called RNA (5'-R(P*CP*UP*CP*AP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	5	Total	C	N	O	P	0	0	0
			102	46	16	35	5			

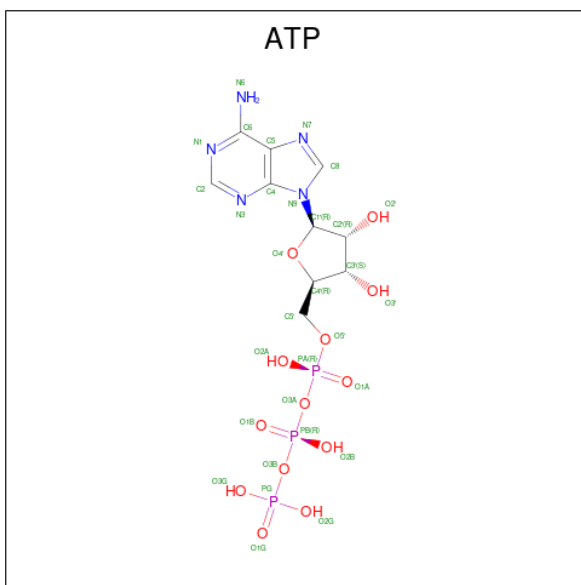
- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	1	Total	Mg	0	0
			1	1		

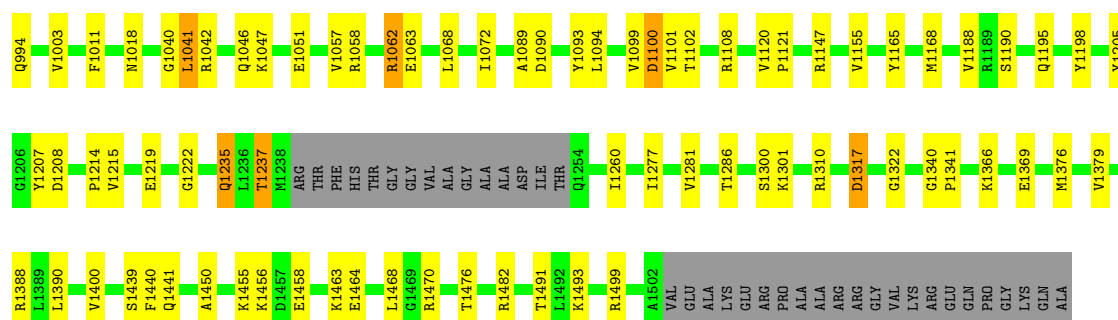
- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	2	Total	Zn	0	0
			2	2		

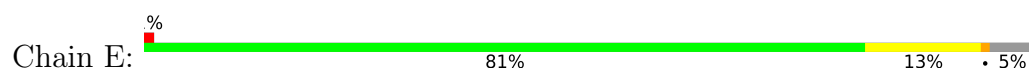
- Molecule 11 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



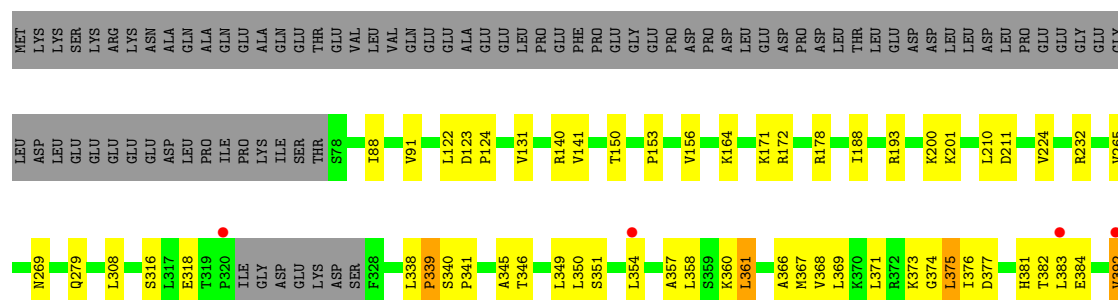
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	I	1	Total 31	C 10	N 5	O 13	P 3	0	0



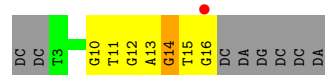
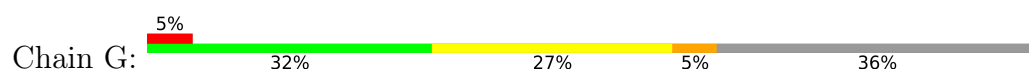
• Molecule 4: DNA-directed RNA polymerase subunit omega



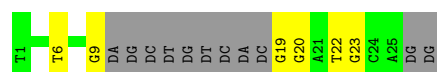
• Molecule 5: RNA polymerase sigma factor SigA



• Molecule 6: DNA (5'-D(*CP*CP*TP*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*GP*CP*AP*GP*CP*CP*A)-3')



• Molecule 7: DNA (5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*AP*GP*G)-3')



- Molecule 8: RNA (5'-R(P*CP*UP*CP*AP*C)-3')

Chain I:  60% 40%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	187.09Å 102.08Å 297.26Å 90.00° 98.14° 90.00°	Depositor
Resolution (Å)	41.98 – 3.00 41.98 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.3 (41.98-3.00) 90.6 (41.98-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1563)	Depositor
R, R_{free}	0.269 , 0.294 0.274 , 0.292	Depositor DCC
R_{free} test set	1883 reflections (1.65%)	wwPDB-VP
Wilson B-factor (Å ²)	59.4	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	28290	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, 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	0.27	0/1814	0.77	0/2466
1	B	0.27	0/1782	0.78	0/2424
2	C	0.27	0/8937	0.75	6/12087 (0.0%)
3	D	0.27	0/11928	0.73	6/16127 (0.0%)
4	E	0.26	0/775	0.76	0/1045
5	F	0.30	1/2791 (0.0%)	0.75	1/3754 (0.0%)
6	G	0.32	0/323	0.65	1/497 (0.2%)
7	H	0.10	0/374	0.52	0/575
8	I	0.60	0/112	0.55	0/171
All	All	0.27	1/28836 (0.0%)	0.74	14/39146 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	339	PRO	C-N	-8.09	1.20	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	14	DG	O3'-P-O5'	-7.10	93.35	104.00
2	C	766	GLU	CA-C-N	6.36	127.79	119.84
2	C	766	GLU	C-N-CA	6.36	127.79	119.84
3	D	1018	ASN	CA-C-N	6.24	125.73	119.24
3	D	1018	ASN	C-N-CA	6.24	125.73	119.24
5	F	339	PRO	O-C-N	-6.14	115.73	123.10
3	D	65	ARG	N-CA-C	5.89	116.02	108.24
3	D	1237	THR	N-CA-C	-5.42	105.97	113.18
2	C	501	THR	CA-C-N	5.17	126.30	119.84
2	C	501	THR	C-N-CA	5.17	126.30	119.84
2	C	154	ARG	CA-C-N	5.05	124.22	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	154	ARG	C-N-CA	5.05	124.22	118.97
3	D	1340	GLY	CA-C-N	5.03	124.20	118.97
3	D	1340	GLY	C-N-CA	5.03	124.20	118.97

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	1782	0	1834	26	0
1	B	1750	0	1797	22	0
2	C	8770	0	8874	157	0
3	D	11722	0	11949	168	0
4	E	761	0	778	9	0
5	F	2747	0	2831	80	0
6	G	289	0	159	9	0
7	H	333	0	183	6	0
8	I	102	0	55	3	0
9	D	1	0	0	0	0
10	D	2	0	0	0	0
11	I	31	0	11	2	0
All	All	28290	0	28471	409	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 7.

All (409) 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)
2:C:776:SER:CB	5:F:373:LYS:NZ	2.02	1.23
2:C:769:PRO:HG2	5:F:374:GLY:O	1.40	1.19
2:C:776:SER:HB2	5:F:373:LYS:NZ	1.58	1.19
2:C:769:PRO:CG	5:F:374:GLY:O	1.93	1.17
3:D:233:LYS:NZ	3:D:240:GLU:OE2	1.88	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:776:SER:CB	5:F:373:LYS:HZ3	1.65	1.02
2:C:776:SER:HB2	5:F:373:LYS:HZ3	0.86	1.01
2:C:776:SER:OG	5:F:373:LYS:NZ	1.94	0.97
5:F:392:VAL:CG1	5:F:396:ARG:HB2	2.05	0.86
6:G:16:DG:H8	6:G:16:DG:H5''	1.41	0.85
5:F:368:VAL:HG21	5:F:400:ILE:HG21	1.63	0.80
2:C:774:LEU:HD22	5:F:350:LEU:HD11	1.63	0.79
5:F:392:VAL:HG22	5:F:396:ARG:HD2	1.65	0.79
2:C:776:SER:CB	5:F:373:LYS:HZ2	1.82	0.78
3:D:671:LYS:HE2	5:F:346:THR:HG21	1.66	0.77
3:D:256:GLU:OE1	3:D:274:ARG:NH1	2.19	0.75
5:F:392:VAL:HG13	5:F:396:ARG:HB2	1.69	0.74
5:F:360:LYS:HD3	5:F:411:HIS:ND1	2.02	0.73
3:D:61:GLY:O	3:D:64:LYS:NZ	2.21	0.73
5:F:371:LEU:HD23	5:F:376:ILE:HD12	1.70	0.72
2:C:577:PRO:HG2	2:C:580:MET:HG2	1.72	0.72
2:C:776:SER:CB	5:F:373:LYS:CE	2.68	0.72
2:C:769:PRO:CG	5:F:374:GLY:C	2.63	0.71
5:F:358:LEU:CD2	5:F:366:ALA:HB1	2.21	0.70
6:G:16:DG:H8	6:G:16:DG:C5'	2.04	0.70
1:A:56:VAL:HG22	1:A:142:VAL:HG12	1.73	0.69
5:F:392:VAL:HG11	5:F:396:ARG:HB2	1.74	0.68
5:F:200:LYS:HG3	5:F:201:LYS:HG3	1.76	0.68
3:D:260:GLU:OE1	3:D:273:ARG:NH1	2.27	0.68
3:D:256:GLU:HG3	3:D:300:LYS:HG3	1.76	0.67
3:D:132:TYR:OH	3:D:568:ARG:NH2	2.28	0.67
6:G:15:DT:O4	11:I:101:ATP:N6	2.24	0.67
2:C:243:ARG:NH2	7:H:9:DG:O6	2.27	0.67
5:F:384:GLU:HG2	5:F:394:ARG:CZ	2.25	0.67
2:C:521:PRO:HB3	3:D:1068:LEU:HD21	1.77	0.66
2:C:557:ARG:HG3	2:C:844:GLY:HA3	1.76	0.66
1:B:88:ARG:NH1	1:B:123:MET:SD	2.68	0.66
3:D:800:LYS:HB3	3:D:822:ALA:HB2	1.76	0.66
2:C:793:PRO:HB2	2:C:796:GLU:HG3	1.77	0.66
3:D:704:ARG:NH2	8:I:5:A:O2'	2.29	0.65
2:C:769:PRO:HB2	5:F:375:LEU:HA	1.77	0.65
1:A:55:SER:HB3	1:A:143:ARG:HB3	1.78	0.65
2:C:905:ILE:HG23	2:C:906:PHE:HD1	1.61	0.65
2:C:154:ARG:NH2	2:C:176:VAL:O	2.31	0.64
2:C:769:PRO:HG3	5:F:374:GLY:O	1.91	0.64
3:D:17:LYS:O	3:D:20:SER:OG	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:358:LEU:HD22	5:F:366:ALA:HB1	1.80	0.64
3:D:455:ARG:HB2	3:D:460:ALA:HB2	1.80	0.63
2:C:236:ILE:HG23	2:C:248:PRO:HB2	1.80	0.63
3:D:411:THR:HB	3:D:437:VAL:H	1.62	0.63
2:C:769:PRO:HB3	5:F:374:GLY:C	2.23	0.63
2:C:683:ASN:HB3	2:C:872:ASN:HB2	1.80	0.62
2:C:281:LEU:HD13	2:C:305:PRO:HB2	1.82	0.62
2:C:17:PRO:HB2	2:C:20:GLU:HB3	1.81	0.62
2:C:710:ILE:HD12	2:C:790:LEU:HB2	1.82	0.62
2:C:614:ARG:NH2	2:C:618:GLY:O	2.32	0.62
2:C:711:GLU:O	2:C:758:ARG:NH1	2.32	0.62
3:D:671:LYS:HE2	5:F:346:THR:CG2	2.30	0.62
3:D:960:LYS:NZ	3:D:1063:GLU:OE1	2.32	0.61
5:F:371:LEU:CD2	5:F:376:ILE:HD12	2.30	0.61
1:A:222:LEU:HD22	1:B:215:VAL:HG23	1.84	0.59
2:C:769:PRO:CB	5:F:375:LEU:HA	2.31	0.59
2:C:846:LYS:NZ	8:I:5:A:OP1	2.30	0.59
3:D:136:ASP:OD2	3:D:138:LYS:HE3	2.02	0.59
2:C:640:ARG:NH1	2:C:657:ASP:O	2.35	0.59
5:F:392:VAL:HG22	5:F:396:ARG:CD	2.33	0.59
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.83	0.59
2:C:413:LEU:HD21	2:C:451:LEU:HD13	1.86	0.58
3:D:1468:LEU:HB3	3:D:1470:ARG:HG3	1.86	0.58
2:C:251:ASP:OD1	2:C:251:ASP:N	2.36	0.58
2:C:939:ARG:HB2	2:C:982:PRO:HG3	1.84	0.58
6:G:16:DG:H5''	6:G:16:DG:C8	2.31	0.58
2:C:769:PRO:HA	2:C:772:ARG:HB2	1.84	0.58
3:D:1491:THR:HG21	4:E:89:MET:HG2	1.86	0.58
2:C:270:GLY:O	2:C:274:ARG:N	2.35	0.58
2:C:683:ASN:HB3	2:C:872:ASN:HD22	1.68	0.58
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.86	0.58
2:C:769:PRO:CB	5:F:374:GLY:C	2.76	0.58
2:C:846:LYS:HE3	3:D:741:ASP:HB2	1.86	0.58
3:D:241:ILE:HG12	3:D:312:ARG:NH1	2.19	0.57
3:D:431:VAL:HG21	3:D:448:GLU:HG2	1.86	0.57
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.86	0.57
5:F:338:LEU:HD23	5:F:339:PRO:HD2	1.85	0.57
3:D:1047:LYS:HD2	3:D:1051:GLU:HG3	1.85	0.57
2:C:595:LEU:HB3	2:C:656:ALA:HB3	1.86	0.57
1:B:84:GLU:OE2	3:D:867:ARG:NH1	2.36	0.57
2:C:904:PRO:HD2	2:C:908:GLY:HA2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:177:GLU:HG3	2:C:178:PRO:HD2	1.85	0.57
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.37	0.57
5:F:420:ASP:O	5:F:422:LEU:N	2.36	0.57
3:D:173:PRO:HA	3:D:209:ARG:HH12	1.70	0.57
7:H:19:DG:H2''	7:H:20:DG:H5'	1.87	0.56
2:C:12:VAL:HG21	2:C:472:ARG:HD3	1.87	0.56
3:D:372:ASP:OD1	3:D:372:ASP:N	2.38	0.56
5:F:360:LYS:HD3	5:F:411:HIS:CE1	2.39	0.56
2:C:422:ARG:HG2	7:H:19:DG:OP2	2.06	0.56
5:F:358:LEU:HD23	5:F:366:ALA:HB1	1.86	0.56
1:B:112:ARG:HB3	1:B:125:PRO:HB2	1.88	0.56
3:D:433:GLY:HA2	3:D:449:SER:H	1.71	0.56
5:F:350:LEU:HD13	5:F:421:PHE:CD1	2.41	0.56
5:F:415:THR:HB	5:F:417:LYS:HE3	1.87	0.56
3:D:216:VAL:HG23	3:D:383:GLY:HA2	1.88	0.55
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.89	0.55
1:B:206:THR:HG22	1:B:209:GLU:H	1.71	0.55
2:C:770:GLU:OE1	5:F:351:SER:OG	2.24	0.55
3:D:619:LEU:HD11	3:D:1439:SER:HB2	1.87	0.55
3:D:244:GLU:HG3	3:D:310:LEU:HG	1.89	0.55
2:C:397:GLU:HG3	2:C:631:SER:HB2	1.89	0.54
3:D:573:MET:SD	5:F:210:LEU:HB3	2.46	0.54
2:C:759:THR:HB	2:C:785:VAL:HB	1.89	0.54
3:D:171:LEU:HD22	3:D:390:PRO:HG2	1.90	0.54
3:D:968:ASP:OD1	3:D:1058:ARG:NH2	2.41	0.54
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.88	0.54
2:C:615:TYR:HH	2:C:623:TYR:HH	1.49	0.54
3:D:1101:VAL:HG13	3:D:1102:THR:HG23	1.88	0.54
3:D:563:PRO:HD2	3:D:566:ILE:HD12	1.88	0.54
6:G:16:DG:C5'	6:G:16:DG:C8	2.88	0.54
2:C:208:ALA:HB2	2:C:222:MET:HE1	1.89	0.54
2:C:428:ARG:NH2	2:C:447:ALA:O	2.39	0.54
2:C:1052:MET:HG3	3:D:623:VAL:HG11	1.89	0.54
3:D:504:ASP:OD1	3:D:1388:ARG:NH2	2.41	0.54
5:F:345:ALA:O	5:F:349:LEU:HG	2.07	0.54
1:B:94:LEU:HD21	1:B:97:VAL:HG13	1.90	0.54
2:C:911:GLU:OE2	3:D:1062:ARG:NH1	2.41	0.53
5:F:392:VAL:HG12	5:F:397:ILE:HG12	1.90	0.53
2:C:129:ILE:HG12	2:C:386:PHE:HB3	1.90	0.53
2:C:69:LEU:HD12	2:C:97:ARG:HG2	1.90	0.53
2:C:971:LYS:HB3	2:C:986:PRO:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:996:LYS:HE2	2:C:1000:MET:HE2	1.89	0.53
3:D:192:ALA:HB3	3:D:195:VAL:HB	1.90	0.53
3:D:241:ILE:HG12	3:D:312:ARG:HH12	1.72	0.53
3:D:9:ARG:HB2	3:D:1456:LYS:HG2	1.90	0.53
5:F:164:LYS:HA	5:F:171:LYS:HE3	1.90	0.53
1:B:88:ARG:NH2	1:B:121:GLU:OE1	2.42	0.53
1:B:138:LEU:HD11	1:B:140:MET:HE3	1.90	0.53
3:D:67:ARG:NH1	5:F:377:ASP:OD1	2.42	0.53
3:D:86:ARG:HB3	3:D:522:PRO:HG2	1.91	0.53
2:C:87:ASP:HA	2:C:131:GLY:HA3	1.91	0.52
3:D:119:SER:HB3	3:D:122:GLU:HG3	1.90	0.52
3:D:236:TYR:HD2	3:D:322:VAL:HG21	1.74	0.52
2:C:286:SER:OG	2:C:301:GLU:OE1	2.28	0.52
3:D:657:LEU:HG	3:D:661:MET:HE2	1.92	0.52
5:F:396:ARG:HA	5:F:399:GLN:HG2	1.91	0.52
5:F:404:ALA:O	5:F:408:LEU:HG	2.10	0.52
3:D:520:LEU:O	3:D:525:ARG:NH1	2.43	0.52
2:C:769:PRO:CB	5:F:374:GLY:O	2.56	0.51
2:C:1095:LEU:HD23	3:D:582:LEU:HD22	1.92	0.51
3:D:339:TRP:HE1	3:D:341:GLU:HG3	1.74	0.51
3:D:822:ALA:HB3	3:D:825:ALA:HB2	1.92	0.51
1:A:94:LEU:O	1:A:146:ARG:NH1	2.34	0.51
3:D:128:TYR:OH	3:D:579:ASP:OD2	2.26	0.51
3:D:486:ARG:HA	3:D:489:ARG:HH21	1.76	0.51
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.93	0.51
2:C:546:LEU:HB2	2:C:565:GLN:HE22	1.76	0.51
2:C:775:ARG:HG2	2:C:782:ALA:HB2	1.93	0.51
3:D:693:GLU:HA	4:E:48:MET:HE1	1.91	0.51
1:A:54:THR:HB	1:A:158:ILE:HD12	1.93	0.51
2:C:133:ASP:HB2	2:C:632:ASN:HD21	1.74	0.51
2:C:740:GLU:OE1	2:C:805:ARG:NH1	2.44	0.51
2:C:774:LEU:HD22	5:F:350:LEU:CD1	2.37	0.50
2:C:942:GLU:HG3	2:C:945:ARG:HH21	1.75	0.50
3:D:102:ILE:HD12	3:D:579:ASP:HB3	1.92	0.50
2:C:631:SER:HB3	2:C:637:LEU:HG	1.93	0.50
3:D:622:ARG:NH1	6:G:13:DA:OP1	2.43	0.50
2:C:175:GLU:O	2:C:183:SER:OG	2.24	0.50
2:C:578:VAL:HG23	2:C:579:VAL:HG23	1.93	0.50
3:D:1219:GLU:OE1	4:E:17:TYR:OH	2.24	0.50
3:D:601:ARG:HD3	5:F:318:GLU:HG2	1.93	0.50
3:D:923:GLY:O	3:D:927:THR:OG1	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1168:MET:HE3	3:D:1168:MET:HA	1.94	0.50
5:F:188:ILE:HG12	5:F:224:VAL:HG21	1.94	0.50
2:C:92:ALA:HB2	2:C:120:LEU:HD11	1.94	0.50
2:C:541:SER:OG	2:C:542:VAL:N	2.37	0.50
2:C:109:LYS:HG2	2:C:368:THR:HG22	1.92	0.50
2:C:16:PRO:HB3	2:C:460:ARG:HH21	1.76	0.49
3:D:710:ARG:HH21	3:D:772:PRO:HG3	1.77	0.49
5:F:265:VAL:O	5:F:269:ASN:ND2	2.31	0.49
1:A:4:SER:O	1:A:189:ARG:NH2	2.45	0.49
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.93	0.49
3:D:462:GLN:HB2	3:D:513:ILE:HG21	1.94	0.49
3:D:474:GLU:HG3	3:D:496:LEU:HD11	1.93	0.49
3:D:1450:ALA:HA	3:D:1455:LYS:HD2	1.94	0.49
2:C:160:ALA:HB2	2:C:310:LEU:HD13	1.94	0.49
2:C:504:GLU:HG2	2:C:509:ALA:HB2	1.93	0.49
3:D:500:ARG:HH12	3:D:1390:LEU:HD21	1.77	0.49
1:B:80:LEU:HD11	3:D:842:VAL:HG12	1.95	0.49
2:C:397:GLU:N	2:C:633:GLN:OE1	2.42	0.49
1:A:44:LEU:HB3	1:A:177:VAL:HG21	1.93	0.49
3:D:218:LYS:HG2	3:D:338:GLU:HG2	1.95	0.49
2:C:740:GLU:HB3	2:C:805:ARG:HH12	1.78	0.49
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	1.94	0.48
3:D:675:ARG:NH2	5:F:420:ASP:O	2.46	0.48
2:C:764:GLU:HB2	3:D:54:LYS:NZ	2.28	0.48
2:C:769:PRO:HB3	5:F:375:LEU:N	2.27	0.48
2:C:1001:VAL:HB	3:D:724:GLN:HB2	1.94	0.48
3:D:231:VAL:O	3:D:236:TYR:OH	2.31	0.48
1:A:26:GLU:HB2	1:A:194:LYS:HG3	1.96	0.48
1:A:218:LEU:HD23	1:B:222:LEU:HD21	1.94	0.48
3:D:323:GLU:HB2	3:D:334:THR:HB	1.96	0.48
2:C:537:LYS:HD3	2:C:583:LEU:HD11	1.95	0.47
1:A:124:ASN:OD1	1:A:124:ASN:N	2.47	0.47
2:C:776:SER:HB3	5:F:373:LYS:CE	2.44	0.47
3:D:759:ALA:HA	3:D:763:MET:HB2	1.96	0.47
3:D:1235:GLN:C	3:D:1237:THR:H	2.21	0.47
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.48	0.47
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.48	0.47
3:D:899:LEU:HD21	3:D:921:ARG:HD3	1.97	0.47
2:C:271:GLU:OE1	2:C:274:ARG:NH1	2.47	0.47
2:C:324:ASP:HB3	2:C:327:HIS:HB2	1.96	0.47
3:D:661:MET:HE3	3:D:673:ALA:HB1	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:703:ASN:HB2	3:D:713:ILE:HG12	1.96	0.47
1:A:99:LEU:HB2	1:A:142:VAL:HG23	1.96	0.47
1:A:215:VAL:HG13	1:B:222:LEU:HD22	1.96	0.47
1:B:78:ILE:HG21	1:B:140:MET:HE1	1.95	0.47
2:C:495:THR:OG1	2:C:517:ARG:NE	2.47	0.47
2:C:769:PRO:HG3	5:F:374:GLY:C	2.38	0.47
3:D:224:ARG:NE	3:D:254:GLU:OE2	2.47	0.47
3:D:284:LEU:HD22	3:D:288:MET:HG2	1.97	0.47
3:D:644:LEU:HD12	3:D:645:PRO:HD2	1.97	0.47
1:B:175:ARG:N	1:B:200:TRP:O	2.43	0.47
2:C:778:PHE:CD1	5:F:412:GLU:OE2	2.68	0.47
3:D:564:GLU:OE2	5:F:140:ARG:NH2	2.47	0.47
5:F:340:SER:HB2	5:F:341:PRO:HD2	1.97	0.47
5:F:357:ALA:O	5:F:361:LEU:HG	2.15	0.47
1:A:83:LYS:NZ	2:C:698:ASP:OD2	2.48	0.47
2:C:399:ASN:O	2:C:402:SER:OG	2.32	0.47
3:D:1300:SER:OG	3:D:1301:LYS:N	2.48	0.47
3:D:526:PRO:HB2	3:D:528:VAL:HG13	1.97	0.46
3:D:1100:ASP:OD1	3:D:1463:LYS:NZ	2.36	0.46
3:D:1208:ASP:HB2	3:D:1215:VAL:HA	1.97	0.46
3:D:520:LEU:HD12	3:D:521:PRO:HD2	1.98	0.46
2:C:351:LEU:HD21	2:C:373:VAL:HG13	1.97	0.46
3:D:485:SER:O	3:D:487:ALA:N	2.49	0.46
3:D:959:GLU:N	3:D:959:GLU:OE1	2.48	0.46
2:C:637:LEU:HA	2:C:659:PRO:HG3	1.97	0.46
2:C:983:ILE:O	2:C:985:GLY:N	2.42	0.46
1:A:54:THR:HG21	1:A:145:ASP:HB2	1.98	0.46
2:C:680:ASP:H	3:D:943:THR:HB	1.80	0.46
2:C:686:ASP:OD1	2:C:879:ARG:NH1	2.35	0.46
4:E:47:LYS:HB3	4:E:54:LEU:HG	1.96	0.46
7:H:19:DG:H2''	7:H:20:DG:H2'	1.98	0.46
2:C:595:LEU:HD21	2:C:623:TYR:HB3	1.97	0.46
3:D:1003:VAL:HG21	3:D:1041:LEU:HG	1.97	0.46
3:D:1147:ARG:NH2	3:D:1369:GLU:OE1	2.44	0.46
1:A:220:GLU:O	1:A:223:THR:OG1	2.34	0.46
1:B:32:PHE:HA	1:B:35:THR:HB	1.98	0.46
2:C:503:LEU:HD23	2:C:508:ILE:HA	1.99	0.45
3:D:233:LYS:HB2	3:D:236:TYR:CZ	2.51	0.45
2:C:709:GLU:HG3	2:C:824:ARG:HG2	1.98	0.45
5:F:357:ALA:HB1	5:F:408:LEU:HD22	1.97	0.45
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ARG:HB3	1:B:190:THR:HG23	1.98	0.45
2:C:884:GLN:O	2:C:888:THR:OG1	2.30	0.45
3:D:355:VAL:HG11	3:D:385:VAL:HG21	1.98	0.45
5:F:384:GLU:HG2	5:F:394:ARG:NH1	2.31	0.45
2:C:876:VAL:HG11	3:D:949:ILE:HG21	1.98	0.45
3:D:7:LYS:NZ	3:D:1458:GLU:OE1	2.49	0.45
3:D:312:ARG:HH11	3:D:312:ARG:HB3	1.81	0.45
3:D:977:ALA:O	3:D:983:LEU:N	2.45	0.45
2:C:21:ILE:HD12	2:C:455:LEU:HD22	1.97	0.45
2:C:35:PRO:HG2	2:C:38:LYS:HD3	1.99	0.45
5:F:357:ALA:HB1	5:F:408:LEU:CD2	2.47	0.45
2:C:769:PRO:HG2	3:D:65:ARG:NH1	2.31	0.45
3:D:131:LYS:HD3	3:D:152:LEU:HB3	1.97	0.45
2:C:727:PRO:HB2	2:C:728:HIS:HD2	1.80	0.45
3:D:661:MET:HG2	3:D:666:ILE:HD12	1.99	0.45
1:B:124:ASN:OD1	1:B:124:ASN:N	2.49	0.45
2:C:1059:ASP:O	2:C:1063:ARG:N	2.42	0.45
3:D:804:LEU:H	3:D:827:ILE:HG22	1.82	0.45
5:F:340:SER:HB2	5:F:341:PRO:CD	2.47	0.45
5:F:367:MET:SD	5:F:376:ILE:HD11	2.57	0.45
2:C:164:PRO:HA	2:C:269:LEU:HD12	1.98	0.44
2:C:502:PRO:HD2	2:C:510:ALA:HB2	1.99	0.44
2:C:577:PRO:HB3	2:C:993:PHE:CG	2.52	0.44
3:D:539:ASP:OD1	5:F:316:SER:OG	2.26	0.44
3:D:1341:PRO:HB3	3:D:1376:MET:HE2	1.99	0.44
2:C:419:THR:H	2:C:422:ARG:HB2	1.83	0.44
3:D:224:ARG:H	3:D:251:PHE:HE1	1.64	0.44
4:E:40:LEU:HG	4:E:67:GLU:HG2	1.99	0.44
5:F:360:LYS:HB3	5:F:411:HIS:CE1	2.53	0.44
1:A:58:ILE:HG21	1:A:68:ILE:HD11	1.99	0.44
3:D:1089:ALA:HA	6:G:10:DG:C8	2.53	0.44
4:E:57:ASP:O	4:E:63:TRP:NE1	2.49	0.44
1:A:31:GLY:O	1:A:35:THR:OG1	2.28	0.44
3:D:704:ARG:HB2	3:D:745:MET:HE2	2.00	0.44
2:C:987:ILE:HD11	3:D:946:GLY:HA2	2.00	0.44
3:D:187:LYS:HB2	3:D:200:ASP:OD2	2.17	0.44
3:D:224:ARG:NH1	3:D:254:GLU:OE2	2.50	0.44
1:A:99:LEU:HD21	1:A:122:ILE:HD11	2.00	0.44
4:E:3:GLU:HA	4:E:4:PRO:HD3	1.90	0.44
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.18	0.43
2:C:230:ARG:HB2	2:C:233:GLU:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:THR:HG22	1:A:209:GLU:H	1.83	0.43
2:C:194:VAL:HG22	2:C:221:LEU:HD22	1.99	0.43
2:C:673:LEU:HD23	2:C:867:VAL:HA	2.00	0.43
2:C:724:ARG:NH2	2:C:734:LEU:O	2.51	0.43
3:D:350:HIS:CD2	5:F:232:ARG:HG2	2.53	0.43
3:D:1165:TYR:CZ	3:D:1214:PRO:HB3	2.53	0.43
2:C:214:TYR:CD2	2:C:218:VAL:HG23	2.54	0.43
3:D:1499:ARG:HH12	4:E:81:PRO:HD2	1.83	0.43
5:F:413:SER:HA	5:F:416:ARG:HG2	2.00	0.43
2:C:492:ASP:HB3	2:C:518:LYS:HG2	2.00	0.43
3:D:1093:TYR:OH	3:D:1441:GLN:NE2	2.35	0.43
3:D:1379:VAL:HG21	3:D:1400:VAL:HG11	2.00	0.43
3:D:787:LEU:HD21	3:D:947:ILE:HG21	1.99	0.43
3:D:809:PRO:HB3	3:D:839:LEU:HD13	2.00	0.43
3:D:1094:LEU:HD22	3:D:1260:ILE:HG12	2.00	0.43
5:F:201:LYS:HE3	5:F:201:LYS:HB2	1.89	0.43
1:A:202:ASP:OD1	1:A:203:GLY:N	2.52	0.43
3:D:339:TRP:NE1	3:D:341:GLU:HG3	2.34	0.43
3:D:1281:VAL:HG22	3:D:1317:ASP:H	1.84	0.43
2:C:439:CYS:HA	2:C:440:PRO:HD3	1.82	0.43
2:C:617:ASP:HB2	2:C:619:ARG:HG2	2.00	0.43
2:C:627:ARG:HD3	2:C:638:ASP:OD1	2.19	0.43
2:C:938:LYS:HE2	2:C:938:LYS:HB3	1.89	0.43
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	2.01	0.43
2:C:474:VAL:HG22	2:C:479:VAL:HG22	2.01	0.43
2:C:1031:ARG:NH2	3:D:620:GLY:O	2.44	0.43
2:C:1101:THR:OG1	2:C:1109:VAL:O	2.36	0.43
3:D:828:LYS:HG2	3:D:833:GLU:HG2	2.01	0.43
5:F:131:VAL:HG13	5:F:178:ARG:HD3	2.00	0.43
2:C:937:ASP:HB3	2:C:940:GLU:HG3	2.00	0.42
3:D:827:ILE:HB	3:D:829:VAL:HG23	2.00	0.42
3:D:954:ALA:HB3	3:D:1062:ARG:HG3	1.99	0.42
5:F:360:LYS:HD3	5:F:411:HIS:CG	2.54	0.42
3:D:84:ILE:HG13	3:D:88:TYR:HE1	1.84	0.42
2:C:144:PRO:HB2	2:C:273:GLY:HA3	2.00	0.42
3:D:171:LEU:HA	3:D:172:PRO:HD3	1.95	0.42
2:C:928:LYS:O	2:C:932:GLU:HB2	2.19	0.42
3:D:260:GLU:HB3	3:D:271:VAL:HB	2.01	0.42
5:F:123:ASP:HA	5:F:124:PRO:HD3	1.91	0.42
5:F:377:ASP:CG	5:F:381:HIS:HE2	2.22	0.42
1:B:97:VAL:HG23	1:B:144:VAL:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:245:LEU:HD22	3:D:249:TYR:HB3	2.01	0.42
3:D:711:LEU:HB3	3:D:714:GLN:HE21	1.85	0.42
2:C:390:GLN:HG3	11:I:101:ATP:H4'	2.02	0.42
3:D:961:LYS:HE3	3:D:961:LYS:HB2	1.91	0.42
2:C:229:MET:HB2	2:C:233:GLU:HB2	2.01	0.42
2:C:810:ASP:HA	2:C:811:PRO:HD3	1.90	0.42
3:D:214:GLU:HB3	3:D:340:THR:HB	2.00	0.42
3:D:238:PRO:HD3	3:D:318:ARG:HG3	2.02	0.42
3:D:714:GLN:HB2	3:D:736:PHE:HZ	1.84	0.42
3:D:795:VAL:HG12	3:D:876:SER:HB3	2.02	0.42
1:A:227:ASN:HA	1:A:228:PRO:HD3	1.77	0.42
2:C:214:TYR:CE2	2:C:311:PHE:HB3	2.54	0.42
2:C:462:ASP:OD2	2:C:468:ARG:NH1	2.52	0.42
3:D:266:GLU:HG3	3:D:314:PRO:HB3	2.02	0.42
2:C:261:ILE:HG23	2:C:290:LEU:HB2	2.01	0.42
3:D:273:ARG:HB3	3:D:278:PRO:HA	2.01	0.42
3:D:527:MET:SD	3:D:537:THR:HB	2.60	0.42
3:D:1205:TYR:CE1	3:D:1366:LYS:HE2	2.55	0.42
2:C:691:SER:HA	2:C:858:MET:HE3	2.02	0.41
3:D:39:PRO:HG3	3:D:47:GLU:HG3	2.01	0.41
3:D:1190:SER:OG	3:D:1369:GLU:OE1	2.38	0.41
1:A:199:ILE:HB	1:A:207:PRO:HB3	2.00	0.41
2:C:1054:THR:OG1	2:C:1055:LEU:N	2.53	0.41
3:D:58:CYS:SG	3:D:62:LYS:N	2.92	0.41
3:D:87:ARG:HG2	3:D:523:ASP:HB2	2.03	0.41
3:D:1102:THR:O	3:D:1222:GLY:HA3	2.20	0.41
2:C:510:ALA:HB3	2:C:513:VAL:HG12	2.02	0.41
2:C:905:ILE:C	2:C:907:ASP:H	2.28	0.41
2:C:944:LEU:HD23	2:C:944:LEU:HA	1.95	0.41
3:D:553:ARG:HH12	5:F:211:ASP:HA	1.84	0.41
7:H:22:DT:H2''	7:H:23:DG:C8	2.55	0.41
2:C:122:THR:OG1	2:C:124:ASP:OD1	2.29	0.41
2:C:572:ILE:HG13	2:C:573:ARG:HG2	2.01	0.41
3:D:230:TRP:CZ2	3:D:232:GLU:HG2	2.55	0.41
6:G:14:DG:N2	8:I:2:C:O2	2.52	0.41
1:B:51:THR:OG1	1:B:87:VAL:O	2.23	0.41
2:C:327:HIS:CE1	2:C:433:THR:HG21	2.55	0.41
2:C:376:ARG:NH2	5:F:279:GLN:OE1	2.54	0.41
3:D:48:ARG:NE	3:D:76:CYS:O	2.54	0.41
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.53	0.41
3:D:896:ALA:O	3:D:900:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:802:ARG:HB2	2:C:826:TYR:HB2	2.02	0.41
3:D:890:VAL:HB	3:D:922:LEU:HD13	2.02	0.41
5:F:91:VAL:O	5:F:193:ARG:NH2	2.38	0.41
1:B:18:ARG:NH1	1:B:204:SER:O	2.53	0.41
2:C:35:PRO:HA	2:C:36:PRO:HD3	1.85	0.41
2:C:224:GLU:CD	2:C:224:GLU:H	2.28	0.41
2:C:1036:GLU:OE2	2:C:1036:GLU:N	2.52	0.41
3:D:272:LEU:HB2	3:D:280:ALA:HB3	2.03	0.41
3:D:321:GLN:HB2	3:D:336:PHE:CD2	2.56	0.41
2:C:657:ASP:OD2	2:C:663:ASN:N	2.50	0.41
1:A:70:GLY:H	2:C:607:ASP:CG	2.29	0.41
1:A:91:ASN:HA	1:A:92:PRO:HD3	1.91	0.41
2:C:1067:TYR:OH	3:D:674:ARG:NH1	2.54	0.41
3:D:222:GLY:HA2	3:D:333:LEU:O	2.21	0.41
3:D:374:GLU:C	3:D:376:GLU:H	2.29	0.41
3:D:750:PRO:O	3:D:756:GLN:NE2	2.54	0.41
4:E:14:ASP:OD2	4:E:14:ASP:N	2.52	0.41
1:B:77:GLU:HG2	3:D:872:ARG:HH11	1.86	0.41
2:C:543:ASN:OD1	2:C:543:ASN:N	2.53	0.41
2:C:1090:LYS:HA	2:C:1090:LYS:HD3	1.93	0.40
3:D:350:HIS:HD2	5:F:232:ARG:HG2	1.85	0.40
5:F:308:LEU:HD23	5:F:308:LEU:HA	1.94	0.40
6:G:11:DT:H2'	6:G:12:DG:C8	2.56	0.40
2:C:405:ARG:HH21	2:C:566:THR:HG21	1.85	0.40
3:D:1120:VAL:HA	3:D:1121:PRO:HD3	1.88	0.40
2:C:283:ILE:HD13	2:C:305:PRO:HG2	2.02	0.40
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.56	0.40
3:D:508:ARG:HA	3:D:509:PRO:HD3	1.98	0.40
3:D:629:SER:HB3	3:D:726:ILE:HG13	2.03	0.40
3:D:935:LYS:HE2	3:D:935:LYS:HB3	1.88	0.40
5:F:193:ARG:HB2	7:H:6:DT:H1'	2.02	0.40
5:F:350:LEU:O	5:F:354:LEU:HG	2.21	0.40
2:C:501:THR:HA	2:C:502:PRO:HD3	1.99	0.40
3:D:897:TRP:CH2	3:D:902:LEU:HD22	2.57	0.40
3:D:1090:ASP:OD1	3:D:1090:ASP:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	224/315 (71%)	209 (93%)	15 (7%)	0	100	100
1	B	220/315 (70%)	207 (94%)	12 (6%)	1 (0%)	24	60
2	C	1107/1119 (99%)	1029 (93%)	70 (6%)	8 (1%)	18	53
3	D	1480/1524 (97%)	1393 (94%)	77 (5%)	10 (1%)	18	53
4	E	92/99 (93%)	89 (97%)	3 (3%)	0	100	100
5	F	334/423 (79%)	316 (95%)	16 (5%)	2 (1%)	21	56
All	All	3457/3795 (91%)	3243 (94%)	193 (6%)	21 (1%)	21	56

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	F	421	PHE
2	C	12	VAL
2	C	211	LEU
3	D	448	GLU
3	D	484	PRO
5	F	361	LEU
2	C	365	ASP
2	C	984	GLU
3	D	320	ALA
3	D	486	ARG
3	D	1440	PHE
1	B	191	ASP
2	C	477	GLY
3	D	530	VAL
2	C	212	GLY
2	C	767	PRO
3	D	665	GLY
3	D	1322	GLY
2	C	769	PRO
3	D	1040	GLY

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Mol	Chain	Res	Type
3	D	668	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	199/273 (73%)	196 (98%)	3 (2%)	57	80
1	B	195/273 (71%)	189 (97%)	6 (3%)	35	68
2	C	936/941 (100%)	902 (96%)	34 (4%)	31	65
3	D	1251/1279 (98%)	1197 (96%)	54 (4%)	26	60
4	E	83/88 (94%)	81 (98%)	2 (2%)	43	73
5	F	294/371 (79%)	281 (96%)	13 (4%)	25	60
All	All	2958/3225 (92%)	2846 (96%)	112 (4%)	29	63

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	LEU
1	A	148	VAL
1	A	206	THR
1	B	80	LEU
1	B	94	LEU
1	B	158	ILE
1	B	186	LEU
1	B	206	THR
1	B	221	HIS
2	C	37	GLU
2	C	55	GLU
2	C	81	ASP
2	C	103	LYS
2	C	113	VAL
2	C	143	SER
2	C	194	VAL
2	C	205	GLU

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Mol	Chain	Res	Type
2	C	214	TYR
2	C	251	ASP
2	C	261	ILE
2	C	285	LEU
2	C	348	LEU
2	C	364	GLU
2	C	442	GLU
2	C	480	THR
2	C	483	VAL
2	C	511	GLU
2	C	513	VAL
2	C	524	VAL
2	C	539	VAL
2	C	581	THR
2	C	584	GLU
2	C	633	GLN
2	C	640	ARG
2	C	644	VAL
2	C	680	ASP
2	C	715	THR
2	C	796	GLU
2	C	801	VAL
2	C	813	VAL
2	C	905	ILE
2	C	939	ARG
2	C	1001	VAL
3	D	32	ILE
3	D	33	ASN
3	D	53	ILE
3	D	64	LYS
3	D	65	ARG
3	D	106	LYS
3	D	141	ILE
3	D	171	LEU
3	D	186	VAL
3	D	198	ARG
3	D	204	LEU
3	D	230	TRP
3	D	231	VAL
3	D	256	GLU
3	D	272	LEU
3	D	312	ARG

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Mol	Chain	Res	Type
3	D	331	VAL
3	D	360	ARG
3	D	372	ASP
3	D	415	VAL
3	D	578	VAL
3	D	632	VAL
3	D	737	ASN
3	D	754	PHE
3	D	810	GLU
3	D	813	LEU
3	D	817	GLU
3	D	864	VAL
3	D	884	ARG
3	D	894	LYS
3	D	904	VAL
3	D	907	GLU
3	D	940	THR
3	D	972	LEU
3	D	974	ILE
3	D	994	GLN
3	D	1011	PHE
3	D	1041	LEU
3	D	1046	GLN
3	D	1062	ARG
3	D	1100	ASP
3	D	1155	VAL
3	D	1188	VAL
3	D	1195	GLN
3	D	1207	TYR
3	D	1235	GLN
3	D	1277	ILE
3	D	1286	THR
3	D	1310	ARG
3	D	1317	ASP
3	D	1464	GLU
3	D	1476	THR
3	D	1482	ARG
3	D	1493	LYS
4	E	50	THR
4	E	54	LEU
5	F	88	ILE
5	F	122	LEU

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Mol	Chain	Res	Type
5	F	141	VAL
5	F	150	THR
5	F	172	ARG
5	F	369	LEU
5	F	375	LEU
5	F	382	THR
5	F	383	LEU
5	F	392	VAL
5	F	394	ARG
5	F	400	ILE
5	F	420	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	212	ASN
2	C	31	GLN
2	C	117	HIS
2	C	187	ASN
2	C	330	ASN
2	C	506	ASN
2	C	556	ASN
2	C	565	GLN
2	C	632	ASN
2	C	728	HIS
2	C	999	HIS
2	C	1026	GLN
2	C	1030	GLN
2	C	1050	GLN
3	D	33	ASN
3	D	294	HIS
3	D	350	HIS
3	D	611	GLN
3	D	714	GLN
3	D	724	GLN
3	D	744	GLN
3	D	1124	GLN
3	D	1202	GLN
3	D	1235	GLN
3	D	1359	GLN
4	E	33	HIS
5	F	218	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	4/5 (80%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 3 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
11	ATP	I	101	-	32,33,33	1.61	1 (3%)	48,52,52	0.86	1 (2%)

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
11	ATP	I	101	-	-	4/22/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	I	101	ATP	C5'-C4'	-8.23	1.26	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	I	101	ATP	C5'-C4'-C3'	-3.95	100.98	115.21

There are no chirality outliers.

All (4) torsion outliers are listed below:

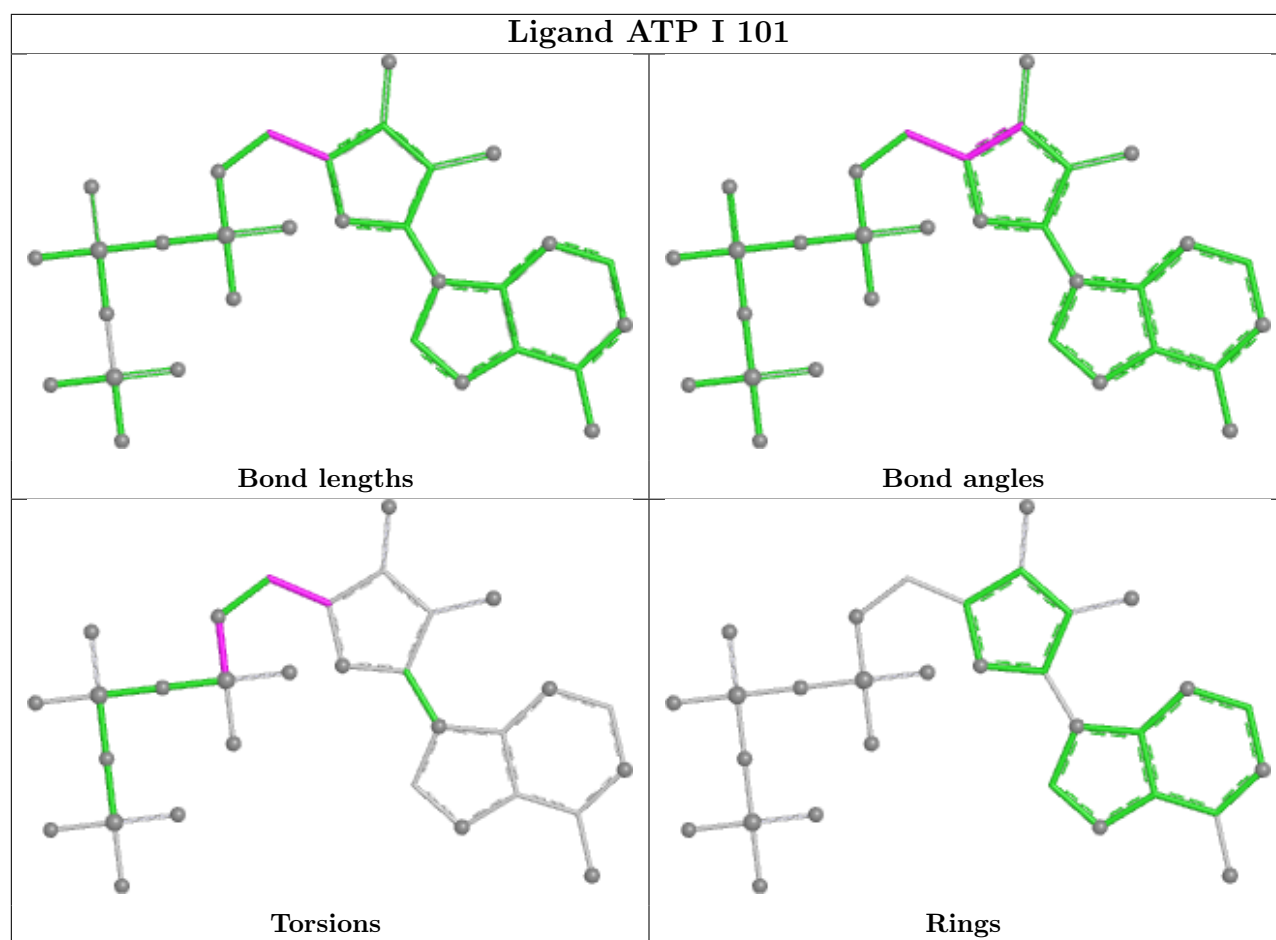
Mol	Chain	Res	Type	Atoms
11	I	101	ATP	C5'-O5'-PA-O3A
11	I	101	ATP	O4'-C4'-C5'-O5'
11	I	101	ATP	C3'-C4'-C5'-O5'
11	I	101	ATP	C5'-O5'-PA-O1A

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	I	101	ATP	2	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	226/315 (71%)	0.20	3 (1%) 75 53	76, 116, 149, 155	0
1	B	222/315 (70%)	-0.02	1 (0%) 87 72	63, 90, 119, 133	0
2	C	1111/1119 (99%)	0.22	18 (1%) 70 47	28, 107, 187, 229	0
3	D	1484/1524 (97%)	0.07	6 (0%) 88 76	30, 90, 161, 225	1 (0%)
4	E	94/99 (94%)	0.09	1 (1%) 78 57	64, 100, 177, 190	0
5	F	338/423 (79%)	0.35	7 (2%) 63 40	94, 135, 226, 265	0
6	G	14/22 (63%)	0.36	1 (7%) 22 11	78, 106, 188, 200	0
7	H	16/27 (59%)	0.23	0 100 100	126, 135, 179, 183	0
8	I	5/5 (100%)	-0.45	0 100 100	60, 65, 75, 76	0
All	All	3510/3849 (91%)	0.15	37 (1%) 78 57	28, 104, 177, 265	1 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	422	LEU	3.3
2	C	536	PRO	3.3
5	F	400	ILE	3.2
1	B	157	GLY	3.2
2	C	107	LEU	3.1
6	G	16	DG	2.9
2	C	211	LEU	2.9
3	D	412	GLY	2.9
3	D	268	ALA	2.8
3	D	282	TYR	2.6
2	C	998	TYR	2.5
5	F	383	LEU	2.5
2	C	68	PHE	2.5
5	F	392	VAL	2.4
2	C	448	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
4	E	94	PRO	2.3
3	D	565	ILE	2.3
2	C	773	LEU	2.3
2	C	1061	GLU	2.2
2	C	196	LEU	2.2
5	F	354	LEU	2.2
2	C	311	PHE	2.2
3	D	184	GLU	2.2
5	F	408	LEU	2.2
1	A	64	GLU	2.2
2	C	593	ALA	2.2
2	C	594	ALA	2.2
1	A	97	VAL	2.2
2	C	65	VAL	2.2
1	A	55	SER	2.2
2	C	272	ALA	2.2
5	F	320	PRO	2.2
2	C	254	VAL	2.1
2	C	322	VAL	2.1
3	D	355	VAL	2.1
2	C	255	ALA	2.0
2	C	777	ILE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	ATP	I	101	31/31	0.58	0.11	72,98,200,233	0

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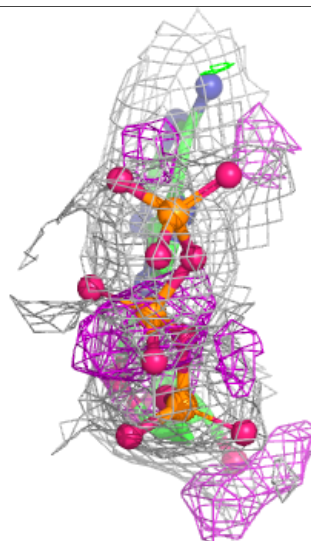
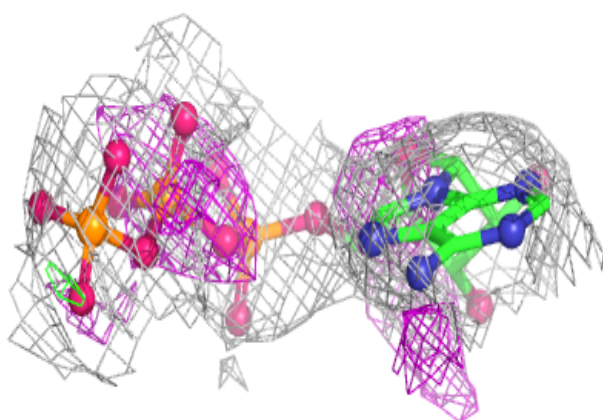
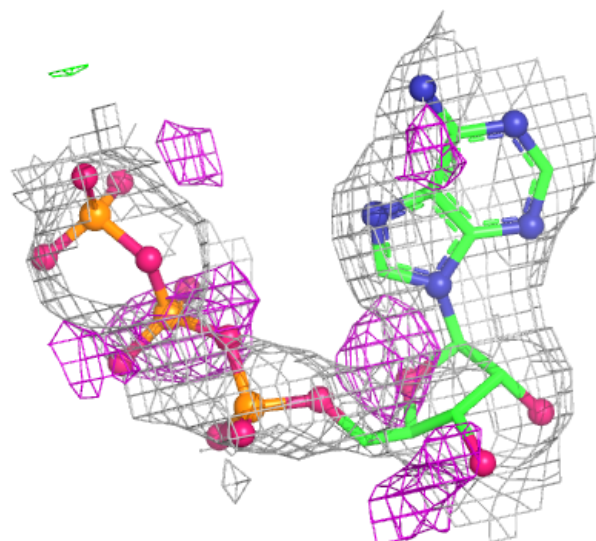
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	ZN	D	2002	1/1	0.98	0.10	238,238,238,238	0
10	ZN	D	2003	1/1	0.99	0.02	47,47,47,47	0
9	MG	D	2001	1/1	0.99	0.04	24,24,24,24	0

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 I 101:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.