Full wwPDB X-ray Structure Validation Report (i)

Feb 21, 2024 – 05:24 AM EST

PDB ID	:	4NH0
Title	:	Cytoplasmic domain of the Thermomonospora curvata Type VII Secretion ATPase EccC
Authors	:	Rosenberg, O.S.; Cox, J.S.; Stroud, R.M.; Strauli, N.; Dovala, D.
Deposited on	:	2013-11-03
Resolution	:	2.90 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:

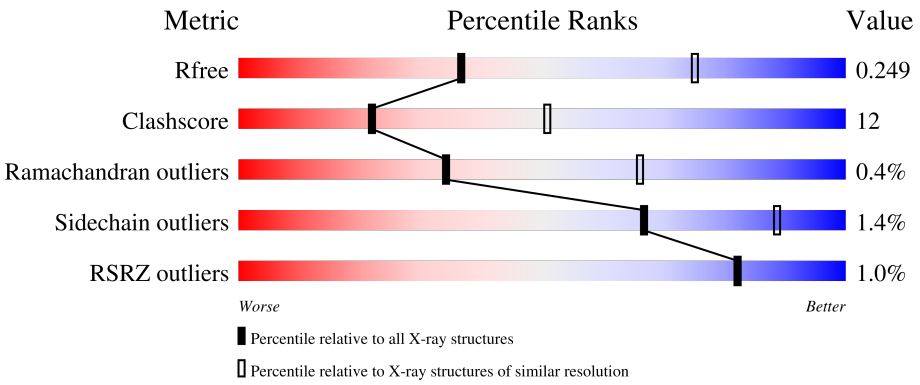
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	1147	60% 14% 25%
1	B	1147	% 56% 17% • 25%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13435 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 Cell divisionFtsK/SpoIIIE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	861	6663	4212	1181	1249	21	0	0	0
1	B	859	6626	4186	1175	1244	21	0	0	0

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	169	MET	-	expression tag	UNP D1A4G7
A	170	HIS	-	expression tag	UNP D1A4G7
A	171	HIS	-	expression tag	UNP D1A4G7
A	172	HIS	-	expression tag	UNP D1A4G7
A	173	HIS	-	expression tag	UNP D1A4G7
A	174	HIS	-	expression tag	UNP D1A4G7
A	175	HIS	-	expression tag	UNP D1A4G7
A	176	HIS	-	expression tag	UNP D1A4G7
A	177	HIS	-	expression tag	UNP D1A4G7
A	178	GLY	-	expression tag	UNP D1A4G7
A	179	GLY	-	expression tag	UNP D1A4G7
A	180	SER	-	expression tag	UNP D1A4G7
A	181	GLU	-	expression tag	UNP D1A4G7
A	182	PHE	-	expression tag	UNP D1A4G7
A	183	SER	-	expression tag	UNP D1A4G7
A	184	ILE	-	expression tag	UNP D1A4G7
A	185	ASP	-	expression tag	UNP D1A4G7
A	186	GLY	-	expression tag	UNP D1A4G7
A	187	GLY	-	expression tag	UNP D1A4G7
A	188	SER	-	expression tag	UNP D1A4G7
A	189	LEU	-	expression tag	UNP D1A4G7
A	190	GLU	-	expression tag	UNP D1A4G7
A	191	VAL	-	expression tag	UNP D1A4G7
A	192	LEU	-	expression tag	UNP D1A4G7
A	193	PHE	-	expression tag	UNP D1A4G7

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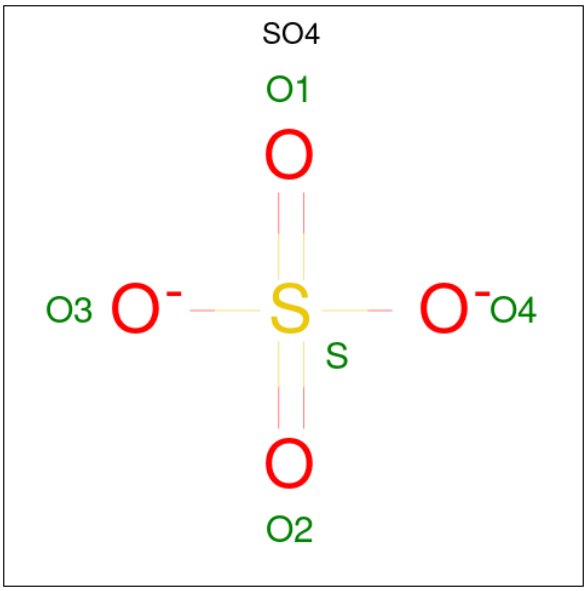
Chain	Residue	Modelled	Actual	Comment	Reference
A	194	GLN	-	expression tag	UNP D1A4G7
A	195	GLY	-	expression tag	UNP D1A4G7
A	196	PRO	-	expression tag	UNP D1A4G7
A	197	SER	-	expression tag	UNP D1A4G7
A	198	SER	-	expression tag	UNP D1A4G7
A	199	PRO	-	expression tag	UNP D1A4G7
B	169	MET	-	expression tag	UNP D1A4G7
B	170	HIS	-	expression tag	UNP D1A4G7
B	171	HIS	-	expression tag	UNP D1A4G7
B	172	HIS	-	expression tag	UNP D1A4G7
B	173	HIS	-	expression tag	UNP D1A4G7
B	174	HIS	-	expression tag	UNP D1A4G7
B	175	HIS	-	expression tag	UNP D1A4G7
B	176	HIS	-	expression tag	UNP D1A4G7
B	177	HIS	-	expression tag	UNP D1A4G7
B	178	GLY	-	expression tag	UNP D1A4G7
B	179	GLY	-	expression tag	UNP D1A4G7
B	180	SER	-	expression tag	UNP D1A4G7
B	181	GLU	-	expression tag	UNP D1A4G7
B	182	PHE	-	expression tag	UNP D1A4G7
B	183	SER	-	expression tag	UNP D1A4G7
B	184	ILE	-	expression tag	UNP D1A4G7
B	185	ASP	-	expression tag	UNP D1A4G7
B	186	GLY	-	expression tag	UNP D1A4G7
B	187	GLY	-	expression tag	UNP D1A4G7
B	188	SER	-	expression tag	UNP D1A4G7
B	189	LEU	-	expression tag	UNP D1A4G7
B	190	GLU	-	expression tag	UNP D1A4G7
B	191	VAL	-	expression tag	UNP D1A4G7
B	192	LEU	-	expression tag	UNP D1A4G7
B	193	PHE	-	expression tag	UNP D1A4G7
B	194	GLN	-	expression tag	UNP D1A4G7
B	195	GLY	-	expression tag	UNP D1A4G7
B	196	PRO	-	expression tag	UNP D1A4G7
B	197	SER	-	expression tag	UNP D1A4G7
B	198	SER	-	expression tag	UNP D1A4G7
B	199	PRO	-	expression tag	UNP D1A4G7

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

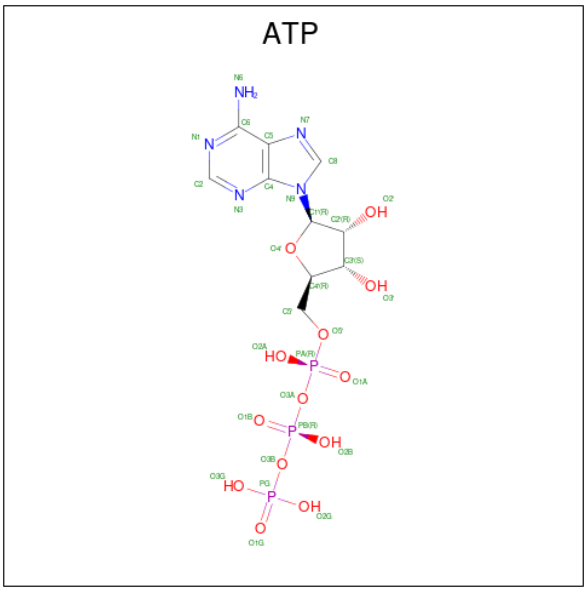


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Mg 2 2	0	0
3	B	2	Total Mg 2 2	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	0	0
			31	10	5	13	3		
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is water.

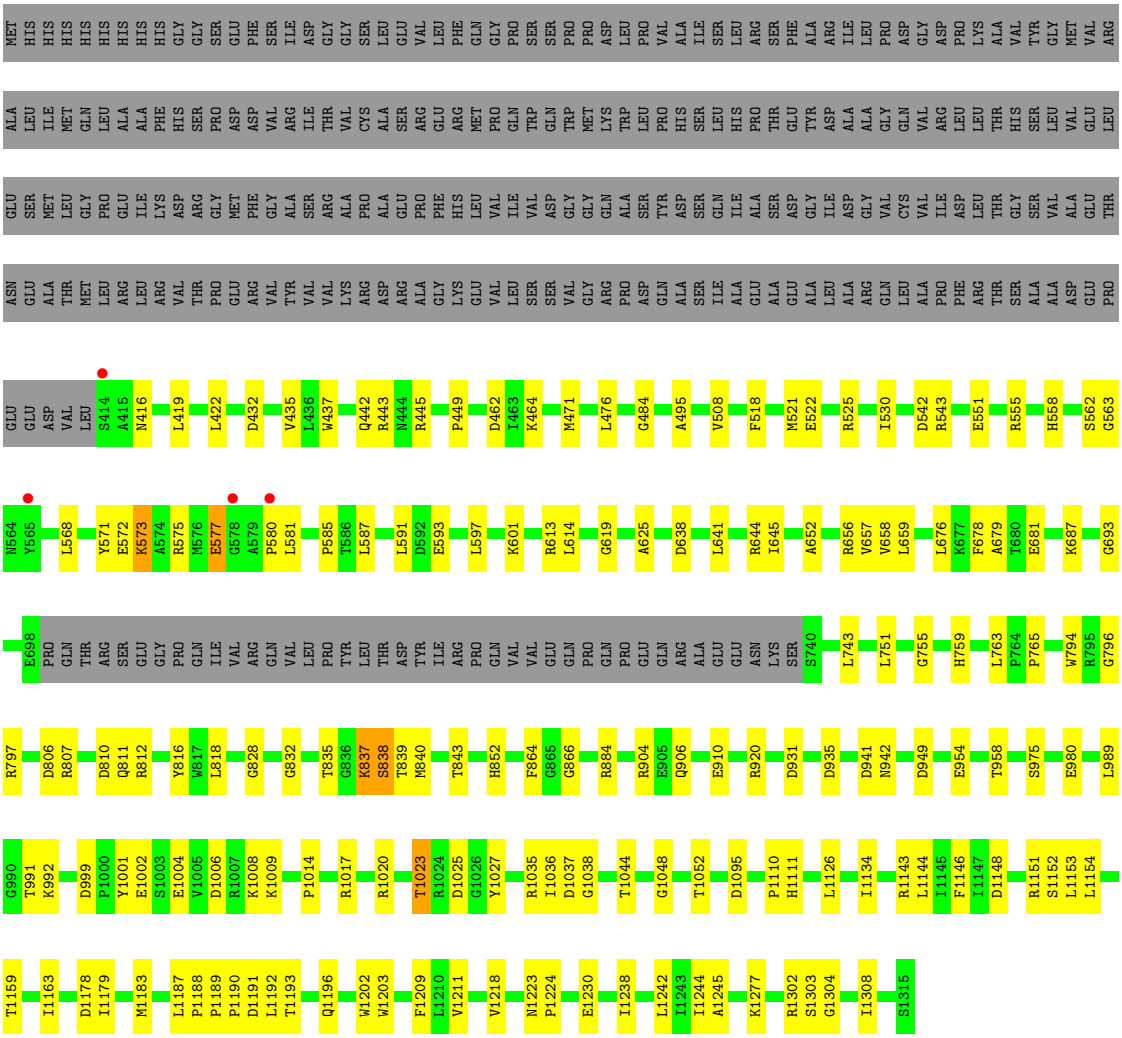
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	O	0	0
			4	4		
5	B	4	Total	O	0	0
			4	4		

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: Cell divisionFtsK/SpoIIIE

Chain A: 60% 14% 25%



- Molecule 1: Cell divisionFtsK/SpoIIIE

Chain B: % 56% 17% • 25%

MET HIS HIS HIS HIS HIS HIS HIS GLY GLY SER GLU PHE SER ILE ASP GLY GLY SER LEU GLU VAL LEU PHE GLN GLY PRO SER SER PRO PRO ASP LEU PRO VAL ALA ILE SER LEU ARG SER PHE ALA ARG ILE ILE LEU PRO ASP GLY ASP PRO LYS ALA VAL TYR GLY MET VAL ARG
ALA LEU ILE MET GLN LEU ALA ALA PHE HIS SER PRO ASP ASP VAL ARG ILE THR VAL CYS ALA SER ARG GLU ARG MET PRO GLN TRP GLN TRP MET LYS TRP LEU PRO HIS SER LEU HIS PRO THR GLU TYR ASP ALA ALA GLY GLN VAL ARG LEU LEU THR HIS SER LEU VAL GLU LEU
GLU SER MET LEU GLY PRO GLU ILE LYS ASP ARG GLY MET PHE GLY ALA SER ARG ALA PRO ALA GLU PRO PHE HIS LEU VAL ILE VAL ASP GLY GLY GLN ALA SER TYR ASP SER GLN ILE ALA SER ASP GLY ILE ASP GLY VAL CYS VAL ILE ASP LEU THR GLY SER VAL ALA GLU THR
ASN GLU ALA THR MET LEU ARG LEU ARG VAL THR PRO GLU ARG VAL TYR VAL VAL LYS ARG ASP ARG ALA GLY LYS GLU VAL LEU SER SER VAL GLY ARG PRO ASP GLN ALA SER ILE ALA GLU ALA GLU ALA LEU ARG GLN LEU ALA PRO PHE ARG THR SER ALA ALA ASP GLU PRO
GLU GLU ASP VAL LEU S414 A415 N416 L419 L422 Y429 D432 P433 A434 V435 Q442 R445 L446 P449 D453 R457 D462 I463 K464 Q468 M471 G475 L476 S483 E487 T491 E503 L524 L534 V541 D542 Y545 R555
L559 R560 H561 S562 Y565 Y571 E572 R575 M576 E577 G578 A579 P580 L581 P585 D592 E593 F594 S595 K601 L607 R613 L614 A625 S626 Q627 R628 L629 E630 E631 G632 K633 L634 R635 G636 L637 D638 T639 H640 L641 S642 Y643 R644 L647 F650 M653 E654
S655 R656 V657 V658 L659 G660 V661 Y665 E666 L667 P668 Y675 R685 Y690 V691 S692 G693 P694 V695 D696 E697 GLU PRO GLN THR ARG SER GLU GLY PRO GLN ILE VAL ARG GLN VAL LEU PRO TYR LEU THR ASP TYR ILE ARG PRO GLN VAL VAL GLU GLN PRO GLN PRO GLU GLN
ARG ALA GLU GLU ASN LYS SER SER E741 S742 L743 F744 D745 V746 V747 P756 E757 P758 P764 P765 L766 P769 L772 S782 A783 G796 R797 L798 H799 L804 V805 D806 R807 P808 F809 D810 Q811 R812 R813 D819 G822 G823 A824 G828 G832 P833 Q834 K837
L850 L851 H852 T853 P854 F859 D863 F864 G867 L872 L875 V878 T883 R884 R891 E905 Q906 E910 R920 R923 F933 G934 D935 D941 N942 Y950 L953 S956 R963 S975 E980 L989 E994 L995 R996 L997
Y1001 E1002 D1006 K1009 V1013 R1020 G1021 F1029 L1030 L1033 P1034 R1035 I1036 D1037 G1038 D1039 T1040 T1044 G1048 T1051 T1052 V1053 K1054 E1058 A1059 W1060 A1065 P1066 L1071 P1072 D1095 E1096 D1117 C1120 G1121 K1122 D1148 S1152 L1153 A1166 L1175
V1176 R1177 K1180 M1183 L1187 P1188 P1189 L1192 R1200 S1201 W1202 P1227 R1236 D1237 I1238 L1242 I1243 I1244 M1248 G1275 G1294 F1298 I1308 Q1309 T1310 S1315

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	251.82Å 116.32Å 174.11Å 90.00° 102.70° 90.00°	Depositor
Resolution (Å)	48.93 – 2.90 48.93 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.93-2.90) 86.2 (48.93-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	0.52 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.226 , 0.246 0.229 , 0.249	Depositor DCC
R_{free} test set	1523 reflections (1.41%)	wwPDB-VP
Wilson B-factor (Å^2)	67.3	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 50.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13435	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 3.30% 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: SO4, MG, ATP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.25	0/6813	0.41	1/9264 (0.0%)
1	B	0.27	0/6774	0.47	2/9215 (0.0%)
All	All	0.26	0/13587	0.44	3/18479 (0.0%)

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	807	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	B	579	ALA	C-N-CD	6.66	142.39	128.40
1	A	563	GLY	N-CA-C	-5.68	98.91	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	807	ARG	Peptide

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	6663	0	6636	118	0
1	B	6626	0	6588	196	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	62	0	24	1	0
4	B	62	0	24	4	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
All	All	13435	0	13272	314	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 12.

All (314) 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:B:629:LEU:HD21	1:B:633:LYS:CB	1.81	1.09
1:B:629:LEU:CD2	1:B:633:LYS:HB2	1.87	1.05
1:B:629:LEU:HD21	1:B:633:LYS:HB2	1.08	1.03
1:B:1122:LYS:NZ	4:B:1404:ATP:O2B	1.97	0.97
1:B:764:PRO:O	1:B:813:ARG:NH2	2.02	0.93
1:B:631:GLU:N	1:B:631:GLU:OE2	2.02	0.92
1:B:628:ARG:NH2	1:B:650:PHE:CG	2.38	0.91
1:B:636:GLY:O	1:B:640:HIS:HD2	1.52	0.91
1:A:1006:ASP:OD2	1:A:1009:LYS:N	2.04	0.89
1:A:442:GLN:O	1:A:464:LYS:NZ	2.07	0.86
1:B:905:GLU:OE2	1:B:963:ARG:NH1	2.08	0.86
1:B:644:ARG:HH11	1:B:644:ARG:HG3	1.38	0.85
1:A:442:GLN:HG3	1:A:445:ARG:HH12	1.42	0.82
1:A:543:ARG:NH1	1:A:806:ASP:OD2	2.13	0.81
1:B:471:MET:O	1:B:642:SER:OG	1.97	0.81
1:B:807:ARG:HG2	1:B:812:ARG:H	1.45	0.81
1:A:1148:ASP:OD2	1:A:1152:SER:N	2.13	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:628:ARG:HH21	1:B:650:PHE:CB	1.95	0.79
1:A:832:GLY:O	1:A:835:THR:OG1	1.99	0.79
1:A:1006:ASP:HB3	1:A:1009:LYS:HG3	1.65	0.79
1:B:561:HIS:CD2	1:B:562:SER:H	2.01	0.78
1:B:636:GLY:O	1:B:640:HIS:CD2	2.35	0.78
1:A:1006:ASP:CB	1:A:1009:LYS:HG3	2.14	0.78
1:B:644:ARG:HG3	1:B:644:ARG:NH1	1.98	0.78
1:B:807:ARG:NE	1:B:811:GLN:H	1.82	0.78
1:B:813:ARG:HG2	1:B:813:ARG:HH11	1.49	0.77
1:B:572:GLU:OE2	1:B:575:ARG:HG2	1.85	0.77
1:A:542:ASP:OD2	1:A:601:LYS:NZ	2.17	0.76
1:B:743:LEU:HD13	1:B:744:PHE:H	1.50	0.75
1:B:629:LEU:HD22	1:B:630:GLU:H	1.52	0.74
1:B:630:GLU:HG2	1:B:633:LYS:HG2	1.69	0.74
1:B:629:LEU:CD2	1:B:630:GLU:H	2.01	0.73
1:B:807:ARG:HE	1:B:811:GLN:H	1.35	0.73
1:A:555:ARG:NH2	1:A:585:PRO:O	2.21	0.73
1:B:629:LEU:HD23	1:B:633:LYS:HG3	1.71	0.73
1:B:575:ARG:HG2	1:B:575:ARG:HH11	1.52	0.72
1:B:837:LYS:NZ	4:B:1405:ATP:O2B	2.20	0.72
1:B:891:ARG:NH1	1:B:1096:GLU:OE2	2.24	0.71
1:B:629:LEU:CD2	1:B:633:LYS:CG	2.68	0.71
1:B:637:LEU:O	1:B:641:LEU:HG	1.90	0.71
1:B:743:LEU:HD13	1:B:744:PHE:N	2.05	0.71
1:B:629:LEU:HD11	1:B:634:LEU:HD21	1.71	0.71
1:B:691:VAL:HG23	1:B:692:SER:H	1.55	0.69
1:B:1033:LEU:O	1:B:1035:ARG:N	2.26	0.69
1:B:629:LEU:CD2	1:B:633:LYS:CB	2.58	0.68
1:B:807:ARG:HD2	1:B:807:ARG:C	2.14	0.68
1:B:807:ARG:HD2	1:B:808:PRO:N	2.08	0.68
1:B:464:LYS:NZ	1:B:468:GLN:O	2.27	0.68
1:A:1001:TYR:HD1	1:A:1002:GLU:H	1.39	0.68
1:B:807:ARG:HE	1:B:810:ASP:N	1.93	0.67
1:A:904:ARG:NE	1:A:931:ASP:OD2	2.23	0.67
1:B:692:SER:OG	1:B:693:GLY:N	2.26	0.66
1:B:1200:ARG:HH21	1:B:1236:ARG:HG2	1.60	0.66
1:B:487:GLU:OE2	1:B:692:SER:N	2.29	0.66
1:B:432:ASP:HB3	1:B:435:VAL:HG22	1.78	0.65
1:B:655:SER:OG	1:B:661:VAL:O	2.14	0.65
1:B:804:LEU:HD11	1:B:813:ARG:HB3	1.78	0.65
1:A:432:ASP:HB3	1:A:435:VAL:HG22	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:975:SER:OG	1:A:980:GLU:OE1	2.16	0.64
1:B:975:SER:OG	1:B:980:GLU:OE1	2.15	0.64
1:B:629:LEU:CD2	1:B:633:LYS:HG3	2.28	0.64
1:A:573:LYS:O	1:A:577:GLU:N	2.30	0.63
1:B:766:LEU:H	1:B:813:ARG:HH22	1.47	0.63
1:A:658:VAL:HG23	1:A:659:LEU:HG	1.81	0.62
1:A:681:GLU:N	1:A:681:GLU:OE1	2.33	0.62
1:A:442:GLN:HG3	1:A:445:ARG:NH1	2.12	0.62
1:B:743:LEU:HA	1:B:746:VAL:HB	1.80	0.62
1:B:1177:ARG:HG2	1:B:1177:ARG:HH11	1.65	0.62
1:B:813:ARG:HG2	1:B:813:ARG:NH1	2.12	0.62
1:B:805:VAL:HA	1:B:1029:PHE:HA	1.82	0.62
1:A:543:ARG:NH2	1:A:763:LEU:O	2.33	0.61
1:A:1006:ASP:CG	1:A:1009:LYS:HG3	2.21	0.61
1:A:645:ILE:HG12	1:A:676:LEU:HD23	1.83	0.61
1:A:1189:PRO:HD2	1:A:1192:LEU:HD11	1.83	0.61
1:B:542:ASP:HA	1:B:545:TYR:HB3	1.82	0.61
1:A:920:ARG:NH1	1:A:935:ASP:OD2	2.34	0.60
1:B:628:ARG:NH2	1:B:650:PHE:CD2	2.68	0.60
1:B:1036:ILE:HG12	1:B:1052:THR:HG22	1.82	0.60
1:B:1020:ARG:CG	1:B:1030:LEU:HA	2.32	0.60
1:B:810:ASP:HB3	1:B:812:ARG:NH1	2.17	0.60
1:B:644:ARG:HH11	1:B:644:ARG:CG	2.12	0.60
1:A:543:ARG:NH1	1:A:765:PRO:HA	2.18	0.59
1:A:1006:ASP:OD2	1:A:1008:LYS:N	2.34	0.59
1:B:628:ARG:NH2	1:B:650:PHE:CB	2.62	0.59
1:B:1148:ASP:OD2	1:B:1152:SER:N	2.34	0.59
1:A:568:LEU:HD13	1:A:619:GLY:HA3	1.84	0.59
1:B:1006:ASP:OD2	1:B:1009:LYS:HG3	2.02	0.59
1:B:772:LEU:HD23	1:B:850:LEU:HD12	1.83	0.59
1:B:923:ARG:NH1	1:B:933:PHE:O	2.35	0.59
1:B:807:ARG:NE	1:B:811:GLN:N	2.49	0.59
1:B:764:PRO:O	1:B:766:LEU:N	2.36	0.59
1:B:575:ARG:HH11	1:B:575:ARG:CG	2.16	0.58
1:A:508:VAL:HG23	1:A:587:LEU:HD11	1.83	0.58
1:A:525:ARG:NH1	1:A:755:GLY:O	2.37	0.58
1:B:629:LEU:HD22	1:B:630:GLU:N	2.18	0.58
1:B:996:ARG:HD3	1:B:1013:VAL:HG22	1.85	0.58
1:B:1037:ASP:OD1	1:B:1038:GLY:N	2.36	0.58
1:A:476:LEU:HB2	1:A:641:LEU:HD13	1.86	0.58
1:B:422:LEU:HD23	1:B:449:PRO:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:541:VAL:HG11	1:B:601:LYS:HG3	1.86	0.57
1:A:1001:TYR:CD1	1:A:1002:GLU:N	2.69	0.57
1:B:804:LEU:O	1:B:1030:LEU:N	2.37	0.57
1:A:837:LYS:O	1:A:840:MET:N	2.38	0.57
1:A:838:SER:OG	4:A:1405:ATP:O1B	2.23	0.57
1:B:572:GLU:O	1:B:575:ARG:HB3	2.05	0.57
1:B:613:ARG:NH1	1:B:614:LEU:HD21	2.20	0.57
1:B:654:GLU:CD	1:B:654:GLU:H	2.07	0.56
1:B:859:PHE:HB2	1:B:878:VAL:HG12	1.86	0.56
1:B:810:ASP:HB3	1:B:812:ARG:HH12	1.70	0.56
1:B:1117:ASP:O	1:B:1122:LYS:HE2	2.05	0.56
1:B:1120:CYS:SG	1:B:1122:LYS:HE3	2.45	0.56
1:B:475:GLY:HA3	1:B:643:TYR:CZ	2.41	0.56
1:B:561:HIS:HD2	1:B:562:SER:H	1.53	0.56
1:B:1020:ARG:HD3	1:B:1030:LEU:HA	1.88	0.56
1:B:804:LEU:HD21	1:B:813:ARG:HD3	1.88	0.56
1:B:864:PHE:H	1:B:941:ASP:HB3	1.71	0.55
1:A:1035:ARG:HH12	1:A:1044:THR:HG23	1.71	0.55
1:A:462:ASP:OD2	1:A:464:LYS:HE2	2.07	0.55
1:B:442:GLN:HA	1:B:445:ARG:NH1	2.22	0.55
1:B:1117:ASP:O	1:B:1122:LYS:CE	2.54	0.55
1:B:757:GLU:HG2	1:B:758:PRO:HD2	1.90	0.54
1:A:573:LYS:O	1:A:577:GLU:HB2	2.07	0.54
1:B:822:GLY:O	1:B:824:ALA:N	2.38	0.54
1:B:483:SER:HB2	1:B:647:LEU:HB3	1.88	0.54
1:B:1054:LYS:NZ	1:B:1058:GLU:OE2	2.38	0.54
1:B:628:ARG:HH21	1:B:650:PHE:HB3	1.71	0.54
1:A:1134:ILE:HG12	1:A:1159:THR:HG21	1.90	0.54
1:B:432:ASP:OD1	1:B:434:ALA:N	2.41	0.53
1:B:631:GLU:HA	1:B:657:VAL:HG21	1.89	0.53
1:A:1126:LEU:HD21	1:A:1245:ALA:HB2	1.90	0.53
1:A:807:ARG:HD3	1:A:1027:TYR:CE2	2.43	0.53
1:B:807:ARG:HE	1:B:809:PHE:C	2.12	0.53
1:A:1144:LEU:HD23	1:A:1209:PHE:HB2	1.90	0.53
1:A:1277:LYS:H	1:A:1277:LYS:HD2	1.73	0.53
1:B:631:GLU:OE1	1:B:653:MET:SD	2.67	0.53
1:B:561:HIS:O	1:B:562:SER:OG	2.26	0.53
1:B:593:GLU:OE2	1:B:627:GLN:CG	2.57	0.53
1:B:643:TYR:C	1:B:644:ARG:HD3	2.29	0.52
1:B:693:GLY:O	1:B:743:LEU:HD12	2.09	0.52
1:A:1126:LEU:HD12	1:A:1211:VAL:HG13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:690:TYR:HD1	1:B:692:SER:HB3	1.73	0.52
1:B:561:HIS:CD2	1:B:562:SER:N	2.75	0.52
1:B:595:SER:OG	1:B:633:LYS:NZ	2.42	0.52
1:B:629:LEU:HD23	1:B:633:LYS:CG	2.36	0.52
1:B:920:ARG:NH1	1:B:935:ASP:OD2	2.43	0.52
1:B:629:LEU:HD11	1:B:634:LEU:CD2	2.40	0.52
1:A:1023:THR:HG22	1:A:1025:ASP:H	1.74	0.51
1:A:1037:ASP:OD1	1:A:1038:GLY:N	2.43	0.51
1:B:1001:TYR:CD2	1:B:1002:GLU:HG3	2.44	0.51
1:B:1071:LEU:HD12	1:B:1072:PRO:HD2	1.91	0.51
1:B:572:GLU:OE2	1:B:572:GLU:HA	2.09	0.51
1:B:593:GLU:OE2	1:B:627:GLN:HG3	2.10	0.51
1:A:1035:ARG:HA	1:A:1052:THR:HG21	1.93	0.51
1:B:1048:GLY:O	1:B:1051:THR:OG1	2.26	0.51
1:A:572:GLU:O	1:A:575:ARG:HB3	2.11	0.51
1:B:1183:MET:HB3	1:B:1238:ILE:HD12	1.93	0.51
1:A:1143:ARG:HE	1:A:1163:ILE:HD11	1.76	0.50
1:B:419:LEU:HD22	1:B:491:THR:HG23	1.93	0.50
1:A:759:HIS:NE2	1:A:811:GLN:OE1	2.42	0.50
1:B:1177:ARG:HG2	1:B:1177:ARG:NH1	2.27	0.50
1:A:558:HIS:ND1	1:A:562:SER:OG	2.44	0.50
1:A:591:LEU:HD21	1:A:597:LEU:HD13	1.93	0.50
1:A:999:ASP:OD1	1:A:1001:TYR:N	2.44	0.50
1:B:572:GLU:HA	1:B:575:ARG:HB3	1.93	0.50
1:B:828:GLY:HA3	1:B:989:LEU:HD13	1.94	0.50
1:B:1180:LYS:HD2	1:B:1227:PRO:HB2	1.93	0.50
1:B:1242:LEU:HD23	1:B:1244:ILE:HD11	1.94	0.50
1:A:796:GLY:HA2	1:A:852:HIS:CD2	2.47	0.49
1:B:807:ARG:HD3	1:B:810:ASP:H	1.76	0.49
1:A:1193:THR:HG23	1:A:1196:GLN:H	1.77	0.49
1:B:832:GLY:O	1:B:837:LYS:NZ	2.46	0.49
1:B:782:SER:OG	1:B:783:ALA:N	2.44	0.49
1:B:872:LEU:HB3	1:B:875:LEU:HD12	1.95	0.49
1:A:638:ASP:CG	1:A:644:ARG:HH22	2.16	0.49
1:B:565:TYR:CD2	1:B:571:TYR:HA	2.47	0.48
1:B:592:ASP:HA	1:B:625:ALA:HB3	1.95	0.48
1:B:654:GLU:O	1:B:658:VAL:HG13	2.13	0.48
1:B:691:VAL:O	1:B:743:LEU:HD11	2.13	0.48
1:A:866:GLY:H	1:A:884:ARG:HH22	1.60	0.48
1:B:1035:ARG:HA	1:B:1052:THR:HG21	1.96	0.48
1:A:522:GLU:HG3	1:A:530:ILE:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:828:GLY:HA3	1:A:989:LEU:HD13	1.94	0.48
1:B:1020:ARG:HG3	1:B:1029:PHE:O	2.12	0.48
1:A:1191:ASP:OD1	1:A:1191:ASP:N	2.42	0.48
1:B:641:LEU:N	1:B:641:LEU:HD23	2.27	0.48
1:B:807:ARG:HE	1:B:811:GLN:N	2.07	0.48
1:B:1148:ASP:OD2	1:B:1153:LEU:N	2.44	0.48
1:B:1035:ARG:NH2	1:B:1044:THR:O	2.47	0.48
1:A:443:ARG:HA	1:A:464:LYS:HZ1	1.79	0.48
1:A:657:VAL:HG23	1:A:658:VAL:HG13	1.95	0.48
1:A:794:TRP:HA	1:A:797:ARG:HG3	1.96	0.48
1:B:690:TYR:CD1	1:B:692:SER:HB3	2.49	0.47
1:B:769:PRO:HA	1:B:1030:LEU:HD23	1.95	0.47
1:A:419:LEU:HD21	1:A:495:ALA:HB2	1.96	0.47
1:A:1095:ASP:HA	1:A:1308:ILE:HA	1.96	0.47
1:A:1151:ARG:HB3	1:A:1154:LEU:HD21	1.95	0.47
1:B:416:ASN:HB3	1:B:690:TYR:CE2	2.49	0.47
1:B:629:LEU:CD2	1:B:630:GLU:N	2.73	0.47
1:B:545:TYR:CE1	1:B:607:LEU:HB2	2.49	0.47
1:B:854:PRO:HG2	1:B:1060:TRP:CD1	2.48	0.47
1:A:1218:VAL:O	1:A:1223:ASN:ND2	2.42	0.47
1:B:807:ARG:HD2	1:B:808:PRO:CA	2.44	0.47
1:B:631:GLU:OE1	1:B:653:MET:CG	2.62	0.47
1:B:1248:MET:HG3	1:B:1275:GLY:HA2	1.97	0.47
1:B:575:ARG:CG	1:B:575:ARG:NH1	2.73	0.47
1:A:558:HIS:O	1:A:562:SER:OG	2.33	0.47
1:A:593:GLU:N	1:A:625:ALA:O	2.47	0.47
1:A:810:ASP:HB3	1:A:812:ARG:NH1	2.30	0.47
1:A:442:GLN:HA	1:A:445:ARG:NH1	2.30	0.46
1:A:1178:ASP:OD1	1:A:1178:ASP:N	2.38	0.46
1:B:675:TYR:CE1	1:B:685:ARG:HD3	2.50	0.46
1:B:807:ARG:NE	1:B:810:ASP:N	2.63	0.46
1:A:1242:LEU:HD12	1:A:1244:ILE:HD11	1.96	0.46
1:B:1187:LEU:HA	1:B:1188:PRO:HD3	1.81	0.46
1:A:1014:PRO:HG2	1:A:1020:ARG:NH1	2.31	0.46
1:B:629:LEU:HD23	1:B:630:GLU:H	1.80	0.46
1:B:995:LEU:HA	1:B:1021:GLY:HA3	1.98	0.46
1:B:1294:GLY:O	1:B:1310:THR:OG1	2.24	0.46
1:A:1277:LYS:HD2	1:A:1277:LYS:N	2.31	0.46
1:B:953:LEU:HA	1:B:956:SER:HB3	1.96	0.46
1:A:837:LYS:HB2	1:A:837:LYS:HE2	1.25	0.46
1:B:675:TYR:HE1	1:B:685:ARG:HD3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1039:ASP:OD1	1:B:1040:THR:N	2.49	0.46
1:A:416:ASN:ND2	1:A:687:LYS:NZ	2.63	0.45
1:B:628:ARG:CG	1:B:629:LEU:N	2.79	0.45
1:B:696:ASP:OD1	1:B:697:GLU:N	2.49	0.45
1:A:1183:MET:HB3	1:A:1238:ILE:HD12	1.98	0.45
1:B:462:ASP:OD1	1:B:464:LYS:HE3	2.17	0.45
1:B:693:GLY:C	1:B:743:LEU:HD12	2.37	0.45
1:B:1122:LYS:NZ	4:B:1404:ATP:O1G	2.49	0.45
1:B:1020:ARG:CD	1:B:1030:LEU:HA	2.47	0.45
1:B:476:LEU:HB2	1:B:641:LEU:HD13	1.99	0.45
1:A:837:LYS:O	1:A:839:THR:N	2.49	0.45
1:B:1200:ARG:HA	1:B:1202:TRP:CZ3	2.52	0.45
1:A:1001:TYR:O	1:A:1002:GLU:HB2	2.17	0.45
1:B:503:GLU:HB2	1:B:756:PRO:HG2	1.98	0.45
1:B:1020:ARG:HD3	1:B:1030:LEU:CA	2.47	0.45
1:A:518:PHE:HB3	1:A:521:MET:HG3	1.99	0.44
1:A:693:GLY:O	1:A:743:LEU:N	2.46	0.44
1:B:667:LEU:HA	1:B:668:PRO:HD3	1.86	0.44
1:B:1166:ALA:HB2	1:B:1175:LEU:HD12	1.98	0.44
1:A:1111:HIS:ND1	1:A:1242:LEU:HB2	2.33	0.44
1:B:1188:PRO:HB3	1:B:1192:LEU:HD12	2.00	0.44
1:A:1202:TRP:CE2	1:A:1203:TRP:HD1	2.35	0.44
1:B:994:GLU:OE2	1:B:997:LEU:HD21	2.18	0.44
1:B:799:HIS:NE2	1:B:819:ASP:OD1	2.51	0.44
1:A:992:LYS:HD2	1:A:1004:GLU:HG2	1.99	0.43
1:B:883:THR:OG1	1:B:884:ARG:N	2.52	0.43
1:B:442:GLN:O	1:B:464:LYS:HE2	2.18	0.43
1:B:691:VAL:HG23	1:B:692:SER:N	2.30	0.43
1:B:542:ASP:HA	1:B:545:TYR:CB	2.47	0.43
1:B:654:GLU:O	1:B:657:VAL:HG12	2.18	0.43
1:A:443:ARG:HA	1:A:464:LYS:NZ	2.33	0.43
1:A:652:ALA:O	1:A:656:ARG:HG3	2.18	0.43
1:B:446:LEU:HD23	1:B:463:ILE:HG13	2.01	0.43
1:B:796:GLY:HA2	1:B:852:HIS:CD2	2.53	0.43
1:A:1230:GLU:H	1:A:1230:GLU:HG2	1.57	0.43
1:B:432:ASP:HB3	1:B:435:VAL:CG2	2.47	0.43
1:B:593:GLU:OE2	1:B:627:GLN:HG2	2.19	0.43
1:B:462:ASP:O	1:B:471:MET:HB2	2.19	0.43
1:B:864:PHE:HB2	1:B:942:ASN:HB3	2.01	0.43
1:B:1189:PRO:HD2	1:B:1192:LEU:HD11	2.00	0.43
1:A:839:THR:O	1:A:843:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1110:PRO:HG2	1:A:1111:HIS:CD2	2.54	0.43
1:B:632:GLY:O	1:B:633:LYS:C	2.57	0.43
1:B:741:GLU:HB2	1:B:742:SER:HB3	2.01	0.43
1:B:834:GLN:HB3	4:B:1405:ATP:H5'1	2.01	0.43
1:B:476:LEU:HB2	1:B:641:LEU:CD1	2.49	0.42
1:A:422:LEU:HD23	1:A:449:PRO:HB2	2.00	0.42
1:A:1148:ASP:OD2	1:A:1153:LEU:N	2.52	0.42
1:A:1302:ARG:O	1:A:1303:SER:OG	2.33	0.42
1:A:543:ARG:HH12	1:A:765:PRO:HA	1.84	0.42
1:A:1035:ARG:NH2	1:A:1037:ASP:OD2	2.49	0.42
1:B:1298:PHE:HB2	1:B:1308:ILE:HD13	2.02	0.42
1:B:453:ASP:OD1	1:B:457:ARG:N	2.52	0.42
1:B:580:PRO:C	1:B:581:LEU:HD12	2.40	0.42
1:B:1095:ASP:HA	1:B:1308:ILE:HA	2.01	0.42
1:A:906:GLN:O	1:A:910:GLU:HG3	2.19	0.42
1:A:1143:ARG:NE	1:A:1163:ILE:HD11	2.34	0.42
1:A:884:ARG:H	1:A:884:ARG:HG2	1.61	0.42
1:A:1223:ASN:HA	1:A:1224:PRO:HD3	1.85	0.42
1:A:471:MET:HA	1:A:678:PHE:CD1	2.55	0.42
1:A:1014:PRO:HB3	1:A:1017:ARG:HG3	2.01	0.42
1:A:1048:GLY:O	1:A:1052:THR:HG23	2.20	0.41
1:B:555:ARG:NH2	1:B:585:PRO:O	2.51	0.41
1:B:798:LEU:HD11	1:B:920:ARG:NH1	2.35	0.41
1:B:863:ASP:OD2	1:B:867:GLY:HA2	2.19	0.41
1:A:1148:ASP:CG	1:A:1152:SER:H	2.17	0.41
1:A:1179:ILE:O	1:A:1183:MET:HG2	2.20	0.41
1:A:1189:PRO:HA	1:A:1190:PRO:HD3	1.87	0.41
1:A:613:ARG:HE	1:A:614:LEU:CD1	2.33	0.41
1:B:743:LEU:O	1:B:747:VAL:N	2.43	0.41
1:A:949:ASP:OD1	1:A:949:ASP:N	2.54	0.41
1:A:1036:ILE:HG13	1:A:1052:THR:HG22	2.02	0.41
1:B:429:TYR:HE1	1:B:695:VAL:HG21	1.85	0.41
1:A:1187:LEU:HA	1:A:1188:PRO:HD3	1.81	0.41
1:B:630:GLU:OE2	1:B:633:LYS:NZ	2.33	0.41
1:A:484:GLY:N	2:A:1401:SO4:O4	2.54	0.41
1:A:818:LEU:HG	1:A:991:THR:HG21	2.03	0.41
1:A:954:GLU:O	1:A:958:THR:OG1	2.27	0.41
1:A:437:TRP:CZ2	1:A:751:LEU:HD12	2.56	0.41
1:A:571:TYR:CE1	1:A:581:LEU:HD13	2.56	0.41
1:B:629:LEU:HD22	1:B:630:GLU:O	2.21	0.41
1:B:1020:ARG:HG2	1:B:1030:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:GLU:OE1	1:A:555:ARG:NH1	2.53	0.40
1:A:679:ALA:HB3	1:A:681:GLU:OE1	2.21	0.40
1:A:1146:PHE:HD2	1:A:1153:LEU:HD23	1.85	0.40
1:A:638:ASP:CG	1:A:644:ARG:NH2	2.75	0.40
1:A:864:PHE:H	1:A:941:ASP:HB3	1.86	0.40
1:B:950:TYR:HB3	1:B:953:LEU:HD13	2.03	0.40
1:A:1302:ARG:C	1:A:1304:GLY:H	2.22	0.40
1:B:1065:ALA:HA	1:B:1066:PRO:HD3	1.97	0.40
1:A:864:PHE:HB2	1:A:942:ASN:H	1.86	0.40
1:B:906:GLN:O	1:B:910:GLU:HG3	2.20	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	857/1147 (75%)	799 (93%)	56 (6%)	2 (0%)	47	78
1	B	855/1147 (74%)	793 (93%)	58 (7%)	4 (0%)	29	61
All	All	1712/2294 (75%)	1592 (93%)	114 (7%)	6 (0%)	34	66

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	808	PRO
1	A	577	GLU
1	B	823	GLY
1	B	1034	PRO
1	A	580	PRO
1	B	693	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	709/953 (74%)	704 (99%)	5 (1%)	84 95
1	B	703/953 (74%)	688 (98%)	15 (2%)	53 81
All	All	1412/1906 (74%)	1392 (99%)	20 (1%)	67 89

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	573	LYS
1	A	816	TYR
1	A	837	LYS
1	A	838	SER
1	A	1023	THR
1	B	534	LEU
1	B	560	ARG
1	B	575	ARG
1	B	576	MET
1	B	577	GLU
1	B	629	LEU
1	B	630	GLU
1	B	631	GLU
1	B	638	ASP
1	B	644	ARG
1	B	658	VAL
1	B	742	SER
1	B	743	LEU
1	B	807	ARG
1	B	1020	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	416	ASN
1	B	561	HIS

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Mol	Chain	Res	Type
1	B	640	HIS

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)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	B	1404	3	26,33,33	0.93	1 (3%)	31,52,52	1.54	5 (16%)
2	SO4	B	1401	-	4,4,4	0.14	0	6,6,6	0.06	0
4	ATP	B	1405	3	26,33,33	0.94	1 (3%)	31,52,52	1.59	5 (16%)
4	ATP	A	1404	3	26,33,33	0.93	1 (3%)	31,52,52	1.62	5 (16%)
2	SO4	A	1401	-	4,4,4	0.15	0	6,6,6	0.06	0
4	ATP	A	1405	3	26,33,33	0.93	1 (3%)	31,52,52	1.60	5 (16%)

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	B	1404	3	-	0/18/38/38	0/3/3/3
4	ATP	A	1404	3	-	0/18/38/38	0/3/3/3
4	ATP	A	1405	3	-	0/18/38/38	0/3/3/3
4	ATP	B	1405	3	-	0/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1405	ATP	C5-C4	2.50	1.47	1.40
4	A	1405	ATP	C5-C4	2.47	1.47	1.40
4	B	1404	ATP	C5-C4	2.45	1.47	1.40
4	A	1404	ATP	C5-C4	2.43	1.47	1.40

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1404	ATP	PA-O3A-PB	-3.89	119.48	132.83
4	B	1405	ATP	PA-O3A-PB	-3.82	119.71	132.83
4	A	1405	ATP	PB-O3B-PG	-3.77	119.88	132.83
4	A	1405	ATP	PA-O3A-PB	-3.75	119.97	132.83
4	B	1404	ATP	PA-O3A-PB	-3.68	120.20	132.83
4	A	1404	ATP	PB-O3B-PG	-3.65	120.31	132.83
4	B	1405	ATP	PB-O3B-PG	-3.42	121.08	132.83
4	A	1404	ATP	C3'-C2'-C1'	3.32	105.98	100.98
4	A	1405	ATP	C3'-C2'-C1'	3.28	105.91	100.98
4	B	1405	ATP	C3'-C2'-C1'	3.21	105.81	100.98
4	B	1404	ATP	C3'-C2'-C1'	3.19	105.78	100.98
4	B	1405	ATP	N3-C2-N1	-3.18	123.70	128.68
4	A	1405	ATP	N3-C2-N1	-3.17	123.73	128.68
4	A	1404	ATP	N3-C2-N1	-3.12	123.80	128.68
4	B	1404	ATP	PB-O3B-PG	-3.11	122.14	132.83
4	B	1404	ATP	N3-C2-N1	-3.11	123.81	128.68
4	A	1404	ATP	C4-C5-N7	-2.74	106.55	109.40
4	B	1405	ATP	C4-C5-N7	-2.66	106.62	109.40
4	B	1404	ATP	C4-C5-N7	-2.65	106.63	109.40
4	A	1405	ATP	C4-C5-N7	-2.65	106.64	109.40

There are no chirality outliers.

There are no torsion outliers.

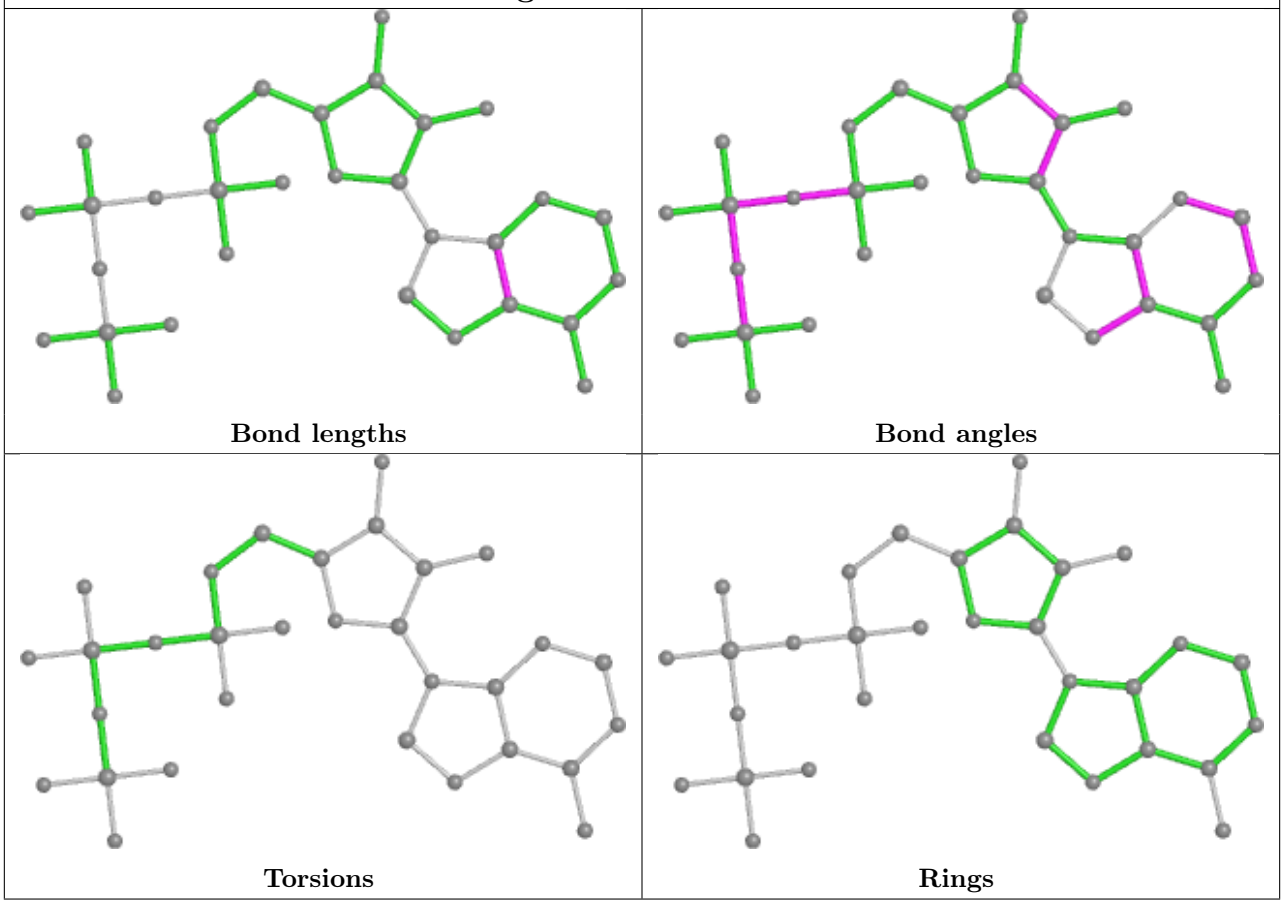
There are no ring outliers.

4 monomers are involved in 6 short contacts:

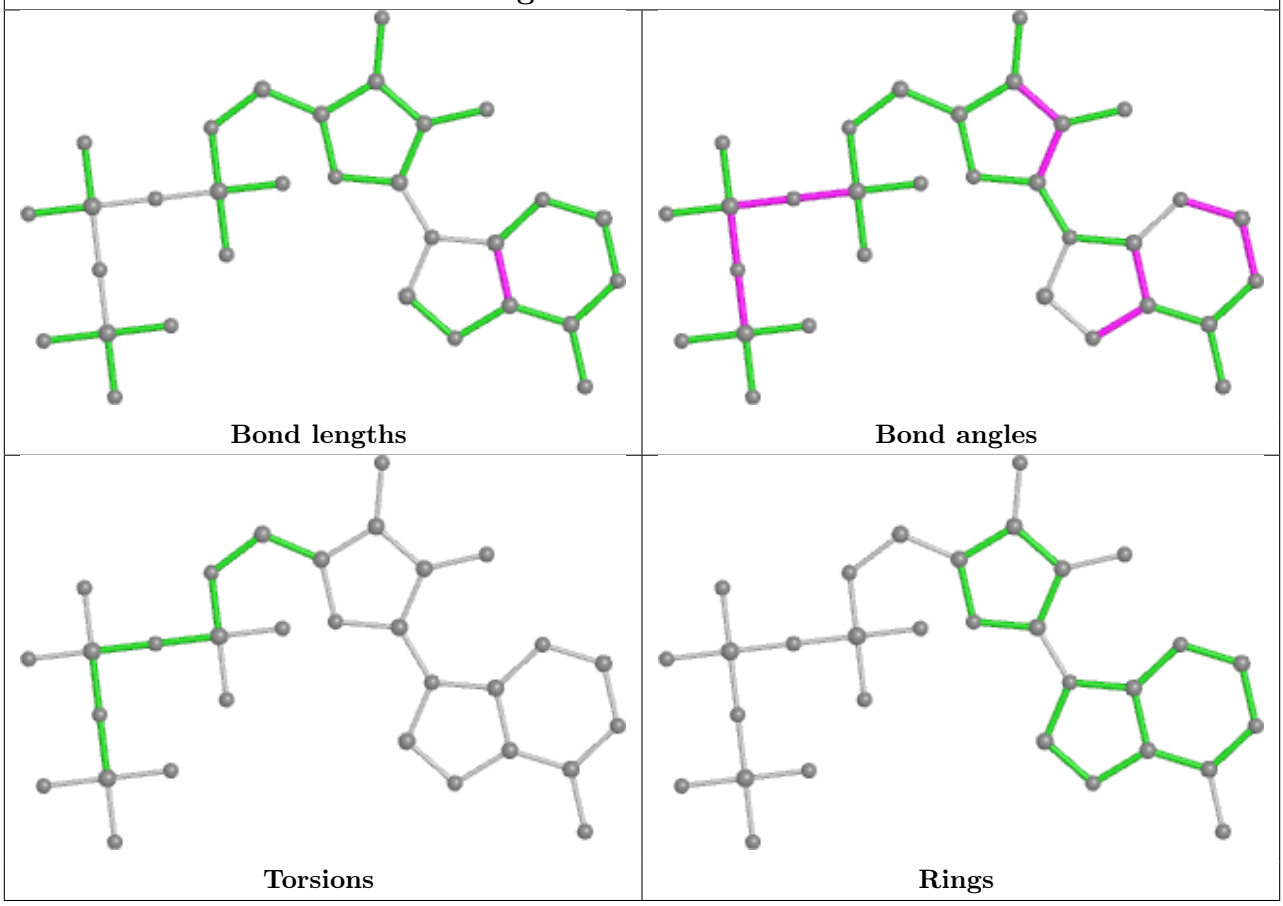
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1404	ATP	2	0
4	B	1405	ATP	2	0
2	A	1401	SO4	1	0
4	A	1405	ATP	1	0

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.

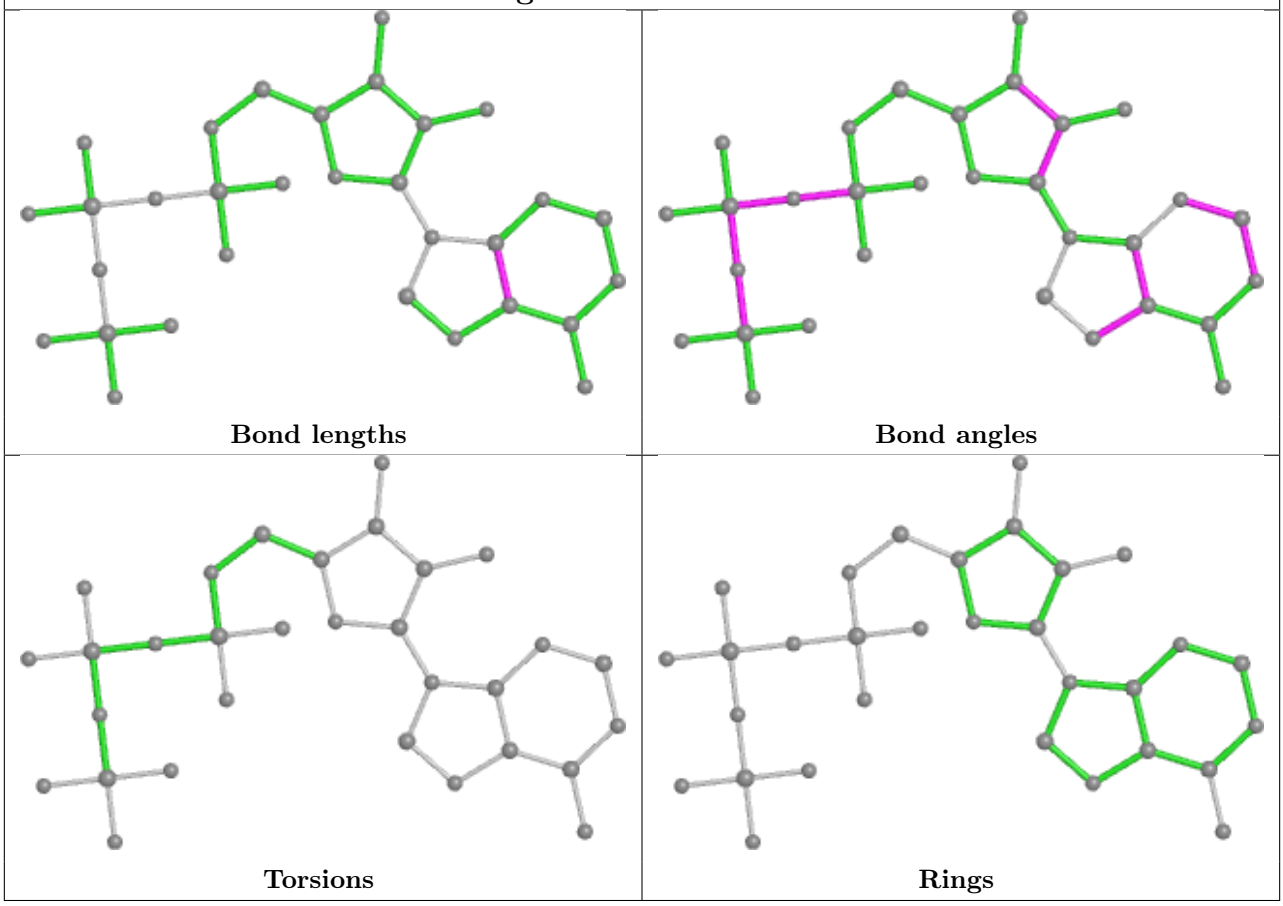
Ligand ATP B 1404



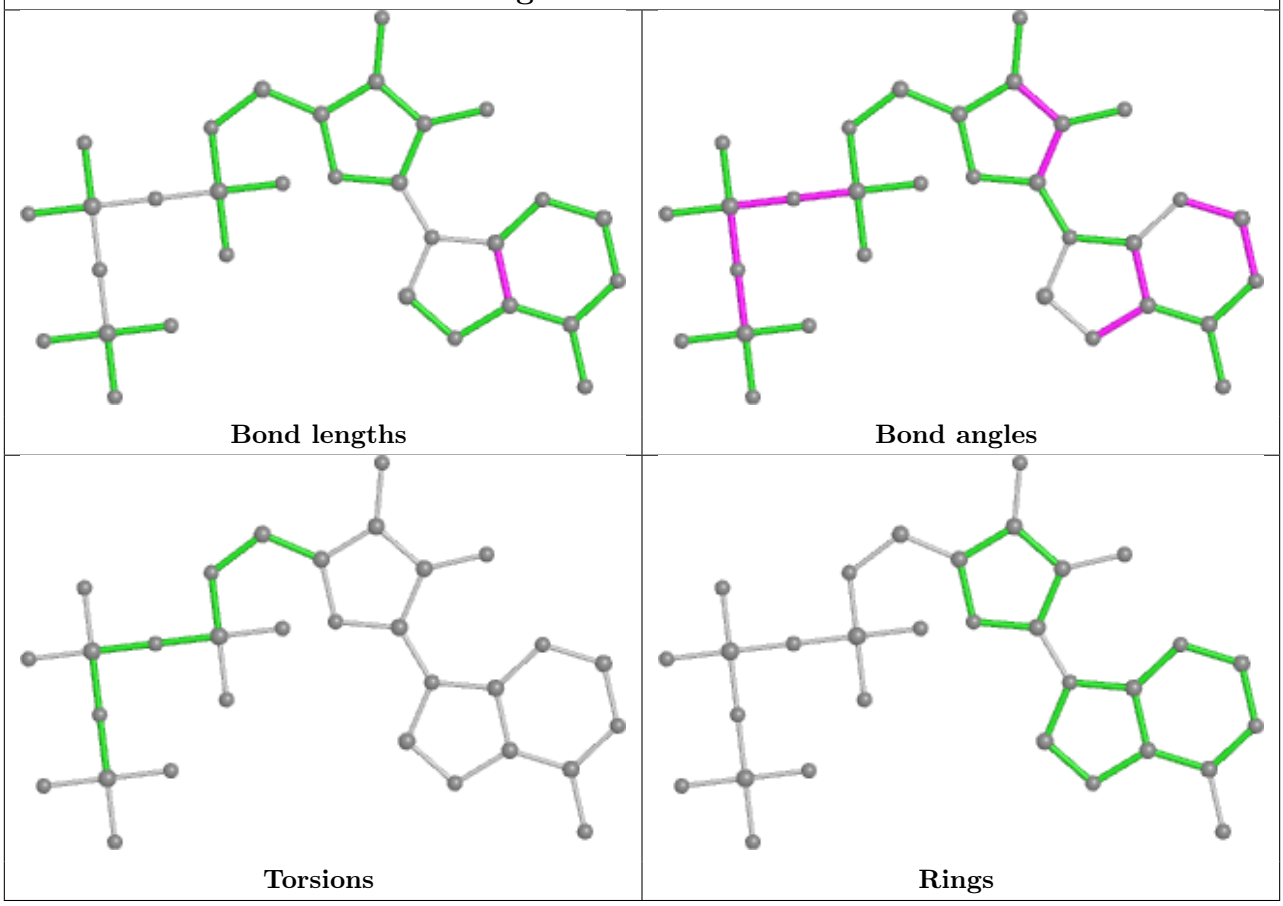
Ligand ATP B 1405



Ligand ATP A 1404



Ligand ATP A 1405



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	861/1147 (75%)	-0.19	4 (0%)	91	91	44, 80, 113, 151	0
1	B	859/1147 (74%)	-0.10	13 (1%)	73	73	35, 84, 128, 161	0
All	All	1720/2294 (74%)	-0.14	17 (0%)	82	82	35, 82, 125, 161	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	578	GLY	3.8
1	B	580	PRO	3.5
1	B	634	LEU	3.3
1	B	565	TYR	2.5
1	A	580	PRO	2.2
1	B	560	ARG	2.2
1	A	565	TYR	2.2
1	B	1001	TYR	2.2
1	B	1059	ALA	2.2
1	B	524	LEU	2.1
1	B	659	LEU	2.1
1	B	665	TYR	2.1
1	A	414	SER	2.1
1	B	559	LEU	2.1
1	B	581	LEU	2.1
1	B	1021	GLY	2.0
1	B	579	ALA	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)

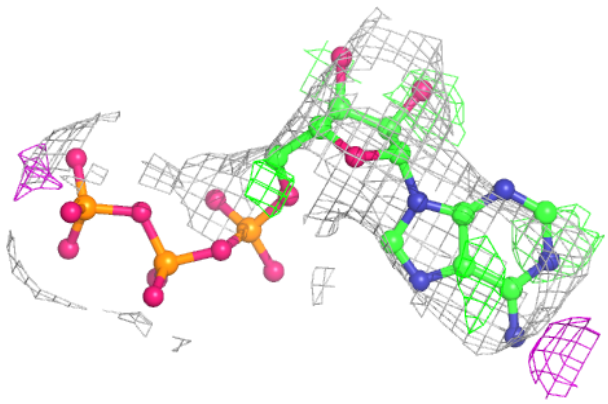
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

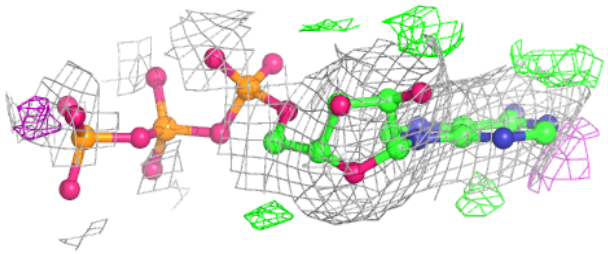
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	B	1401	5/5	0.92	0.11	97,105,124,150	0
2	SO4	A	1401	5/5	0.96	0.11	72,86,91,93	0
3	MG	A	1403	1/1	0.96	0.11	77,77,77,77	0
4	ATP	B	1405	31/31	0.96	0.14	69,117,135,141	0
3	MG	B	1402	1/1	0.97	0.11	59,59,59,59	0
3	MG	B	1403	1/1	0.97	0.06	86,86,86,86	0
4	ATP	A	1404	31/31	0.97	0.14	61,73,96,101	0
4	ATP	A	1405	31/31	0.97	0.14	65,92,108,113	0
4	ATP	B	1404	31/31	0.97	0.16	34,63,78,97	0
3	MG	A	1402	1/1	0.97	0.05	82,82,82,82	0

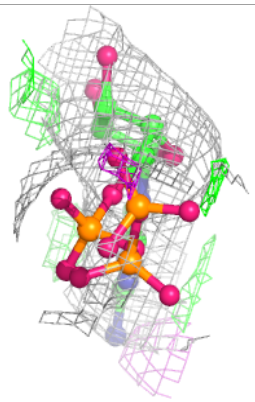
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP B 1405:

$2mF_o$-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 1404:

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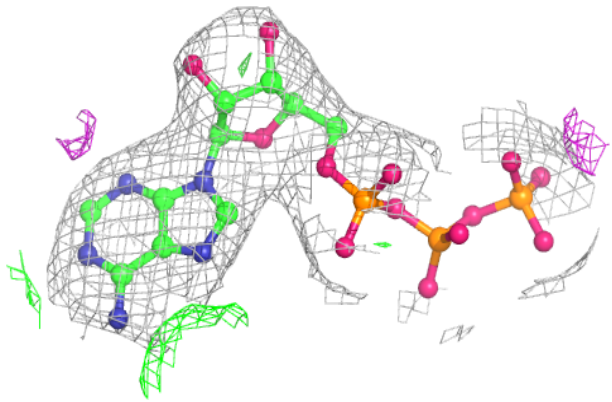
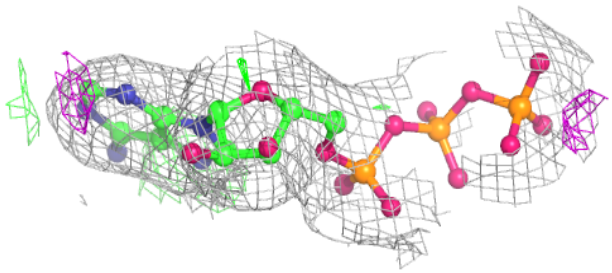
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around ATP A 1405:

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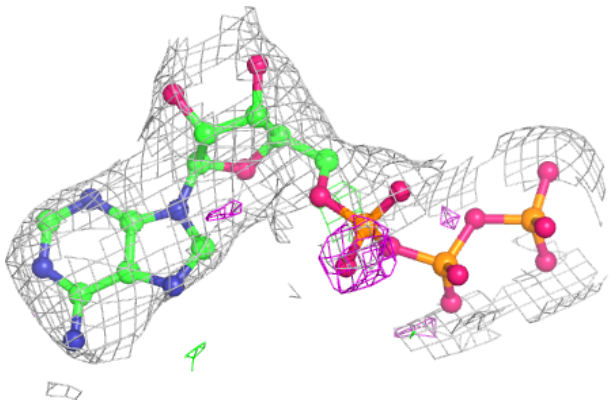
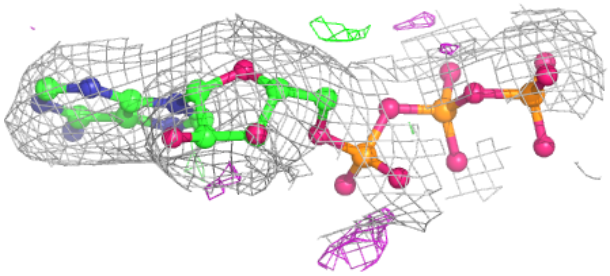
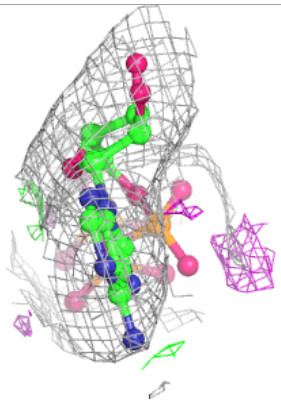
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around ATP B 1404:

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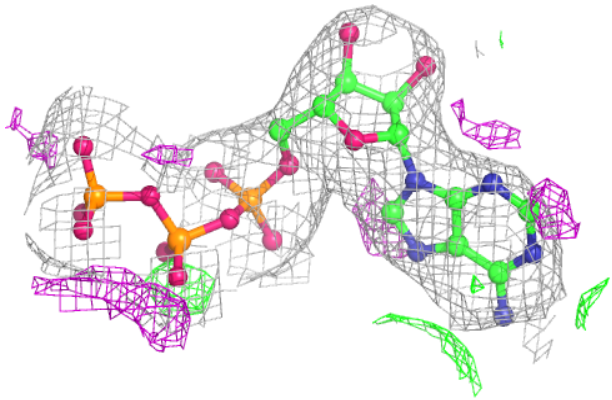
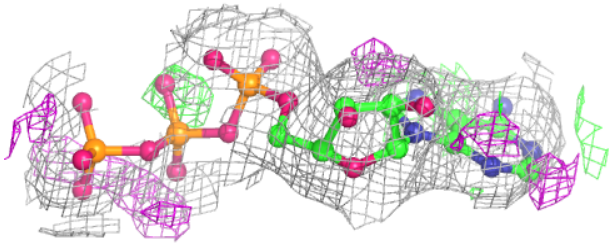
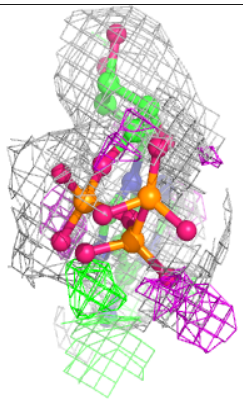
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.