



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 07:06 PM UTC

PDB ID : 1II0 / pdb_00001ii0
Title : CRYSTAL STRUCTURE OF THE ESCHERICHIA COLI ARSENITE-TRANSLOCATING ATPASE
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Deposited on : 2001-04-20
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

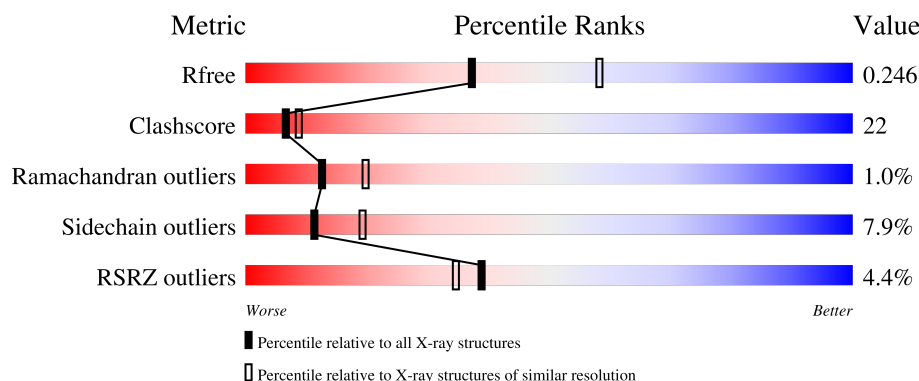
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	589	
1	B	589	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	B	1599	-	-	-	X
3	CL	B	4001	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8927 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 ARSENICAL PUMP-DRIVING ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	550	Total	C	N	O	S	0	0	0
			4201	2642	743	801	15			
1	B	553	Total	C	N	O	S	0	0	0
			4224	2655	748	806	15			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	ASN	ILE	SEE REMARK 999	UNP P08690
A	584	HIS	-	expression tag	UNP P08690
A	585	HIS	-	expression tag	UNP P08690
A	586	HIS	-	expression tag	UNP P08690
A	587	HIS	-	expression tag	UNP P08690
A	588	HIS	-	expression tag	UNP P08690
A	589	HIS	-	expression tag	UNP P08690
B	1060	ASN	ILE	SEE REMARK 999	UNP P08690
B	1584	HIS	-	expression tag	UNP P08690
B	1585	HIS	-	expression tag	UNP P08690
B	1586	HIS	-	expression tag	UNP P08690
B	1587	HIS	-	expression tag	UNP P08690
B	1588	HIS	-	expression tag	UNP P08690
B	1589	HIS	-	expression tag	UNP P08690

- Molecule 2 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	9	Total	Cd	0	0
			9	9		
2	B	8	Total	Cd	0	0
			8	8		

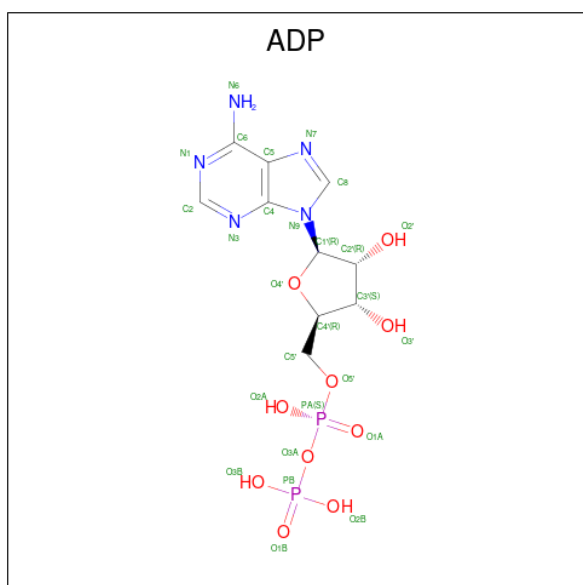
- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Cl	0	0
			3	3		
3	B	4	Total	Cl	0	0
			4	4		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		
4	B	2	Total	Mg	0	0
			2	2		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



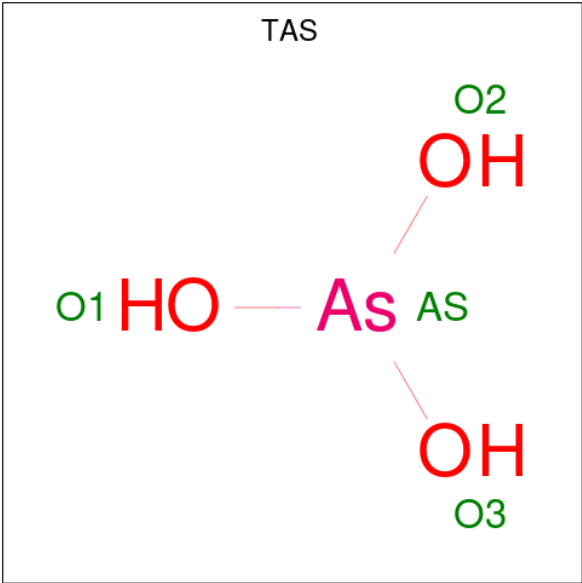
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 7 is TRIHYDROXYARSENITE(III) (CCD ID: TAS) (formula: AsH₃O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	As	O	0	0
			4	1	3		
7	B	1	Total	As	O	0	0
			4	1	3		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	171	Total 171	O 171	0	0
8	B	179	Total 179	O 179	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	76.73Å 222.19Å 74.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.61 – 2.40 28.61 – 2.40	Depositor EDS
% Data completeness (in resolution range)	90.0 (28.61-2.40) 89.9 (28.61-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.210 , 0.252 0.204 , 0.246	Depositor DCC
R_{free} test set	4564 reflections (9.73%)	wwPDB-VP
Wilson B-factor (Å ²)	34.3	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.020 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8927	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TAS, ATP, ADP, MG, CD, CL

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	0.43	0/4273	0.94	11/5810 (0.2%)
1	B	0.42	0/4296	0.95	13/5841 (0.2%)
All	All	0.42	0/8569	0.94	24/11651 (0.2%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1278	GLN	CA-C-N	6.87	126.11	118.97
1	B	1278	GLN	C-N-CA	6.87	126.11	118.97
1	A	559	ALA	N-CA-C	6.61	120.30	109.72
1	B	1406	LEU	N-CA-C	-6.35	98.26	108.55
1	B	1559	ALA	N-CA-C	6.22	118.76	108.99
1	A	96	VAL	N-CA-C	-6.01	107.64	113.53
1	A	90	VAL	N-CA-C	5.97	117.51	111.00
1	B	1155	LEU	N-CA-C	5.97	118.08	109.48
1	A	278	GLN	CA-C-N	5.95	125.15	118.97
1	A	278	GLN	C-N-CA	5.95	125.15	118.97
1	A	419	ARG	N-CA-C	-5.92	105.37	113.30
1	B	1419	ARG	N-CA-C	-5.81	104.75	112.94
1	A	134	THR	N-CA-C	-5.68	106.18	113.23
1	A	558	HIS	N-CA-C	5.58	120.10	113.12
1	B	1045	ASP	CA-C-N	5.55	125.39	119.28
1	B	1045	ASP	C-N-CA	5.55	125.39	119.28
1	B	1039	VAL	N-CA-C	5.52	116.43	108.48
1	B	1490	ARG	N-CA-C	5.48	118.01	111.71
1	B	1155	LEU	CA-C-N	5.26	125.06	119.28
1	B	1155	LEU	C-N-CA	5.26	125.06	119.28
1	A	536	ARG	N-CA-C	-5.13	107.19	113.50
1	B	1172	CYS	N-CA-C	5.12	118.84	112.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	393	ARG	N-CA-C	-5.02	105.81	111.28
1	A	39	VAL	N-CA-C	5.01	115.69	108.48

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	4201	0	4261	180	0
1	B	4224	0	4279	187	0
2	A	9	0	0	0	0
2	B	8	0	0	0	0
3	A	3	0	0	0	0
3	B	4	0	0	3	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	27	0	12	2	0
5	B	27	0	12	2	0
6	A	31	0	12	0	0
6	B	31	0	12	1	0
7	A	4	0	0	1	0
7	B	4	0	0	0	0
8	A	171	0	0	10	0
8	B	179	0	0	14	0
All	All	8927	0	8588	370	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 22.

All (370) 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:1329:LEU:HD11	1:B:1446:MET:HE3	1.43	0.99
1:A:385:ILE:HD11	1:A:428:VAL:HG13	1.45	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1209:LYS:HG2	1:B:1213:GLN:HE21	1.31	0.94
1:A:381:GLN:NE2	1:A:442:ARG:HH22	1.67	0.93
1:B:1170:ALA:HB3	1:B:1402:LYS:HZ3	1.34	0.92
1:A:49:ASN:HD22	1:A:49:ASN:H	1.17	0.90
1:A:235:ASN:HD21	5:A:590:ADP:HN61	1.17	0.89
1:B:1205:ALA:HB2	1:B:1215:VAL:HG21	1.56	0.86
1:B:1169:GLY:HA3	1:B:1398:VAL:HG21	1.56	0.85
1:A:170:ALA:HB3	1:A:402:LYS:HZ1	1.41	0.85
1:B:1307:GLN:HG2	1:B:1308:GLN:H	1.41	0.82
1:A:235:ASN:ND2	5:A:590:ADP:HN61	1.77	0.82
1:B:1151:ARG:O	1:B:1154:GLN:HG2	1.80	0.81
1:A:381:GLN:HE21	1:A:442:ARG:HH22	1.29	0.79
1:B:1527:ASN:ND2	1:B:1528:ASN:H	1.81	0.78
1:A:56:GLN:HE22	1:A:65:ILE:HA	1.49	0.78
1:A:16:LYS:HG2	1:A:19:VAL:HG13	1.63	0.77
1:A:131:SER:O	1:A:134:THR:HB	1.84	0.77
1:A:170:ALA:HB3	1:A:402:LYS:NZ	2.00	0.76
1:B:1261:ALA:C	1:B:1262:ASN:HD22	1.94	0.75
1:B:1243:ALA:HB1	1:B:1250:ALA:HA	1.68	0.75
1:B:1027:ALA:HB1	1:B:1292:LEU:HD21	1.69	0.75
1:B:1527:ASN:HD21	6:B:1591:ATP:HN61	1.32	0.75
1:A:275:LEU:HD13	1:A:291:LEU:HD22	1.66	0.75
1:A:56:GLN:NE2	1:A:65:ILE:HA	2.03	0.74
1:B:1322:ILE:HD13	1:B:1330:ILE:HD11	1.70	0.74
1:B:1532:ILE:HG23	1:B:1566:PRO:HB3	1.70	0.73
1:B:1459:ASP:HA	1:B:1480:THR:HG21	1.68	0.73
1:B:1209:LYS:HG2	1:B:1213:GLN:NE2	2.04	0.73
1:A:386:ASP:HB3	1:A:389:GLU:HG2	1.72	0.72
1:A:436:ILE:HG12	1:A:446:MET:HE1	1.71	0.72
1:B:1170:ALA:HB3	1:B:1402:LYS:NZ	2.05	0.72
1:A:128:THR:HG22	1:A:188:TYR:HD2	1.54	0.71
1:A:264:PRO:HG2	1:A:267:LEU:HD12	1.72	0.71
1:B:1436:ILE:HG12	1:B:1446:MET:CE	2.20	0.71
1:A:79:GLN:O	1:A:83:GLN:HG3	1.90	0.71
1:B:1425:GLU:HG2	8:B:2306:HOH:O	1.90	0.71
1:B:1169:GLY:C	1:B:1171:SER:H	1.99	0.70
1:A:326:GLU:HG2	1:A:356:PHE:CE1	2.26	0.70
1:A:459:ASP:HA	1:A:480:THR:HG21	1.74	0.70
1:B:1163:ILE:HD12	1:B:1173:LEU:CD1	2.23	0.69
3:B:1599:CL:CL	8:B:2333:HOH:O	2.48	0.69
1:A:357:ASP:O	1:A:442:ARG:HB2	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1169:GLY:CA	1:B:1398:VAL:HG21	2.22	0.68
1:B:1322:ILE:HD11	1:B:1351:LEU:HD21	1.73	0.68
1:B:1063:GLN:HG2	8:B:2314:HOH:O	1.93	0.68
1:B:1211:THR:O	1:B:1215:VAL:HG23	1.94	0.68
1:B:1333:MET:HE1	1:B:1514:LEU:HD21	1.76	0.68
1:B:1019:VAL:HG11	8:B:2061:HOH:O	1.93	0.66
1:B:1170:ALA:CB	1:B:1402:LYS:HZ3	2.06	0.66
1:B:1114:THR:OG1	1:B:1175:PRO:HG3	1.95	0.66
3:B:4001:CL:CL	8:B:2195:HOH:O	2.50	0.66
1:A:537:SER:OG	1:A:540:LEU:HD23	1.95	0.66
1:A:433:SER:HA	1:A:436:ILE:HG13	1.77	0.65
1:B:1436:ILE:HG12	1:B:1446:MET:HE1	1.76	0.65
1:A:49:ASN:HD22	1:A:49:ASN:N	1.85	0.65
1:B:1262:ASN:HD22	1:B:1262:ASN:N	1.90	0.65
1:B:1166:ASN:HB2	1:B:1402:LYS:NZ	2.12	0.65
1:B:1235:ASN:ND2	1:B:1236:GLY:H	1.94	0.65
1:A:576:ASP:HB2	1:A:577:LYS:NZ	2.11	0.64
1:A:169:GLY:HA3	1:A:398:VAL:HG11	1.77	0.64
1:A:169:GLY:C	1:A:171:SER:H	2.06	0.64
1:B:1169:GLY:HA3	1:B:1398:VAL:CG2	2.27	0.64
1:B:1411:LYS:O	1:B:1415:GLU:HG3	1.97	0.63
1:B:1001:MET:HB2	1:B:1004:LEU:HD22	1.80	0.63
1:B:1121:ASP:OD1	1:B:1181:LYS:HE2	1.98	0.63
3:B:4001:CL:CL	8:B:3029:HOH:O	2.52	0.63
1:A:502:THR:HB	1:A:503:PRO:HD3	1.80	0.63
1:A:205:ALA:HB2	1:A:215:VAL:HG21	1.80	0.63
1:A:318:LEU:HD22	1:A:522:TRP:HZ3	1.64	0.63
1:A:163:ILE:HD12	1:A:173:LEU:CD1	2.29	0.62
1:B:1235:ASN:HD21	5:B:1590:ADP:HN61	1.46	0.62
1:A:166:ASN:HB3	1:A:167:PRO:HD2	1.82	0.62
1:B:1307:GLN:CG	1:B:1308:GLN:H	2.12	0.62
1:B:1400:GLU:HG3	1:B:1401:THR:N	2.14	0.62
1:A:16:LYS:HG2	1:A:19:VAL:CG1	2.30	0.61
1:B:1404:LYS:HE3	1:B:1404:LYS:HA	1.81	0.61
1:B:1151:ARG:NH1	1:B:1416:GLU:OE2	2.33	0.61
1:A:170:ALA:HA	1:A:417:ASP:OD2	2.01	0.61
1:A:436:ILE:HG12	1:A:446:MET:CE	2.31	0.60
1:A:513:ASP:OD1	1:A:516:ARG:NH1	2.34	0.60
1:A:166:ASN:N	1:A:166:ASN:HD22	1.98	0.60
1:B:1307:GLN:HB2	8:B:2346:HOH:O	2.00	0.60
1:B:1235:ASN:HD22	1:B:1275:LEU:HB2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1086:ARG:HG2	1:B:1106:ASN:ND2	2.17	0.60
1:B:1318:LEU:O	1:B:1322:ILE:HG23	2.01	0.60
1:A:532:ILE:HG12	1:A:532:ILE:O	2.02	0.59
1:B:1131:SER:O	1:B:1134:THR:HB	2.03	0.59
1:A:319:VAL:HG13	1:A:351:LEU:HD13	1.84	0.58
1:B:1548:LEU:HB2	1:B:1549:PRO:HD3	1.83	0.58
1:A:499:PRO:HB2	1:A:547:GLU:HB3	1.85	0.58
1:B:1307:GLN:HG2	1:B:1308:GLN:N	2.17	0.58
1:B:1575:ILE:O	1:B:1579:LYS:HG3	2.03	0.57
1:A:220:LEU:HD11	1:A:266:ASP:OD1	2.04	0.57
1:A:151:ARG:HD2	1:A:416:GLU:OE1	2.03	0.57
1:B:1107:GLU:OE1	1:B:1516:ARG:NH2	2.36	0.57
1:A:238:LEU:HD22	1:A:239:PRO:HD2	1.87	0.57
1:A:450:PRO:HB2	1:A:455:LEU:HD22	1.87	0.57
1:B:1163:ILE:HD12	1:B:1173:LEU:HD13	1.86	0.57
1:A:19:VAL:HG11	8:A:2153:HOH:O	2.03	0.57
1:A:168:GLU:O	1:A:402:LYS:HD2	2.05	0.57
1:B:1502:THR:HB	1:B:1503:PRO:HD3	1.86	0.57
1:A:260:LEU:HD13	1:A:260:LEU:C	2.29	0.56
1:B:1329:LEU:CD1	1:B:1446:MET:HE3	2.26	0.56
1:A:319:VAL:CG1	1:A:351:LEU:HD13	2.35	0.56
1:A:548:LEU:HB2	1:A:549:PRO:HD3	1.87	0.56
1:B:1555:LYS:HE3	1:B:1556:ARG:NH1	2.21	0.56
1:A:455:LEU:HB3	1:A:482:MET:HE1	1.86	0.56
1:B:1397:HIS:O	1:B:1401:THR:HG22	2.04	0.56
1:B:1051:GLY:HA2	1:B:1058:ILE:HG12	1.86	0.56
1:B:1332:LEU:HD13	1:B:1344:ALA:HB2	1.87	0.56
1:B:1319:VAL:HG13	1:B:1351:LEU:HD13	1.86	0.56
1:B:1235:ASN:ND2	5:B:1590:ADP:HN61	2.04	0.56
1:A:350:ARG:NH1	8:A:3014:HOH:O	2.29	0.55
1:B:1001:MET:HE3	1:B:1294:THR:HG22	1.87	0.55
1:B:1367:ALA:C	1:B:1384:ARG:HH12	2.14	0.55
1:A:441:LYS:HD3	8:A:2252:HOH:O	2.07	0.55
1:A:571:GLU:O	1:A:573:THR:N	2.36	0.55
1:A:404:LYS:HB3	1:A:405:GLU:OE1	2.06	0.55
1:B:1284:GLY:O	1:B:1288:LEU:HD22	2.07	0.55
1:A:240:LYS:HB2	1:A:253:TRP:HE1	1.72	0.55
1:A:515:GLU:OE1	1:A:520:HIS:CE1	2.60	0.55
1:A:181:LYS:HB2	1:A:186:TYR:CZ	2.42	0.55
1:A:318:LEU:HD22	1:A:522:TRP:CZ3	2.42	0.55
1:A:275:LEU:HD13	1:A:291:LEU:CD2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ILE:HD11	1:A:126:LEU:HD21	1.89	0.55
1:A:151:ARG:O	1:A:154:GLN:HG2	2.06	0.55
1:B:1169:GLY:HA2	1:B:1418:LEU:HD21	1.89	0.54
1:B:1385:ILE:HD13	1:B:1390:GLU:HG3	1.89	0.54
1:B:1527:ASN:HD22	1:B:1528:ASN:H	1.52	0.54
1:A:68:VAL:HG22	1:A:68:VAL:O	2.07	0.54
1:A:153:LEU:HD23	1:A:176:MET:HE1	1.88	0.54
1:A:571:GLU:HA	1:A:571:GLU:OE2	2.06	0.54
1:A:8:PRO:O	1:A:138:HIS:HD2	1.90	0.54
1:A:561:ARG:NH1	8:A:3003:HOH:O	2.35	0.54
1:A:172:CYS:SG	8:A:2223:HOH:O	2.58	0.54
1:A:49:ASN:N	1:A:49:ASN:ND2	2.56	0.54
1:B:1558:HIS:HD2	8:B:2109:HOH:O	1.90	0.54
1:A:255:ARG:HD3	8:A:2278:HOH:O	2.07	0.54
1:B:1169:GLY:C	1:B:1171:SER:N	2.66	0.53
1:A:319:VAL:HG11	1:A:350:ARG:HG3	1.91	0.53
1:A:431:ALA:O	1:A:434:ARG:HB2	2.08	0.53
1:A:425:GLU:CG	1:A:450:PRO:HA	2.39	0.53
1:B:1252:ILE:O	1:B:1256:GLU:HG3	2.09	0.53
1:A:207:LEU:HG	1:A:234:ILE:HG21	1.89	0.53
1:B:1051:GLY:CA	1:B:1058:ILE:HG12	2.39	0.53
1:A:120:PHE:CD1	1:A:153:LEU:HD12	2.44	0.53
1:A:385:ILE:CD1	1:A:428:VAL:HG13	2.29	0.52
1:A:404:LYS:HE3	1:A:405:GLU:CD	2.34	0.52
1:B:1527:ASN:ND2	1:B:1528:ASN:N	2.56	0.52
1:A:350:ARG:HH11	1:A:350:ARG:HB2	1.75	0.52
1:B:1574:GLY:H	1:B:1577:LYS:HE3	1.75	0.52
1:B:1275:LEU:HD13	1:B:1291:LEU:HD22	1.92	0.52
1:B:1068:VAL:HG11	1:B:1071:LEU:HD23	1.91	0.52
1:B:1308:GLN:OE1	1:B:1545:GLN:HG3	2.09	0.52
1:B:1262:ASN:N	1:B:1262:ASN:ND2	2.53	0.52
1:B:1459:ASP:HA	1:B:1480:THR:CG2	2.36	0.52
1:B:1166:ASN:HB3	1:B:1167:PRO:HD2	1.92	0.52
1:B:1398:VAL:HG11	1:B:1418:LEU:HD21	1.92	0.52
1:A:173:LEU:HG	1:A:417:ASP:CG	2.35	0.52
1:A:26:CYS:O	1:A:30:ILE:HG13	2.10	0.51
1:B:1164:ASP:HB3	1:B:1166:ASN:HD21	1.74	0.51
1:B:1417:ASP:O	1:B:1420:SER:HB2	2.10	0.51
1:A:333:MET:HE1	1:A:514:LEU:HD21	1.91	0.51
1:A:128:THR:HG22	1:A:188:TYR:CD2	2.42	0.51
1:A:240:LYS:HA	1:A:253:TRP:CD1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:GLU:HG2	1:A:356:PHE:CZ	2.46	0.51
1:A:404:LYS:HE3	1:A:405:GLU:OE1	2.11	0.51
1:A:425:GLU:HG3	1:A:450:PRO:HA	1.92	0.51
1:B:1320:ASP:O	1:B:1323:ALA:HB3	2.11	0.51
1:A:381:GLN:HE21	1:A:442:ARG:NH2	2.03	0.51
1:B:1150:ILE:HG21	1:B:1225:ILE:HG21	1.92	0.51
1:B:1205:ALA:CB	1:B:1215:VAL:HG21	2.37	0.51
1:B:1385:ILE:HD12	1:B:1385:ILE:C	2.36	0.51
1:A:262:ASN:N	1:A:262:ASN:HD22	2.07	0.51
1:A:98:PRO:O	1:A:102:VAL:HG23	2.12	0.50
1:A:235:ASN:ND2	1:A:236:GLY:H	2.08	0.50
1:A:283:VAL:HG22	1:A:283:VAL:O	2.10	0.50
1:B:1053:VAL:HG13	1:B:1288:LEU:HD21	1.92	0.50
1:A:451:THR:O	1:A:455:LEU:HD23	2.12	0.50
1:B:1395:ARG:HG2	1:B:1418:LEU:HB3	1.93	0.50
1:B:1085:TYR:CD2	1:B:1178:GLY:HA3	2.47	0.50
1:A:534:ASP:OD2	1:A:534:ASP:N	2.37	0.50
1:B:1054:PHE:O	1:B:1055:SER:C	2.55	0.50
1:B:1064:ALA:HA	1:B:1072:SER:HA	1.94	0.50
1:A:576:ASP:HB2	1:A:577:LYS:HZ3	1.76	0.50
1:B:1151:ARG:HH11	1:B:1416:GLU:CD	2.20	0.50
1:B:1436:ILE:HG12	1:B:1446:MET:HE2	1.92	0.50
1:B:1147:GLY:HA2	1:B:1225:ILE:CD1	2.42	0.50
1:A:90:VAL:HG13	1:A:102:VAL:HG13	1.94	0.49
1:A:169:GLY:C	1:A:171:SER:N	2.70	0.49
1:A:536:ARG:HA	1:A:541:ARG:NH2	2.27	0.49
1:A:59:GLY:C	1:A:61:THR:H	2.19	0.49
1:A:436:ILE:CG1	1:A:446:MET:HE1	2.41	0.49
1:B:1086:ARG:HG2	1:B:1106:ASN:HD21	1.77	0.49
1:B:1252:ILE:HD12	1:B:1540:LEU:HD21	1.94	0.49
1:A:163:ILE:HD12	1:A:173:LEU:HD13	1.94	0.49
1:A:395:ARG:HB3	1:A:395:ARG:NH1	2.28	0.49
1:B:1003:PHE:CE1	1:B:1004:LEU:HD13	2.47	0.49
1:B:1166:ASN:N	1:B:1166:ASN:HD22	2.10	0.49
1:A:14:THR:HB	1:A:144:ALA:HB3	1.95	0.49
1:A:261:ALA:C	1:A:262:ASN:HD22	2.20	0.49
1:A:422:CYS:HA	1:A:425:GLU:HB3	1.94	0.49
1:B:1068:VAL:CG1	1:B:1071:LEU:HD23	2.42	0.49
1:A:16:LYS:CG	1:A:19:VAL:HG13	2.41	0.49
1:B:1438:GLU:HA	1:B:1441:LYS:CE	2.43	0.49
1:A:166:ASN:N	1:A:166:ASN:ND2	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:SER:HA	1:A:436:ILE:CG1	2.42	0.48
1:B:1008:PRO:HB2	1:B:1009:PRO:HD2	1.94	0.48
1:B:1561:ARG:HG2	1:B:1561:ARG:HH11	1.78	0.48
1:A:552:GLU:OE1	1:A:556:ARG:HD2	2.13	0.48
1:B:1165:SER:C	1:B:1166:ASN:HD22	2.21	0.48
1:B:1361:THR:HG21	1:B:1435:VAL:HG21	1.95	0.48
1:B:1085:TYR:CE2	1:B:1178:GLY:HA3	2.49	0.48
1:A:117:ILE:HD13	1:A:149:THR:HG23	1.95	0.48
1:A:114:THR:OG1	1:A:175:PRO:HG3	2.13	0.48
1:B:1398:VAL:HG11	1:B:1418:LEU:CD2	2.44	0.48
1:B:1394:TYR:O	1:B:1398:VAL:HG12	2.13	0.48
1:B:1422:CYS:O	1:B:1426:ILE:HG13	2.14	0.48
1:A:542:MET:HE1	1:A:545:GLN:OE1	2.13	0.48
1:B:1174:GLY:N	1:B:1175:PRO:CD	2.76	0.48
1:A:260:LEU:HD13	1:A:260:LEU:O	2.14	0.48
1:A:240:LYS:HB2	1:A:253:TRP:NE1	2.29	0.47
1:B:1088:ARG:HD3	1:B:1180:GLU:OE2	2.14	0.47
1:B:1166:ASN:HB2	1:B:1402:LYS:CE	2.43	0.47
1:A:169:GLY:O	1:A:171:SER:N	2.47	0.47
1:B:1001:MET:CE	1:B:1294:THR:HG22	2.43	0.47
1:B:1555:LYS:HE3	1:B:1556:ARG:HH11	1.79	0.47
1:B:1459:ASP:CA	1:B:1480:THR:HG21	2.40	0.47
1:A:151:ARG:NH2	1:A:221:GLU:CD	2.72	0.47
1:B:1229:ASN:C	1:B:1229:ASN:HD22	2.23	0.47
1:A:8:PRO:HB2	1:A:9:PRO:HD2	1.96	0.47
1:A:150:ILE:HB	1:A:225:ILE:HD13	1.97	0.47
1:A:162:PHE:HA	8:A:2316:HOH:O	2.14	0.47
1:A:240:LYS:C	1:A:242:GLU:H	2.22	0.47
1:A:364:ASP:OD1	1:A:365:PRO:HD2	2.15	0.47
1:A:395:ARG:HB3	1:A:395:ARG:HH11	1.79	0.47
1:B:1240:LYS:HA	1:B:1253:TRP:CD1	2.49	0.47
1:B:1260:LEU:HD13	1:B:1260:LEU:O	2.15	0.47
1:B:1490:ARG:HB3	8:B:2154:HOH:O	2.14	0.47
1:A:37:LYS:HE3	8:A:2296:HOH:O	2.15	0.47
1:B:1486:GLN:O	1:B:1488:PRO:HD3	2.14	0.47
1:B:1173:LEU:O	1:B:1176:MET:HG2	2.15	0.47
1:A:386:ASP:HB3	1:A:389:GLU:CG	2.44	0.46
1:B:1098:PRO:HB2	1:B:1101:VAL:HG23	1.98	0.46
1:B:1351:LEU:HB3	1:B:1358:VAL:HG21	1.97	0.46
1:A:325:ASN:O	1:A:326:GLU:HB2	2.15	0.46
1:B:1243:ALA:CB	1:B:1250:ALA:HA	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:LYS:O	1:A:19:VAL:HG22	2.15	0.46
1:B:1456:LEU:HD21	1:B:1517:ALA:HA	1.97	0.46
1:A:1:MET:HB2	1:A:4:LEU:CD2	2.45	0.46
1:B:1400:GLU:O	1:B:1404:LYS:HD2	2.15	0.46
1:A:1:MET:HB2	1:A:4:LEU:HD23	1.98	0.46
1:B:1164:ASP:HB3	1:B:1166:ASN:ND2	2.30	0.46
1:B:1438:GLU:HA	1:B:1441:LYS:HE2	1.97	0.46
1:A:235:ASN:HD22	1:A:275:LEU:HB2	1.81	0.45
1:B:1312:ILE:HG22	1:B:1313:PRO:O	2.16	0.45
1:B:1432:PHE:O	1:B:1435:VAL:HG22	2.15	0.45
1:A:120:PHE:CE1	1:A:153:LEU:HD12	2.51	0.45
1:B:1536:ARG:HA	1:B:1541:ARG:HH21	1.81	0.45
1:A:88:ARG:HD2	1:A:180:GLU:OE1	2.15	0.45
1:B:1333:MET:HE2	8:B:2270:HOH:O	2.16	0.45
1:A:459:ASP:HB2	1:A:482:MET:HE2	1.98	0.45
1:B:1058:ILE:HD12	1:B:1073:ALA:HB3	1.98	0.45
1:A:339:GLY:O	1:A:343:MET:HG2	2.15	0.45
1:B:1315:LEU:HB3	1:B:1582:ALA:HA	1.98	0.45
1:B:1432:PHE:O	1:B:1436:ILE:HG13	2.16	0.45
1:A:47:ALA:HB3	1:A:505:LEU:HD21	1.99	0.45
1:B:1169:GLY:O	1:B:1171:SER:N	2.50	0.45
1:B:1031:ARG:O	1:B:1035:GLN:HG3	2.17	0.45
1:B:1270:LEU:HD12	1:B:1270:LEU:N	2.32	0.45
1:A:577:LYS:HD3	1:A:577:LYS:N	2.32	0.44
1:A:411:LYS:O	1:A:415:GLU:HG3	2.17	0.44
1:B:1350:ARG:HD3	8:B:2101:HOH:O	2.17	0.44
1:A:456:LEU:HD21	1:A:517:ALA:HA	1.98	0.44
1:A:164:ASP:HB3	1:A:166:ASN:HD21	1.83	0.44
1:A:350:ARG:NH1	1:A:350:ARG:HB2	2.32	0.44
1:B:1068:VAL:HA	1:B:1069:PRO:HD2	1.89	0.44
1:A:416:GLU:O	1:A:419:ARG:HB3	2.18	0.44
1:B:1151:ARG:NH2	1:B:1221:GLU:OE1	2.50	0.44
1:B:1404:LYS:HE3	1:B:1404:LYS:CA	2.46	0.44
1:A:391:THR:HG22	1:A:395:ARG:HD2	1.99	0.44
1:B:1016:LYS:HA	8:B:2288:HOH:O	2.17	0.44
1:B:1151:ARG:HD2	1:B:1416:GLU:OE1	2.18	0.44
1:B:1536:ARG:HA	1:B:1541:ARG:NH2	2.32	0.44
1:A:433:SER:HA	1:A:436:ILE:CD1	2.48	0.43
1:B:1282:MET:HE3	1:B:1291:LEU:HG	1.99	0.43
1:A:278:GLN:HA	1:A:279:PRO:HD3	1.87	0.43
1:B:1343:MET:HE1	1:B:1581:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:ILE:HB	1:A:225:ILE:CD1	2.49	0.43
1:B:1361:THR:OG1	1:B:1446:MET:HG2	2.18	0.43
1:B:1058:ILE:HG22	1:B:1075:GLU:HB2	2.00	0.43
1:B:1524:TRP:CD1	1:B:1559:ALA:HB2	2.53	0.43
1:A:151:ARG:HH22	1:A:221:GLU:CD	2.26	0.43
1:A:216:ALA:HA	1:A:267:LEU:HD21	2.00	0.43
1:B:1155:LEU:HA	1:B:1156:PRO:HD3	1.77	0.43
1:B:1552:GLU:OE2	1:B:1556:ARG:NH1	2.52	0.43
1:A:201:LEU:C	1:A:201:LEU:HD13	2.44	0.43
1:B:1332:LEU:HD13	1:B:1344:ALA:CA	2.48	0.43
1:B:1322:ILE:HD12	1:B:1443:PHE:CE2	2.53	0.43
1:A:90:VAL:HG21	1:A:106:ASN:HD22	1.82	0.43
1:A:91:ASP:HB2	1:A:92:PRO:HD3	2.00	0.43
1:A:151:ARG:HA	1:A:154:GLN:HG2	2.00	0.43
1:B:1255:ARG:HD2	1:B:1571:GLU:HG3	2.01	0.43
1:A:345:ALA:HB1	1:A:578:LEU:HD21	2.01	0.42
1:A:395:ARG:HH11	1:A:395:ARG:CB	2.31	0.42
1:B:1332:LEU:HD13	1:B:1344:ALA:CB	2.48	0.42
1:B:1401:THR:HG23	1:B:1402:LYS:HG3	2.00	0.42
1:A:243:ALA:HB1	1:A:250:ALA:HA	2.01	0.42
1:A:575:ILE:O	1:A:579:LYS:HG3	2.19	0.42
1:B:1016:LYS:O	1:B:1019:VAL:HG22	2.19	0.42
1:B:1139:ILE:HD12	1:B:1139:ILE:N	2.34	0.42
1:A:515:GLU:OE1	1:A:520:HIS:NE2	2.52	0.42
1:B:1350:ARG:NH2	1:B:1583:GLY:O	2.53	0.42
1:A:417:ASP:C	1:A:419:ARG:H	2.27	0.42
1:A:295:GLN:HA	1:A:296:PRO:HD3	1.94	0.42
1:A:377:LEU:HB3	1:A:378:ASN:H	1.67	0.42
1:B:1170:ALA:HA	1:B:1417:ASP:OD2	2.20	0.42
1:A:253:TRP:CH2	1:A:257:GLN:HG2	2.54	0.42
1:B:1235:ASN:ND2	1:B:1236:GLY:N	2.65	0.42
1:A:530:LEU:CD2	1:A:540:LEU:HD12	2.49	0.42
1:B:1386:ASP:HA	1:B:1387:PRO:HD2	1.91	0.42
1:B:1090:VAL:HG21	1:B:1106:ASN:HD22	1.85	0.42
1:B:1511:GLN:HG3	1:B:1521:PRO:HG2	2.01	0.42
1:B:1362:THR:O	1:B:1384:ARG:HA	2.20	0.42
1:B:1459:ASP:CG	1:B:1482:MET:HG3	2.45	0.42
1:A:165:SER:C	1:A:166:ASN:HD22	2.28	0.41
1:B:1058:ILE:HD12	1:B:1073:ALA:CB	2.50	0.41
1:B:1212:LEU:HD12	1:B:1212:LEU:HA	1.91	0.41
1:B:1307:GLN:HE21	1:B:1307:GLN:HB3	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1311:ASP:C	1:B:1312:ILE:HD12	2.44	0.41
1:B:1152:LEU:HD11	8:B:2333:HOH:O	2.20	0.41
1:A:255:ARG:HG2	8:A:2327:HOH:O	2.21	0.41
1:A:422:CYS:O	1:A:426:ILE:HG13	2.20	0.41
1:A:510:LEU:HD12	1:A:510:LEU:HA	1.87	0.41
1:B:1240:LYS:HD2	1:B:1253:TRP:CZ2	2.55	0.41
1:A:366:ALA:HB3	8:A:2081:HOH:O	2.20	0.41
1:A:451:THR:O	1:A:455:LEU:CD2	2.69	0.41
1:B:1256:GLU:O	1:B:1259:ALA:HB3	2.20	0.41
1:B:1307:GLN:CG	1:B:1308:GLN:N	2.82	0.41
1:A:520:HIS:O	1:A:521:PRO:C	2.60	0.41
1:A:530:LEU:HD22	1:A:540:LEU:HD12	2.02	0.41
1:B:1350:ARG:O	1:B:1354:MET:HG2	2.21	0.41
1:B:1166:ASN:HB2	1:B:1402:LYS:HZ1	1.82	0.41
1:A:219:HIS:HD1	1:A:230:GLN:CD	2.29	0.41
1:A:568:LEU:HD23	1:A:569:ALA:H	1.85	0.41
1:A:49:ASN:O	1:A:53:VAL:HG13	2.21	0.41
1:A:184:GLU:CD	1:A:184:GLU:H	2.28	0.41
1:A:207:LEU:HD23	1:A:207:LEU:HA	1.93	0.41
1:A:312:ILE:HA	1:A:313:PRO:HD3	1.85	0.41
1:B:1027:ALA:HB1	1:B:1292:LEU:CD2	2.42	0.41
1:B:1552:GLU:O	1:B:1556:ARG:HB2	2.21	0.41
1:B:1576:ASP:CG	1:B:1577:LYS:N	2.79	0.41
1:A:255:ARG:HH12	1:A:570:SER:C	2.28	0.41
1:A:262:ASN:N	1:A:262:ASN:ND2	2.68	0.41
1:A:385:ILE:O	1:A:385:ILE:HG13	2.19	0.41
1:B:1053:VAL:CG1	1:B:1288:LEU:HD21	2.51	0.41
1:B:1319:VAL:CG1	1:B:1351:LEU:HD13	2.49	0.41
1:B:1253:TRP:O	1:B:1257:GLN:HB2	2.21	0.40
1:A:7:ILE:HD13	1:A:11:LEU:HD22	2.03	0.40
1:A:562:VAL:HG12	1:A:563:ALA:N	2.36	0.40
1:B:1495:LEU:HA	1:B:1495:LEU:HD12	1.82	0.40
1:B:1030:ILE:HD13	1:B:1285:VAL:HG13	2.04	0.40
1:A:47:ALA:O	1:A:48:SER:C	2.64	0.40
1:A:532:ILE:HG23	1:A:566:PRO:HB3	2.03	0.40
1:B:1242:GLU:HG3	1:B:1537:SER:OG	2.22	0.40
1:B:1426:ILE:O	1:B:1430:GLN:HG3	2.21	0.40
1:A:543:ARG:NH2	7:A:701:TAS:AS	3.14	0.40
1:B:1152:LEU:CD1	8:B:2333:HOH:O	2.69	0.40
1:B:1450:PRO:HB2	1:B:1455:LEU:HD13	2.03	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	542/589 (92%)	509 (94%)	27 (5%)	6 (1%)	11	18
1	B	545/589 (92%)	514 (94%)	26 (5%)	5 (1%)	14	22
All	All	1087/1178 (92%)	1023 (94%)	53 (5%)	11 (1%)	12	20

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	164	ASP
1	A	244	ALA
1	A	48	SER
1	A	170	ALA
1	B	1170	ALA
1	A	60	ASN
1	B	1378	ASN
1	B	1055	SER
1	B	1366	ALA
1	A	572	PRO
1	B	1572	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	456/487 (94%)	418 (92%)	38 (8%)	10	17
1	B	458/487 (94%)	424 (93%)	34 (7%)	13	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	914/974 (94%)	842 (92%)	72 (8%)	11	19

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	40	LEU
1	A	49	ASN
1	A	53	VAL
1	A	68	VAL
1	A	126	LEU
1	A	132	LEU
1	A	134	THR
1	A	166	ASN
1	A	209	LYS
1	A	212	LEU
1	A	225	ILE
1	A	257	GLN
1	A	258	GLU
1	A	270	LEU
1	A	291	LEU
1	A	312	ILE
1	A	315	LEU
1	A	316	SER
1	A	318	LEU
1	A	350	ARG
1	A	351	LEU
1	A	404	LYS
1	A	406	LEU
1	A	414	LEU
1	A	437	ARG
1	A	457	LEU
1	A	495	LEU
1	A	510	LEU
1	A	534	ASP
1	A	536	ARG
1	A	552	GLU
1	A	553	SER
1	A	556	ARG
1	A	561	ARG
1	A	564	LEU
1	A	568	LEU

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Mol	Chain	Res	Type
1	A	571	GLU
1	B	1004	LEU
1	B	1005	GLN
1	B	1040	LEU
1	B	1068	VAL
1	B	1083	GLN
1	B	1126	LEU
1	B	1134	THR
1	B	1135	ARG
1	B	1164	ASP
1	B	1212	LEU
1	B	1217	ARG
1	B	1260	LEU
1	B	1262	ASN
1	B	1263	LEU
1	B	1288	LEU
1	B	1291	LEU
1	B	1307	GLN
1	B	1315	LEU
1	B	1322	ILE
1	B	1332	LEU
1	B	1351	LEU
1	B	1377	LEU
1	B	1398	VAL
1	B	1399	LEU
1	B	1400	GLU
1	B	1404	LYS
1	B	1414	LEU
1	B	1455	LEU
1	B	1457	LEU
1	B	1483	MET
1	B	1510	LEU
1	B	1536	ARG
1	B	1560	SER
1	B	1564	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	35	GLN
1	A	49	ASN

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Mol	Chain	Res	Type
1	A	52	GLN
1	A	56	GLN
1	A	63	GLN
1	A	79	GLN
1	A	83	GLN
1	A	84	GLN
1	A	154	GLN
1	A	166	ASN
1	A	229	ASN
1	A	235	ASN
1	A	257	GLN
1	A	262	ASN
1	A	325	ASN
1	A	327	HIS
1	A	381	GLN
1	A	486	GLN
1	A	509	ASN
1	A	557	GLN
1	B	1035	GLN
1	B	1049	ASN
1	B	1052	GLN
1	B	1079	GLN
1	B	1106	ASN
1	B	1108	GLN
1	B	1138	HIS
1	B	1154	GLN
1	B	1166	ASN
1	B	1185	GLN
1	B	1213	GLN
1	B	1229	ASN
1	B	1230	GLN
1	B	1235	ASN
1	B	1257	GLN
1	B	1262	ASN
1	B	1307	GLN
1	B	1325	ASN
1	B	1378	ASN
1	B	1388	HIS
1	B	1430	GLN
1	B	1486	GLN
1	B	1509	ASN
1	B	1527	ASN

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Mol	Chain	Res	Type
1	B	1557	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 28 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	$\# Z > 2$
7	TAS	A	701	-	0,3,3	-	-	0,3,3	-	-
6	ATP	B	1591	4	32,33,33	0.74	0	48,52,52	1.81	13 (27%)
5	ADP	B	1590	4	28,29,29	1.21	3 (10%)	43,45,45	3.06	21 (48%)
7	TAS	B	1701	-	0,3,3	-	-	0,3,3	-	-
6	ATP	A	591	4	32,33,33	0.69	0	48,52,52	1.77	7 (14%)
5	ADP	A	590	4	28,29,29	1.22	4 (14%)	43,45,45	3.70	24 (55%)

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
5	ADP	A	590	4	-	2/16/32/32	0/3/3/3
6	ATP	A	591	4	-	1/22/38/38	0/3/3/3
6	ATP	B	1591	4	-	1/22/38/38	0/3/3/3
5	ADP	B	1590	4	-	1/16/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1590	ADP	C8-N9	-2.84	1.32	1.37
5	A	590	ADP	C8-N9	-2.63	1.33	1.37
5	A	590	ADP	C1'-N9	2.58	1.53	1.46
5	B	1590	ADP	C1'-N9	2.40	1.53	1.46
5	A	590	ADP	C2'-C3'	2.19	1.59	1.53
5	A	590	ADP	C8-N7	-2.11	1.27	1.31
5	B	1590	ADP	C2'-C3'	2.06	1.58	1.53

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	590	ADP	C4'-O4'-C1'	10.37	132.36	109.47
5	B	1590	ADP	C4'-O4'-C1'	7.72	126.51	109.47
5	A	590	ADP	O4'-C4'-C3'	-7.69	89.88	105.15
5	A	590	ADP	O4'-C1'-C2'	-7.07	91.49	106.62
5	A	590	ADP	O2A-PA-O5'	6.57	137.33	107.57
5	A	590	ADP	C5'-C4'-C3'	6.20	137.54	115.21
6	A	591	ATP	N3-C2-N1	-6.19	119.21	128.58
5	A	590	ADP	N3-C2-N1	-5.94	119.59	128.58
5	B	1590	ADP	N3-C2-N1	-5.91	119.63	128.58
5	B	1590	ADP	O4'-C4'-C3'	-5.75	93.75	105.15
6	B	1591	ATP	N3-C2-N1	-5.69	119.96	128.58
5	B	1590	ADP	O2A-PA-O3A	-5.40	92.67	107.27
5	B	1590	ADP	C5'-C4'-C3'	5.37	134.54	115.21
5	A	590	ADP	O4'-C1'-N9	-5.35	97.81	108.09
5	B	1590	ADP	O4'-C1'-N9	-4.86	98.76	108.09
5	A	590	ADP	C6-C5-C4	-4.84	110.57	117.18
5	A	590	ADP	O3A-PA-O1A	-4.57	96.95	110.70
6	A	591	ATP	O2'-C2'-C3'	4.52	126.30	111.82
5	B	1590	ADP	O4'-C1'-C2'	-4.44	97.11	106.62
5	B	1590	ADP	O4'-C4'-C5'	-4.11	96.17	109.33
5	A	590	ADP	C1'-N9-C8	4.04	136.05	127.09
5	A	590	ADP	O2'-C2'-C1'	4.02	123.95	110.10
5	A	590	ADP	C6-C5-N7	4.00	139.79	132.09
5	A	590	ADP	O4'-C4'-C5'	-3.99	96.55	109.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1590	ADP	C6-C5-C4	-3.98	111.75	117.18
5	A	590	ADP	PA-O5'-C5'	3.85	143.43	121.35
5	B	1590	ADP	C1'-N9-C8	3.76	135.44	127.09
5	B	1590	ADP	O2'-C2'-C1'	3.72	122.91	110.10
5	B	1590	ADP	PA-O5'-C5'	3.72	142.64	121.35
5	A	590	ADP	O5'-C5'-C4'	-3.67	96.50	108.99
5	A	590	ADP	O2A-PA-O3A	-3.54	97.69	107.27
6	A	591	ATP	C6-C5-C4	-3.48	112.43	117.18
5	B	1590	ADP	C2'-C3'-C4'	3.44	109.26	102.61
5	B	1590	ADP	C4-N9-C1'	-3.41	118.65	126.63
5	B	1590	ADP	O5'-C5'-C4'	-3.37	97.52	108.99
6	A	591	ATP	C2-N3-C4	3.34	119.98	111.83
5	A	590	ADP	O5'-PA-O1A	-3.33	95.72	108.94
5	B	1590	ADP	C6-C5-N7	3.27	138.40	132.09
6	B	1591	ATP	O2A-PA-O5'	3.14	121.80	107.57
5	A	590	ADP	C4-N9-C1'	-3.14	119.30	126.63
6	B	1591	ATP	O4'-C1'-N9	-3.05	102.22	108.09
6	B	1591	ATP	C6-C5-N7	2.86	137.60	132.09
6	B	1591	ATP	C2-N3-C4	2.83	118.74	111.83
6	B	1591	ATP	C6-C5-C4	-2.81	113.34	117.18
5	B	1590	ADP	O5'-PA-O1A	-2.59	98.68	108.94
5	A	590	ADP	C2'-C3'-C4'	2.56	107.55	102.61
6	A	591	ATP	C6-C5-N7	2.55	137.01	132.09
5	B	1590	ADP	C2-N3-C4	2.53	118.01	111.83
5	A	590	ADP	C2'-C1'-N9	2.51	119.55	113.30
5	B	1590	ADP	C2-N1-C6	2.50	122.83	118.73
5	B	1590	ADP	O2A-PA-O1A	2.47	123.91	112.44
5	B	1590	ADP	O2A-PA-O5'	2.43	118.57	107.57
6	B	1591	ATP	C4'-O4'-C1'	2.39	114.75	109.47
5	A	590	ADP	C2-N3-C4	2.34	117.54	111.83
6	B	1591	ATP	N6-C6-N1	-2.31	113.23	118.38
6	A	591	ATP	O2B-PB-O1B	2.25	122.92	112.44
5	A	590	ADP	C2-N1-C6	2.24	122.41	118.73
6	B	1591	ATP	O5'-C5'-C4'	2.22	116.56	108.99
6	B	1591	ATP	O3B-PB-O1B	-2.19	104.10	110.70
6	A	591	ATP	O3B-PB-O1B	-2.17	104.17	110.70
5	A	590	ADP	C3'-C2'-C1'	2.15	105.53	101.46
5	A	590	ADP	N9-C8-N7	2.11	116.94	113.94
6	B	1591	ATP	C2-N1-C6	2.05	122.09	118.73
6	B	1591	ATP	O2B-PB-O1B	2.03	121.89	112.44
6	B	1591	ATP	C2'-C1'-N9	2.00	118.28	113.30

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	590	ADP	O4'-C4'-C5'-O5'
5	B	1590	ADP	O4'-C4'-C5'-O5'
6	B	1591	ATP	C4'-C5'-O5'-PA
6	A	591	ATP	C4'-C5'-O5'-PA
5	A	590	ADP	PB-O3A-PA-O2A

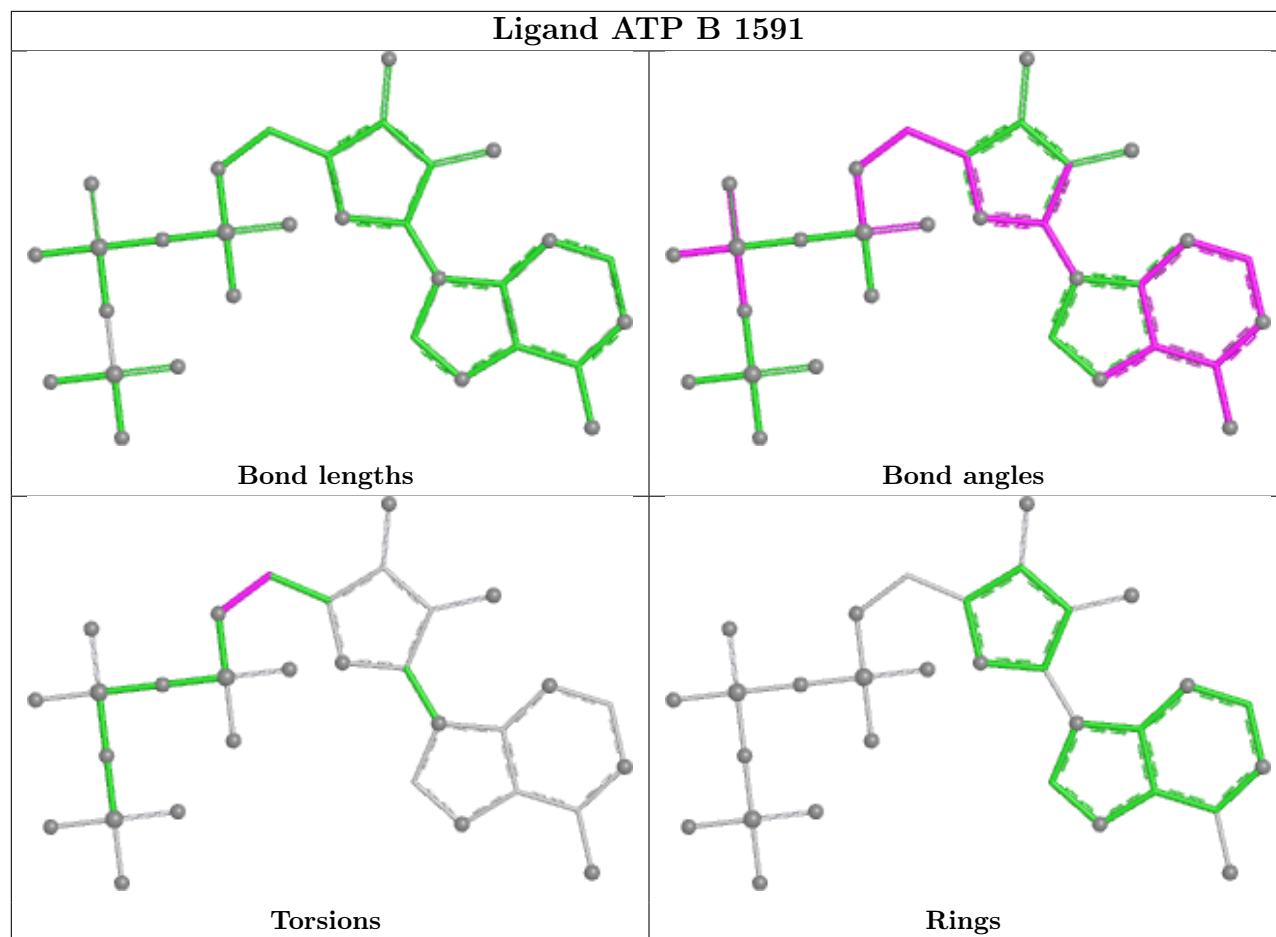
There are no ring outliers.

4 monomers are involved in 6 short contacts:

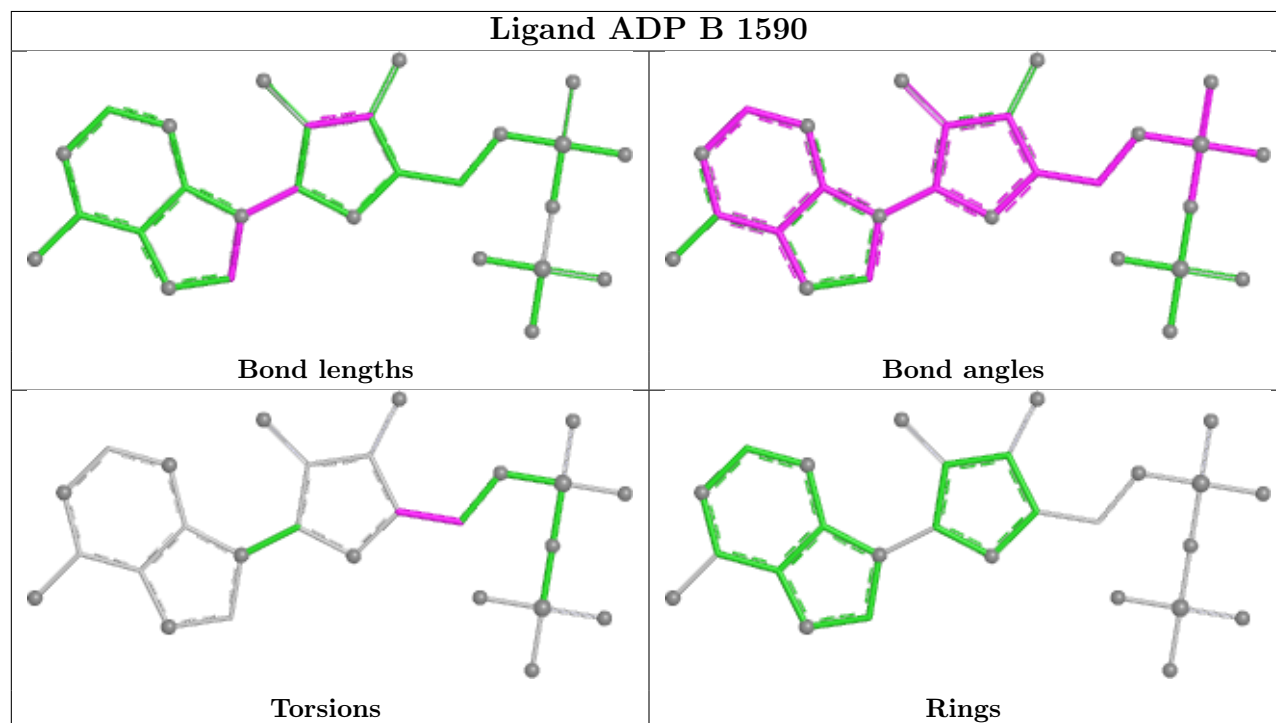
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	701	TAS	1	0
6	B	1591	ATP	1	0
5	B	1590	ADP	2	0
5	A	590	ADP	2	0

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.

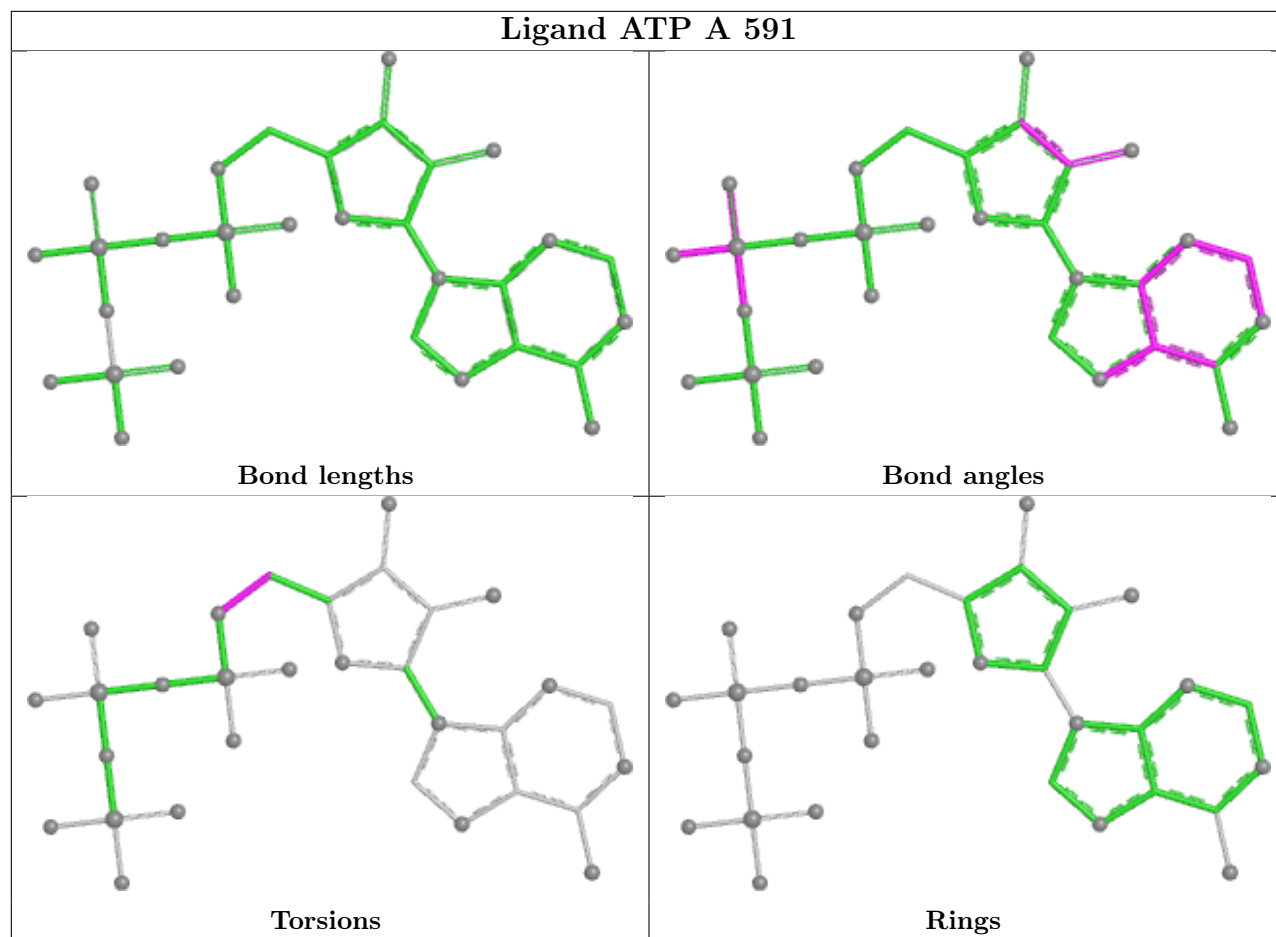
Ligand ATP B 1591



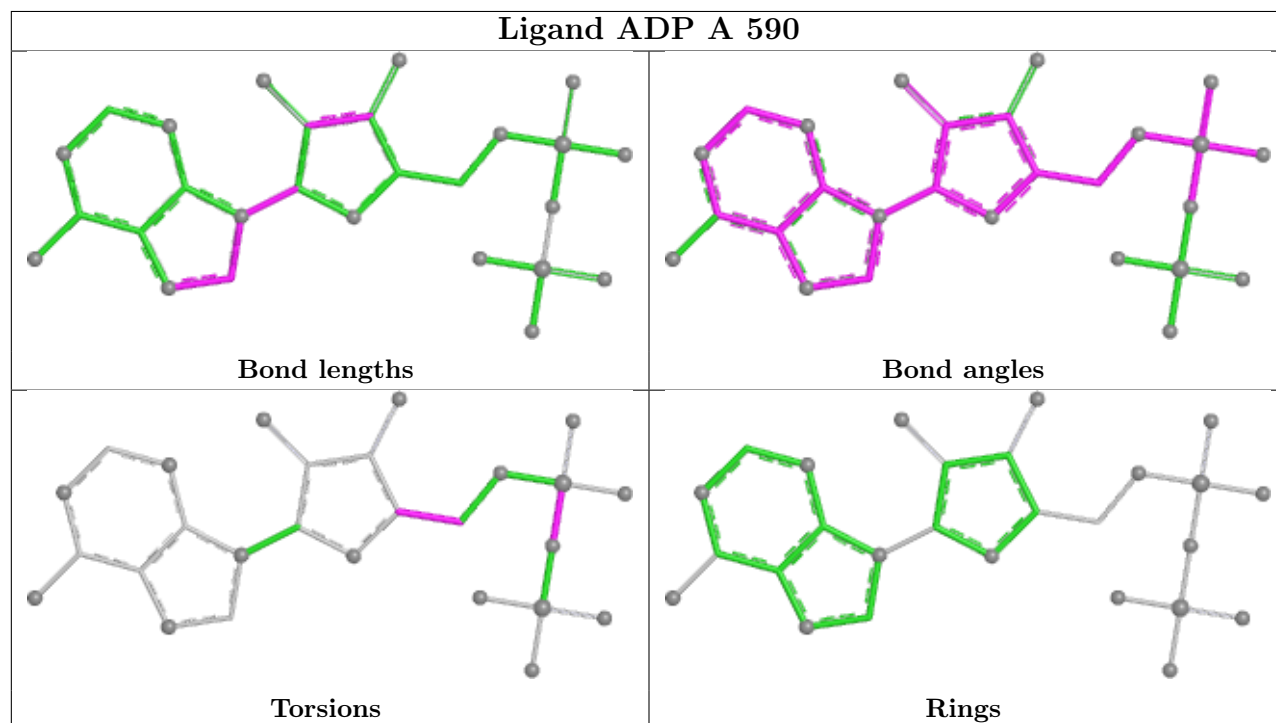
Ligand ADP B 1590



Ligand ATP A 591



Ligand ADP A 590



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	550/589 (93%)	0.17	18 (3%)	49 45	20, 36, 66, 81	0
1	B	553/589 (93%)	0.24	31 (5%)	30 26	21, 38, 67, 95	0
All	All	1103/1178 (93%)	0.21	49 (4%)	39 34	20, 38, 66, 95	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1169	GLY	7.3
1	B	1170	ALA	6.6
1	A	169	GLY	6.1
1	A	170	ALA	5.0
1	B	1167	PRO	4.5
1	A	167	PRO	4.4
1	B	1161	SER	3.8
1	B	1377	LEU	3.7
1	B	1162	PHE	3.7
1	B	1163	ILE	3.5
1	A	479	THR	3.3
1	A	480	THR	3.3
1	B	1168	GLU	3.3
1	B	1307	GLN	3.2
1	B	1401	THR	3.0
1	B	1296	PRO	3.0
1	B	1243	ALA	2.9
1	A	405	GLU	2.8
1	B	1308	GLN	2.8
1	B	1048	SER	2.7
1	B	1068	VAL	2.7
1	A	366	ALA	2.6
1	B	1365	PRO	2.5
1	A	296	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	1378	ASN	2.5
1	B	1058	ILE	2.4
1	A	293	SER	2.4
1	B	1046	PRO	2.4
1	B	1245	ASN	2.4
1	A	166	ASN	2.3
1	A	377	LEU	2.3
1	A	436	ILE	2.3
1	A	164	ASP	2.3
1	A	365	PRO	2.3
1	B	1366	ALA	2.2
1	B	1569	ALA	2.2
1	A	165	SER	2.2
1	B	1049	ASN	2.2
1	B	1165	SER	2.2
1	A	435	VAL	2.1
1	B	1367	ALA	2.1
1	B	1180	GLU	2.1
1	A	168	GLU	2.1
1	B	1244	ALA	2.0
1	B	1261	ALA	2.0
1	B	1480	THR	2.0
1	A	540	LEU	2.0
1	B	1292	LEU	2.0
1	B	1164	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

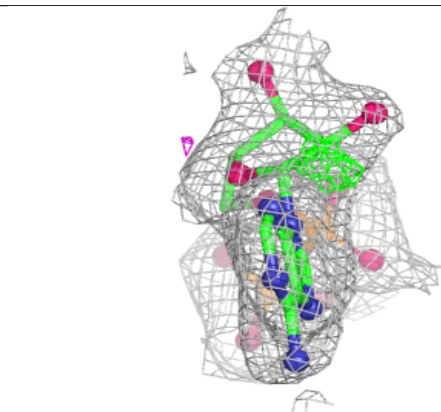
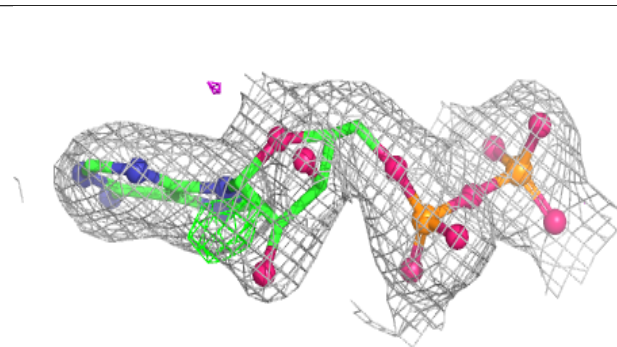
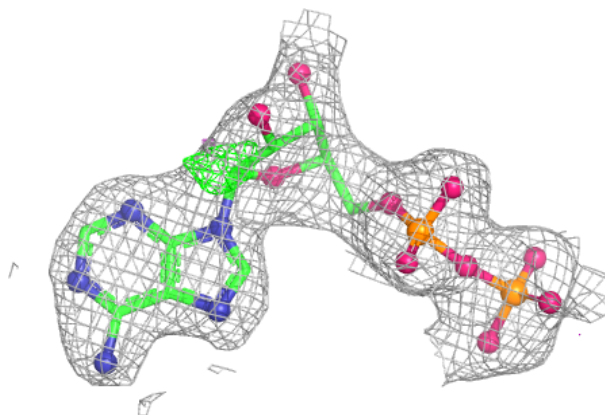
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	TAS	A	701	4/4	0.59	0.34	79,79,79,80	4
3	CL	B	1599	1/1	0.73	0.40	63,63,63,63	1
7	TAS	B	1701	4/4	0.74	0.27	63,63,63,65	4
3	CL	B	4001	1/1	0.76	0.35	50,50,50,50	1
2	CD	B	1608	1/1	0.83	0.16	90,90,90,90	1
5	ADP	A	590	27/27	0.96	0.07	26,36,38,39	0
5	ADP	B	1590	27/27	0.96	0.08	32,37,39,39	0
2	CD	B	1603	1/1	0.97	0.05	75,75,75,75	0
2	CD	A	605	1/1	0.98	0.05	45,45,45,45	1
6	ATP	A	591	31/31	0.98	0.06	29,35,39,39	0
6	ATP	B	1591	31/31	0.98	0.06	27,35,38,39	0
2	CD	A	603	1/1	0.98	0.04	91,91,91,91	0
2	CD	A	604	1/1	0.98	0.03	42,42,42,42	0
4	MG	A	592	1/1	0.99	0.04	17,17,17,17	0
4	MG	A	593	1/1	0.99	0.03	29,29,29,29	0
4	MG	B	1592	1/1	0.99	0.02	16,16,16,16	0
3	CL	A	597	1/1	0.99	0.03	26,26,26,26	0
3	CL	A	598	1/1	0.99	0.04	30,30,30,30	0
3	CL	A	4000	1/1	0.99	0.05	22,22,22,22	0
3	CL	B	1597	1/1	0.99	0.04	31,31,31,31	0
2	CD	B	1607	1/1	0.99	0.03	33,33,33,33	1
2	CD	B	1596	1/1	0.99	0.02	30,30,30,30	0
2	CD	A	600	1/1	1.00	0.01	22,22,22,22	0
2	CD	B	1601	1/1	1.00	0.01	26,26,26,26	0
2	CD	B	1602	1/1	1.00	0.02	29,29,29,29	0
2	CD	A	601	1/1	1.00	0.02	22,22,22,22	0
2	CD	A	602	1/1	1.00	0.03	31,31,31,31	0
4	MG	B	1593	1/1	1.00	0.02	23,23,23,23	0
2	CD	A	594	1/1	1.00	0.01	32,32,32,32	0
2	CD	A	595	1/1	1.00	0.02	27,27,27,27	0
2	CD	A	596	1/1	1.00	0.01	29,29,29,29	0
2	CD	B	1594	1/1	1.00	0.02	28,28,28,28	0
2	CD	B	1595	1/1	1.00	0.01	24,24,24,24	0
3	CL	B	1598	1/1	1.00	0.04	24,24,24,24	0

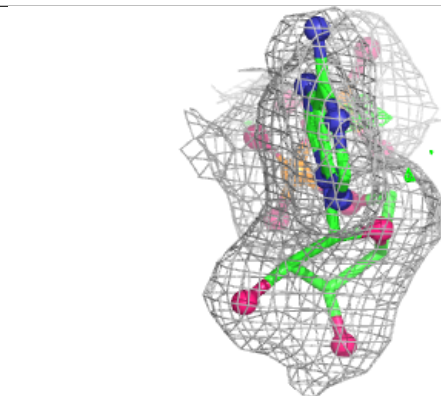
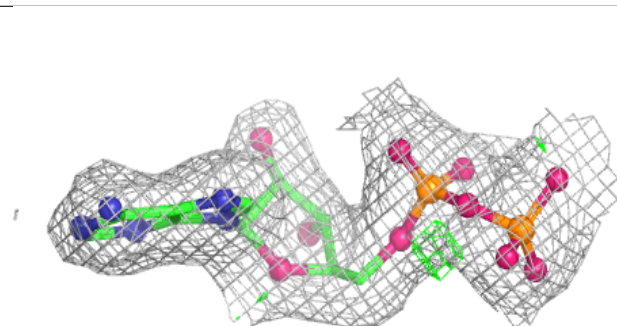
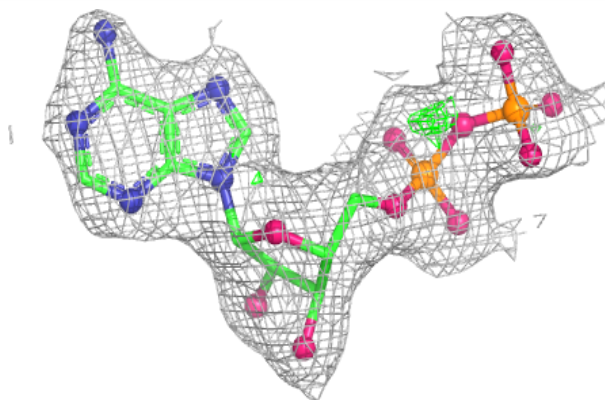
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP A 590:

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

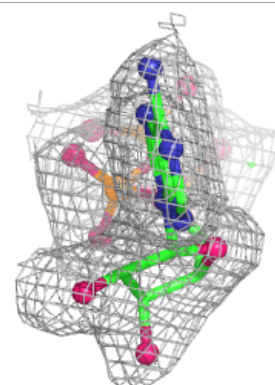
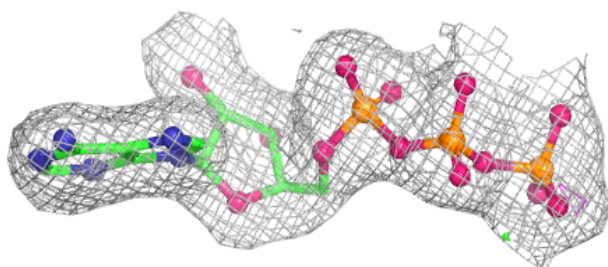
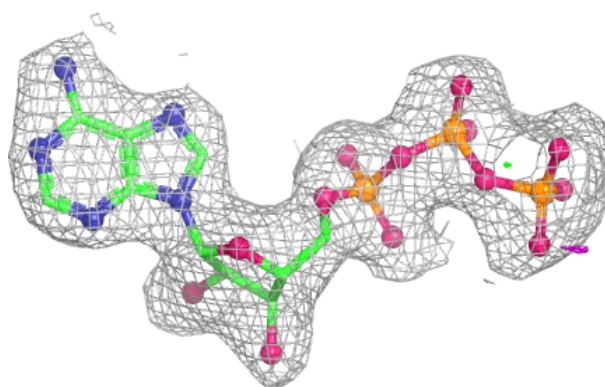
**Electron density around ADP B 1590:**

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

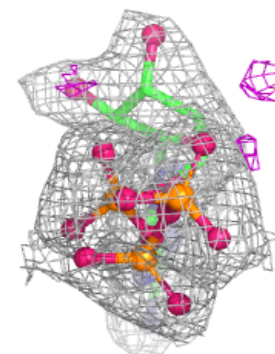
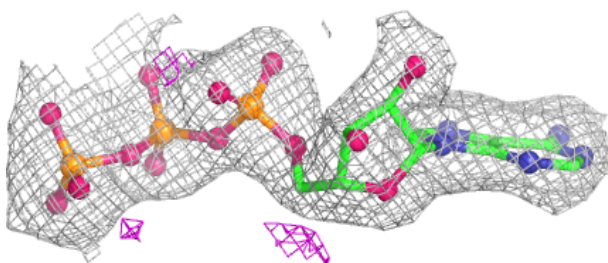
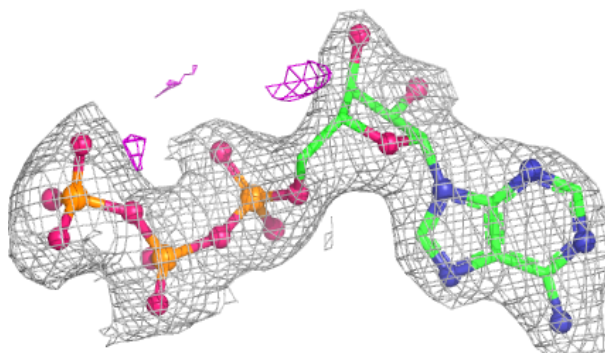


Electron density around ATP A 591:

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

**Electron density around ATP B 1591:**

$2mF_o-DF_c$ (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.