



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 04:12 AM UTC

PDB ID : 3H39 / pdb_00003h39
Title : The complex structure of CCA-adding enzyme with ATP
Authors : Toh, Y.; Tomita, K.
Deposited on : 2009-04-16
Resolution : 2.85 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

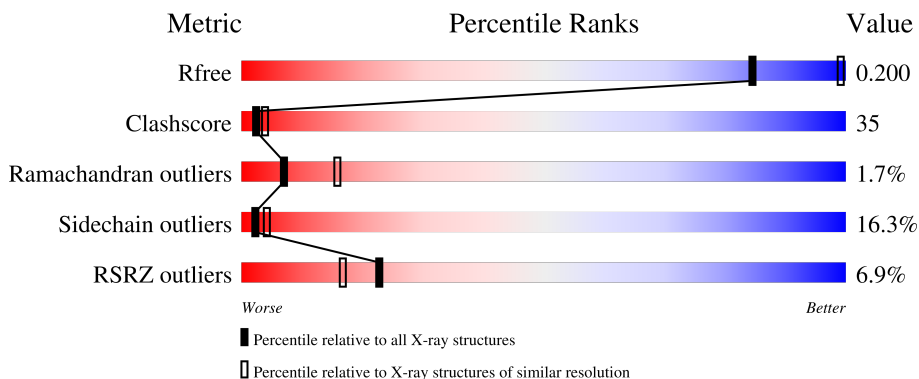
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	441	6% 46% 35% 11% • 6%
1	B	441	7% 45% 39% 10% • 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6970 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 TRNA nucleotidyl transferase-related protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	415	Total	C	N	O	S	0	0	0
			3418	2208	580	619	11			
1	B	420	Total	C	N	O	S	0	0	0
			3450	2228	586	625	11			

There are 28 discrepancies between the modelled and reference sequences:

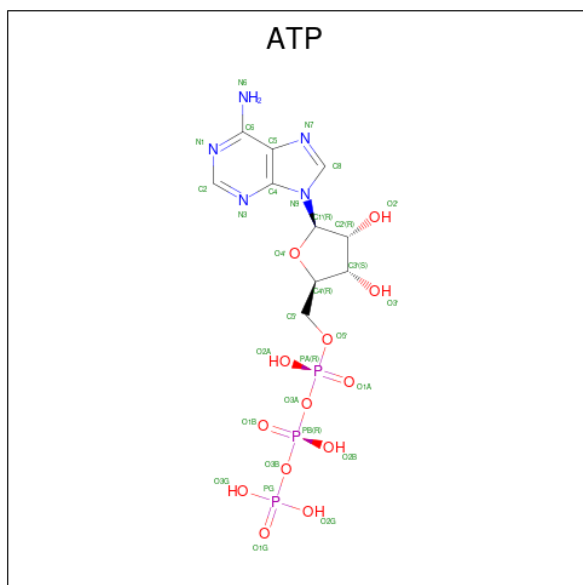
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q9WZH4
A	429	LYS	-	expression tag	UNP Q9WZH4
A	430	LEU	-	expression tag	UNP Q9WZH4
A	431	ALA	-	expression tag	UNP Q9WZH4
A	432	ALA	-	expression tag	UNP Q9WZH4
A	433	ALA	-	expression tag	UNP Q9WZH4
A	434	LEU	-	expression tag	UNP Q9WZH4
A	435	GLU	-	expression tag	UNP Q9WZH4
A	436	HIS	-	expression tag	UNP Q9WZH4
A	437	HIS	-	expression tag	UNP Q9WZH4
A	438	HIS	-	expression tag	UNP Q9WZH4
A	439	HIS	-	expression tag	UNP Q9WZH4
A	440	HIS	-	expression tag	UNP Q9WZH4
A	441	HIS	-	expression tag	UNP Q9WZH4
B	1	MET	-	expression tag	UNP Q9WZH4
B	429	LYS	-	expression tag	UNP Q9WZH4
B	430	LEU	-	expression tag	UNP Q9WZH4
B	431	ALA	-	expression tag	UNP Q9WZH4
B	432	ALA	-	expression tag	UNP Q9WZH4
B	433	ALA	-	expression tag	UNP Q9WZH4
B	434	LEU	-	expression tag	UNP Q9WZH4
B	435	GLU	-	expression tag	UNP Q9WZH4
B	436	HIS	-	expression tag	UNP Q9WZH4
B	437	HIS	-	expression tag	UNP Q9WZH4
B	438	HIS	-	expression tag	UNP Q9WZH4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	439	HIS	-	expression tag	UNP Q9WZH4
B	440	HIS	-	expression tag	UNP Q9WZH4
B	441	HIS	-	expression tag	UNP Q9WZH4

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

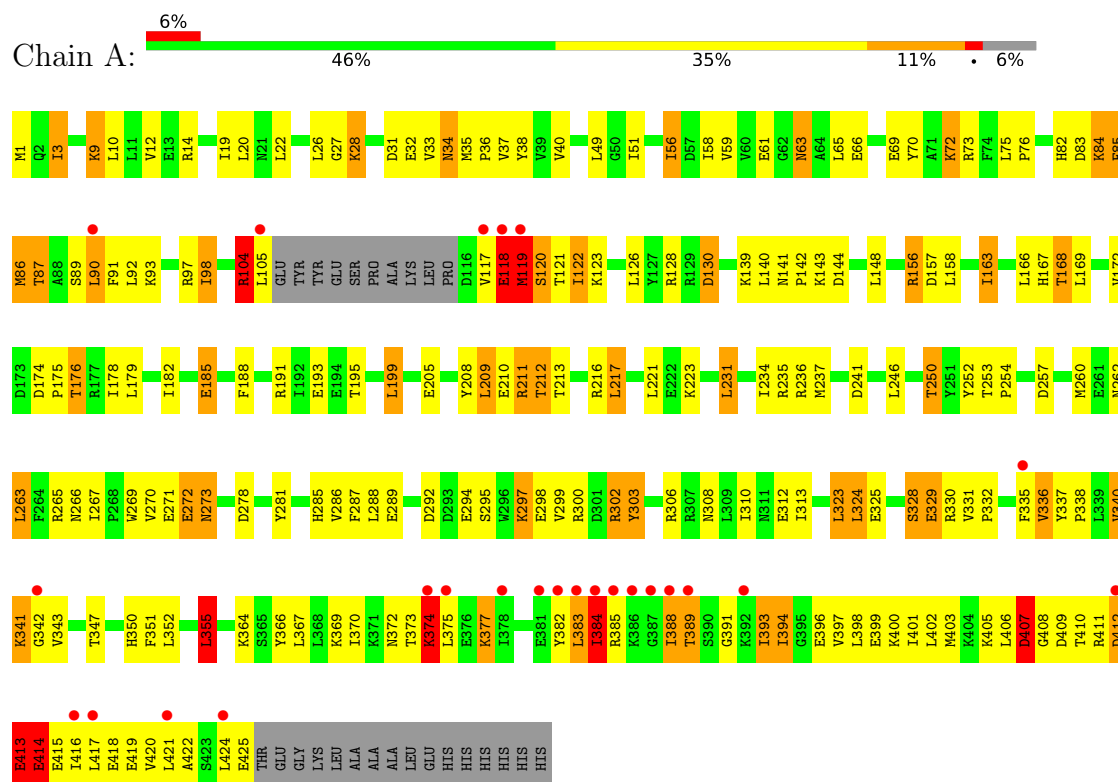
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total	O	0	0
			30	30		
3	B	10	Total	O	0	0
			10	10		

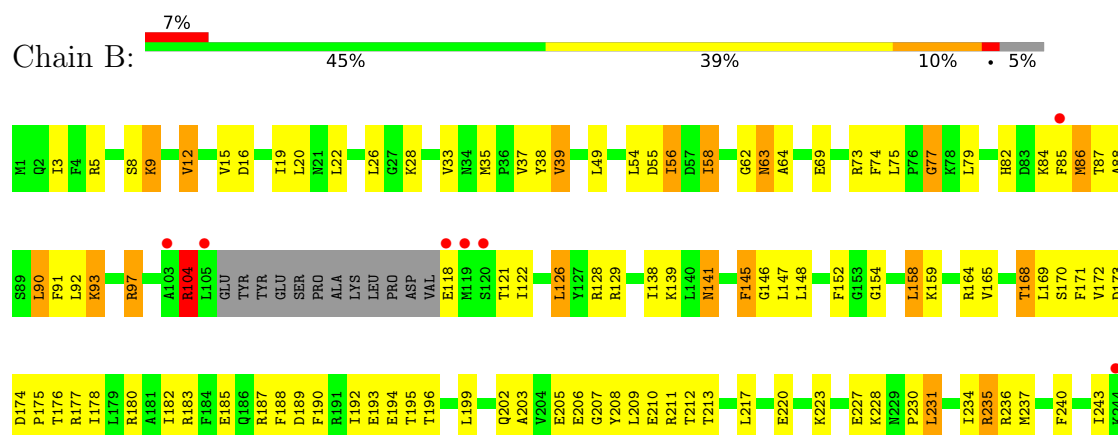
3 Residue-property plots

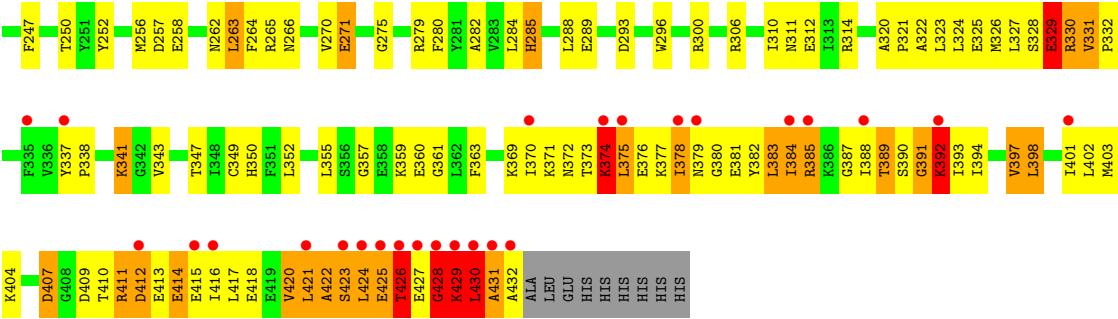
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: TRNA nucleotidyl transferase-related protein



• Molecule 1: TRNA nucleotidyl transferase-related protein





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	186.09Å 64.07Å 151.77Å 90.00° 100.88° 90.00°	Depositor
Resolution (Å)	36.03 – 2.85 36.03 – 2.85	Depositor EDS
% Data completeness (in resolution range)	96.9 (36.03-2.85) 96.8 (36.03-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.210 , 0.252 0.207 , 0.200	Depositor DCC
R_{free} test set	1963 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	63.7	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 70.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6970	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 3.79% 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: 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	0.87	2/3479 (0.1%)	1.17	37/4674 (0.8%)
1	B	0.66	1/3511 (0.0%)	1.12	21/4716 (0.4%)
All	All	0.77	3/6990 (0.0%)	1.15	58/9390 (0.6%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	188	PHE	CA-C	-6.01	1.45	1.52
1	A	3	ILE	CA-CB	-5.37	1.47	1.54
1	B	3	ILE	CA-CB	-5.18	1.47	1.54

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	104	ARG	CB-CA-C	-18.83	76.31	109.64
1	B	425	GLU	N-CA-C	-15.92	94.29	113.88
1	A	121	THR	N-CA-C	-11.45	99.54	114.31
1	B	392	LYS	CB-CA-C	-11.06	88.41	110.42
1	A	119	MET	N-CA-C	-10.83	100.26	113.15
1	B	422	ALA	N-CA-C	-10.45	100.47	113.01
1	A	414	GLU	N-CA-C	-10.26	100.10	111.28
1	A	384	ILE	N-CA-C	9.88	119.90	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	430	LEU	CB-CA-C	9.83	129.98	110.42
1	B	341	LYS	N-CA-C	9.31	121.04	111.07
1	B	104	ARG	CA-C-N	9.28	138.40	121.70
1	B	104	ARG	C-N-CA	9.28	138.40	121.70
1	A	188	PHE	N-CA-C	-8.96	95.70	109.95
1	B	145	PHE	N-CA-C	8.26	119.90	111.07
1	B	228	LYS	N-CA-C	7.86	119.48	111.07
1	B	411	ARG	N-CA-C	7.83	119.90	111.36
1	B	387	GLY	N-CA-C	-7.80	99.91	112.31
1	A	246	LEU	N-CA-C	-7.61	103.84	113.43
1	A	104	ARG	N-CA-C	7.55	119.70	110.41
1	B	86	MET	N-CA-C	7.49	121.58	111.24
1	B	3	ILE	CB-CA-C	-7.17	102.90	111.94
1	A	303	TYR	N-CA-C	-7.06	99.19	110.14
1	A	19	ILE	N-CA-C	7.05	117.85	110.72
1	A	288	LEU	N-CA-C	7.04	121.89	113.16
1	A	391	GLY	N-CA-C	6.96	123.96	111.02
1	A	341	LYS	CB-CA-C	-6.88	99.94	110.26
1	A	328	SER	N-CA-C	-6.31	102.03	110.24
1	B	428	GLY	N-CA-C	6.29	128.08	113.18
1	A	377	LYS	CB-CA-C	-6.26	109.34	116.54
1	A	374	LYS	N-CA-C	-6.19	105.79	113.15
1	B	19	ILE	N-CA-C	6.17	116.33	110.53
1	A	372	ASN	N-CA-C	6.11	118.90	111.82
1	A	130	ASP	N-CA-C	6.06	120.83	111.56
1	A	329	GLU	CB-CA-C	-5.95	103.42	112.11
1	A	188	PHE	CA-C-N	-5.88	113.26	122.08
1	A	188	PHE	C-N-CA	-5.88	113.26	122.08
1	A	355	LEU	N-CA-C	5.72	118.39	109.52
1	A	328	SER	CA-C-N	-5.72	114.39	122.63
1	A	328	SER	C-N-CA	-5.72	114.39	122.63
1	A	303	TYR	CA-C-N	-5.67	114.97	122.85
1	A	303	TYR	C-N-CA	-5.67	114.97	122.85
1	A	272	GLU	CB-CA-C	-5.60	100.26	110.63
1	A	388	ILE	CB-CA-C	-5.47	104.04	111.15
1	B	401	ILE	CB-CA-C	-5.47	104.72	111.94
1	A	185	GLU	CB-CA-C	-5.41	100.63	110.63
1	A	120	SER	CB-CA-C	5.39	120.20	112.12
1	B	392	LYS	N-CA-C	5.36	122.23	110.80
1	A	407	ASP	N-CA-C	5.32	118.11	111.24
1	B	374	LYS	N-CA-C	-5.30	104.55	111.02
1	A	120	SER	CA-C-N	5.27	130.51	122.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	SER	C-N-CA	5.27	130.51	122.24
1	A	413	GLU	CB-CA-C	-5.26	98.99	110.41
1	A	34	ASN	N-CA-C	5.14	118.68	111.74
1	A	370	ILE	N-CA-C	5.14	115.92	110.72
1	A	83	ASP	N-CA-C	5.12	117.60	111.71
1	A	388	ILE	N-CA-C	5.07	115.58	108.89
1	B	121	THR	N-CA-C	-5.04	106.97	113.23
1	B	77	GLY	N-CA-C	5.00	117.89	110.63

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	104	ARG	Peptide

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	3418	0	3517	244	0
1	B	3450	0	3554	247	0
2	A	31	0	12	1	0
2	B	31	0	12	3	0
3	A	30	0	0	0	0
3	B	10	0	0	1	0
All	All	6970	0	7095	492	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 35.

All (492) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:LEU:HD11	1:A:92:LEU:CD2	1.62	1.27
1:B:427:GLU:CG	1:B:428:GLY:H	1.47	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:LEU:HD21	1:B:431:ALA:CB	1.71	1.19
1:B:104:ARG:HD3	1:B:128:ARG:HD3	1.19	1.18
1:B:381:GLU:HG3	1:B:382:TYR:H	1.01	1.18
1:A:383:LEU:H	1:A:383:LEU:CD1	1.52	1.16
1:B:202:GLN:O	1:B:206:GLU:HG3	1.42	1.16
1:A:383:LEU:N	1:A:383:LEU:HD12	1.57	1.13
1:B:425:GLU:O	1:B:426:THR:HG22	1.48	1.13
1:A:341:LYS:O	1:A:341:LYS:HG3	1.50	1.11
1:A:410:THR:CG2	1:A:411:ARG:H	1.64	1.11
1:A:90:LEU:HD11	1:A:92:LEU:HD21	1.12	1.09
1:B:411:ARG:HD2	1:B:411:ARG:O	1.51	1.09
1:B:424:LEU:CD2	1:B:431:ALA:HB1	1.83	1.08
1:B:427:GLU:HG2	1:B:428:GLY:H	0.93	1.08
1:A:90:LEU:CD1	1:A:92:LEU:CD2	2.29	1.07
1:B:430:LEU:HD12	1:B:431:ALA:H	1.17	1.07
1:B:429:LYS:O	1:B:430:LEU:HB3	1.52	1.04
1:B:330:ARG:O	1:B:330:ARG:HG2	1.58	1.04
1:A:410:THR:HG22	1:A:411:ARG:H	0.92	1.03
1:B:427:GLU:CG	1:B:428:GLY:N	2.13	1.02
1:A:90:LEU:CD1	1:A:92:LEU:HD21	1.89	1.01
1:A:331:VAL:HB	1:A:332:PRO:HD2	1.39	1.00
1:A:410:THR:HG22	1:A:411:ARG:N	1.57	1.00
1:A:82:HIS:HD2	1:A:87:THR:CG2	1.74	0.99
1:A:117:VAL:O	1:A:118:GLU:HB3	1.59	0.99
1:A:273:ASN:N	1:A:273:ASN:HD22	1.60	0.98
1:A:117:VAL:O	1:A:118:GLU:CB	2.10	0.98
1:B:427:GLU:HG2	1:B:428:GLY:N	1.69	0.98
1:A:384:ILE:HD11	1:A:397:VAL:HG21	1.45	0.97
1:B:424:LEU:HD21	1:B:431:ALA:HB1	0.97	0.97
1:A:383:LEU:H	1:A:383:LEU:HD12	0.82	0.96
1:A:373:THR:HG22	1:A:373:THR:O	1.66	0.95
1:B:104:ARG:HD3	1:B:128:ARG:CD	1.96	0.95
1:B:381:GLU:HG3	1:B:382:TYR:N	1.82	0.93
1:B:176:THR:HG23	1:B:220:GLU:HG3	1.51	0.92
1:B:388:ILE:O	1:B:389:THR:HG23	1.69	0.92
1:B:381:GLU:CG	1:B:382:TYR:H	1.76	0.91
1:B:388:ILE:O	1:B:389:THR:OG1	1.88	0.91
1:B:328:SER:O	1:B:329:GLU:HB2	1.66	0.91
1:B:411:ARG:HD2	1:B:411:ARG:C	1.89	0.91
1:A:82:HIS:CD2	1:A:87:THR:CG2	2.55	0.90
1:A:90:LEU:HD11	1:A:92:LEU:HD23	1.53	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:HIS:HD2	1:A:87:THR:HG23	1.37	0.88
1:B:425:GLU:C	1:B:426:THR:HG22	1.96	0.88
1:B:381:GLU:O	1:B:384:ILE:HG23	1.77	0.85
1:B:429:LYS:O	1:B:430:LEU:CB	2.24	0.85
1:B:93:LYS:H	1:B:93:LYS:HD2	1.40	0.85
1:A:9:LYS:H	1:A:9:LYS:CD	1.90	0.85
1:A:90:LEU:CD1	1:A:92:LEU:HD23	2.07	0.85
1:A:37:VAL:H	1:A:141:ASN:HD21	1.24	0.84
1:B:37:VAL:H	1:B:141:ASN:HD21	1.26	0.84
1:A:272:GLU:HB2	1:A:273:ASN:ND2	1.93	0.84
1:B:430:LEU:HD12	1:B:431:ALA:N	1.93	0.83
1:A:63:ASN:OD1	1:A:86:MET:HE2	1.78	0.82
1:A:118:GLU:C	1:A:120:SER:H	1.87	0.81
1:B:69:GLU:OE1	1:B:79:LEU:CD2	2.28	0.81
1:A:417:LEU:HA	1:A:420:VAL:HG22	1.61	0.80
1:B:174:ASP:OD1	1:B:176:THR:HB	1.80	0.80
1:B:388:ILE:O	1:B:389:THR:CG2	2.29	0.80
1:A:297:LYS:HG3	1:A:298:GLU:N	1.97	0.79
1:A:93:LYS:H	1:A:93:LYS:HD2	1.46	0.79
1:A:139:LYS:HD3	1:A:144:ASP:HB2	1.64	0.79
1:A:373:THR:O	1:A:373:THR:CG2	2.30	0.79
1:B:411:ARG:O	1:B:411:ARG:CD	2.30	0.79
1:A:91:PHE:HZ	1:A:97:ARG:HH11	1.27	0.79
1:B:420:VAL:O	1:B:423:SER:HB2	1.82	0.78
1:B:425:GLU:O	1:B:426:THR:CG2	2.29	0.78
1:A:49:LEU:HD21	1:A:158:LEU:HD22	1.64	0.78
1:B:330:ARG:O	1:B:330:ARG:CG	2.32	0.78
1:B:411:ARG:C	1:B:411:ARG:CD	2.52	0.78
1:B:427:GLU:HG3	1:B:428:GLY:N	1.98	0.77
1:B:93:LYS:H	1:B:93:LYS:CD	1.97	0.77
1:A:262:ASN:HD22	1:A:265:ARG:HH22	1.31	0.77
1:A:337:TYR:CD2	1:A:403:MET:HE1	2.19	0.77
1:B:331:VAL:HG12	1:B:332:PRO:HD2	1.67	0.76
1:B:380:GLY:O	1:B:381:GLU:HG2	1.84	0.76
1:B:12:VAL:HA	1:B:20:LEU:HD11	1.66	0.76
1:A:56:ILE:HG12	1:A:56:ILE:O	1.85	0.76
1:B:328:SER:O	1:B:329:GLU:CB	2.35	0.75
1:B:424:LEU:N	1:B:424:LEU:HD13	2.02	0.75
1:A:384:ILE:HG21	1:A:394:ILE:HG23	1.68	0.74
1:A:90:LEU:HB3	1:A:98:ILE:CG2	2.17	0.74
1:A:294:GLU:OE1	1:A:297:LYS:HE2	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:THR:HG21	1:B:414:GLU:HG2	1.70	0.74
1:B:209:LEU:HD12	1:B:209:LEU:H	1.52	0.74
1:B:388:ILE:HG22	1:B:389:THR:N	2.03	0.74
1:B:74:PHE:C	1:B:75:LEU:HD12	2.13	0.74
1:B:413:GLU:O	1:B:416:ILE:HG22	1.88	0.74
1:A:117:VAL:O	1:A:118:GLU:CG	2.36	0.73
1:B:409:ASP:OD1	1:B:409:ASP:C	2.29	0.73
1:A:341:LYS:O	1:A:341:LYS:CG	2.30	0.73
1:A:211:ARG:CG	1:A:211:ARG:HH21	2.01	0.73
1:B:388:ILE:O	1:B:389:THR:CB	2.37	0.72
1:B:380:GLY:O	1:B:381:GLU:CG	2.37	0.72
1:B:247:PHE:O	1:B:250:THR:HG22	1.89	0.72
1:A:82:HIS:CD2	1:A:87:THR:HG22	2.24	0.72
1:A:328:SER:O	1:A:329:GLU:CB	2.34	0.72
1:A:82:HIS:HB2	1:A:87:THR:HG22	1.70	0.72
1:A:117:VAL:O	1:A:118:GLU:HG2	1.89	0.72
1:B:427:GLU:HG3	1:B:428:GLY:H	1.48	0.72
1:A:410:THR:HG21	1:A:414:GLU:HB3	1.72	0.72
1:B:424:LEU:N	1:B:424:LEU:CD1	2.53	0.72
1:A:340:VAL:HG23	1:A:340:VAL:O	1.89	0.71
1:A:355:LEU:HD22	1:A:355:LEU:H	1.56	0.71
1:A:273:ASN:N	1:A:273:ASN:ND2	2.30	0.71
1:B:388:ILE:CG2	1:B:389:THR:H	2.02	0.71
1:A:424:LEU:O	1:A:425:GLU:HG2	1.91	0.70
1:B:380:GLY:C	1:B:381:GLU:HG2	2.15	0.70
1:B:428:GLY:O	1:B:429:LYS:HB3	1.92	0.70
1:B:194:GLU:HG3	1:B:195:THR:N	2.05	0.70
1:B:202:GLN:HG2	1:B:206:GLU:OE2	1.92	0.69
1:A:84:LYS:HD2	1:A:84:LYS:C	2.17	0.69
1:B:388:ILE:CG2	1:B:389:THR:N	2.55	0.69
1:A:9:LYS:H	1:A:9:LYS:HD2	1.57	0.69
1:B:262:ASN:HD22	1:B:265:ARG:HH12	1.41	0.69
1:A:85:PHE:O	1:A:86:MET:C	2.35	0.69
1:B:54:LEU:O	1:B:56:ILE:HD12	1.92	0.69
1:B:56:ILE:CG2	1:B:58:ILE:HD12	2.23	0.69
1:B:56:ILE:HG22	1:B:56:ILE:O	1.91	0.69
1:B:376:GLU:HA	1:B:376:GLU:OE1	1.91	0.68
1:A:90:LEU:C	1:A:90:LEU:HD13	2.17	0.68
1:A:174:ASP:OD1	1:A:176:THR:HB	1.94	0.68
1:A:410:THR:CG2	1:A:414:GLU:HB3	2.23	0.68
1:A:420:VAL:O	1:A:424:LEU:HB2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:PHE:O	1:A:87:THR:HB	1.95	0.67
1:A:388:ILE:HG23	1:A:388:ILE:O	1.94	0.67
1:B:410:THR:HG22	1:B:411:ARG:H	1.58	0.67
1:A:117:VAL:C	1:A:118:GLU:CG	2.65	0.67
1:B:175:PRO:HD2	1:B:212:THR:HG21	1.75	0.67
1:B:384:ILE:HD11	1:B:394:ILE:HA	1.77	0.67
1:B:407:ASP:OD2	1:B:407:ASP:N	2.26	0.67
1:A:384:ILE:HG23	1:A:394:ILE:HD13	1.77	0.66
1:B:428:GLY:O	1:B:429:LYS:CB	2.44	0.66
1:A:84:LYS:HD2	1:A:84:LYS:O	1.95	0.66
1:B:378:ILE:HG21	1:B:411:ARG:HH21	1.59	0.66
1:A:213:THR:OG1	1:A:216:ARG:HG3	1.95	0.65
1:B:337:TYR:CD2	1:B:403:MET:HE1	2.32	0.65
1:A:328:SER:O	1:A:329:GLU:HB3	1.97	0.64
1:A:117:VAL:HG23	1:A:118:GLU:HG3	1.80	0.64
1:A:252:TYR:CE2	1:A:257:ASP:HB2	2.32	0.64
1:B:388:ILE:C	1:B:389:THR:OG1	2.39	0.64
1:A:403:MET:HA	1:A:406:LEU:HD12	1.79	0.63
1:B:381:GLU:CG	1:B:382:TYR:N	2.49	0.63
1:A:90:LEU:HD13	1:A:91:PHE:N	2.13	0.63
1:A:411:ARG:O	1:A:413:GLU:N	2.32	0.63
1:A:84:LYS:C	1:A:84:LYS:CD	2.72	0.63
1:B:172:VAL:HG13	1:B:208:TYR:CE1	2.34	0.62
1:B:252:TYR:HA	1:B:256:MET:HG2	1.82	0.62
1:A:262:ASN:ND2	1:A:265:ARG:HH12	1.97	0.62
1:A:272:GLU:HB2	1:A:273:ASN:HD22	1.62	0.62
1:B:391:GLY:O	1:B:392:LYS:HB2	1.99	0.61
1:B:62:GLY:O	1:B:63:ASN:HB2	2.00	0.61
1:A:331:VAL:HB	1:A:332:PRO:CD	2.17	0.61
1:B:169:LEU:C	1:B:173:ASP:OD1	2.43	0.61
1:B:331:VAL:CG1	1:B:332:PRO:HD2	2.30	0.61
1:A:36:PRO:HD3	1:A:119:MET:HE2	1.83	0.61
1:A:1:MET:SD	1:A:156:ARG:HD2	2.41	0.60
1:A:323:LEU:HD12	1:A:351:PHE:CD2	2.35	0.60
1:A:302:ARG:HG2	1:A:303:TYR:CE1	2.35	0.60
1:B:410:THR:HG22	1:B:411:ARG:N	2.15	0.60
1:B:69:GLU:OE1	1:B:79:LEU:HD23	2.01	0.60
1:A:384:ILE:CG2	1:A:394:ILE:HD13	2.32	0.60
1:B:194:GLU:CG	1:B:195:THR:N	2.64	0.60
1:A:272:GLU:C	1:A:273:ASN:HD22	2.08	0.60
1:B:329:GLU:O	1:B:331:VAL:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:TYR:N	1:B:338:PRO:HD2	2.17	0.60
1:A:211:ARG:HH21	1:A:211:ARG:HG2	1.66	0.60
1:A:407:ASP:OD2	1:A:407:ASP:N	2.30	0.60
1:A:297:LYS:HG3	1:A:298:GLU:H	1.67	0.59
1:B:296:TRP:CE2	1:B:310:ILE:HB	2.37	0.59
1:A:63:ASN:HD21	1:A:65:LEU:HB2	1.67	0.59
1:A:93:LYS:HD2	1:A:93:LYS:N	2.14	0.59
1:A:355:LEU:HD22	1:A:355:LEU:N	2.15	0.59
1:B:285:HIS:HB3	1:B:350:HIS:CD2	2.37	0.59
1:B:63:ASN:OD1	1:B:63:ASN:C	2.46	0.59
1:A:417:LEU:HA	1:A:420:VAL:CG2	2.31	0.59
1:B:49:LEU:HD21	1:B:158:LEU:HD22	1.84	0.59
1:A:424:LEU:C	1:A:425:GLU:HG2	2.27	0.59
1:A:117:VAL:C	1:A:118:GLU:HG2	2.28	0.59
1:A:234:ILE:HA	1:A:237:MET:HE3	1.85	0.59
1:A:383:LEU:CD1	1:A:383:LEU:N	2.30	0.59
1:B:393:ILE:O	1:B:397:VAL:HG13	2.03	0.59
1:A:384:ILE:O	1:A:389:THR:OG1	2.21	0.58
1:A:130:ASP:HB3	2:A:501:ATP:C2	2.38	0.58
1:B:262:ASN:ND2	1:B:265:ARG:HH12	2.01	0.58
1:B:263:LEU:HD11	1:B:282:ALA:O	2.02	0.58
1:A:120:SER:HA	1:A:122:ILE:CD1	2.34	0.58
1:B:174:ASP:OD1	1:B:174:ASP:C	2.43	0.58
1:B:87:THR:HG22	1:B:88:ALA:N	2.17	0.58
1:B:195:THR:O	1:B:199:LEU:HB2	2.03	0.58
1:B:380:GLY:C	1:B:381:GLU:CG	2.76	0.58
1:A:294:GLU:OE1	1:A:297:LYS:CE	2.51	0.58
1:B:243:ILE:HG22	1:B:250:THR:HG23	1.85	0.58
1:B:337:TYR:HD2	1:B:403:MET:HE1	1.69	0.58
1:A:384:ILE:HG22	1:A:385:ARG:N	2.19	0.58
1:A:156:ARG:HG2	1:A:157:ASP:N	2.14	0.57
1:B:390:SER:O	1:B:391:GLY:O	2.22	0.57
1:A:382:TYR:O	1:A:383:LEU:C	2.46	0.57
1:A:413:GLU:HB3	1:A:416:ILE:HB	1.85	0.57
1:A:401:ILE:HG23	1:A:415:GLU:OE2	2.04	0.57
1:B:430:LEU:O	1:B:431:ALA:HB3	2.04	0.57
1:B:431:ALA:O	1:B:432:ALA:C	2.47	0.57
1:A:411:ARG:O	1:A:412:ASP:C	2.48	0.57
1:A:337:TYR:N	1:A:338:PRO:HD2	2.19	0.56
1:B:183:ARG:HG3	1:B:227:GLU:HG3	1.87	0.56
1:B:262:ASN:ND2	1:B:265:ARG:HH22	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:HIS:HD2	1:B:350:HIS:HB2	1.70	0.56
1:B:320:ALA:HB3	1:B:321:PRO:HD3	1.86	0.56
1:A:36:PRO:CD	1:A:119:MET:HE2	2.35	0.56
1:A:373:THR:C	1:A:375:LEU:H	2.14	0.56
1:A:297:LYS:HE3	1:A:298:GLU:HG2	1.86	0.56
1:A:421:LEU:HD12	1:A:424:LEU:HD13	1.88	0.56
1:A:33:VAL:HG23	1:A:35:MET:HG3	1.86	0.56
1:A:90:LEU:HD12	1:A:92:LEU:HG	1.87	0.56
1:A:292:ASP:OD1	1:A:295:SER:HB2	2.05	0.56
1:A:9:LYS:CD	1:A:9:LYS:N	2.65	0.56
1:B:324:LEU:HD12	1:B:359:LYS:HE2	1.88	0.56
1:A:263:LEU:O	1:A:267:ILE:HG13	2.06	0.55
1:B:139:LYS:O	1:B:145:PHE:O	2.24	0.55
1:A:84:LYS:O	1:A:84:LYS:CD	2.54	0.55
1:A:211:ARG:CG	1:A:211:ARG:NH2	2.68	0.55
1:A:352:LEU:HA	1:A:355:LEU:HD21	1.87	0.55
1:A:118:GLU:C	1:A:120:SER:N	2.54	0.55
1:A:289:GLU:OE1	1:A:350:HIS:HE1	1.89	0.55
1:B:371:LYS:O	1:B:374:LYS:HD3	2.06	0.55
1:A:253:THR:HB	1:A:254:PRO:HD2	1.89	0.55
1:A:9:LYS:H	1:A:9:LYS:HD3	1.67	0.55
1:A:104:ARG:HH11	1:A:128:ARG:HD3	1.72	0.55
1:B:56:ILE:HG23	1:B:58:ILE:CD1	2.37	0.55
1:A:10:LEU:HD11	1:A:14:ARG:NE	2.22	0.55
1:B:231:LEU:O	1:B:235:ARG:HG3	2.07	0.55
1:B:381:GLU:C	1:B:383:LEU:N	2.62	0.55
1:A:388:ILE:O	1:A:388:ILE:CG2	2.56	0.54
1:A:31:ASP:OD2	1:A:142:PRO:HD2	2.07	0.54
1:A:269:TRP:CH2	1:A:364:LYS:HG2	2.42	0.54
1:A:369:LYS:O	1:A:373:THR:HB	2.07	0.54
1:A:37:VAL:N	1:A:141:ASN:HD21	1.99	0.54
1:A:167:HIS:HD2	1:A:169:LEU:H	1.56	0.54
1:A:278:ASP:OD1	1:A:281:TYR:HD2	1.91	0.54
1:A:285:HIS:ND1	1:A:350:HIS:HD2	2.06	0.54
1:B:420:VAL:O	1:B:423:SER:CB	2.55	0.54
1:B:33:VAL:HG23	1:B:35:MET:HG3	1.90	0.54
1:B:388:ILE:HG22	1:B:389:THR:H	1.68	0.54
1:A:63:ASN:HB3	1:A:66:GLU:HB2	1.89	0.54
1:A:409:ASP:OD1	1:A:409:ASP:C	2.50	0.54
1:A:211:ARG:HG2	1:A:211:ARG:NH2	2.23	0.54
1:B:391:GLY:O	1:B:392:LYS:CB	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:VAL:H	1:A:141:ASN:ND2	1.99	0.53
1:A:120:SER:HA	1:A:122:ILE:HD12	1.90	0.53
1:B:8:SER:HB3	1:B:146:GLY:HA3	1.89	0.53
1:B:169:LEU:O	1:B:173:ASP:OD1	2.25	0.53
1:A:104:ARG:O	1:A:105:LEU:C	2.51	0.53
1:A:410:THR:CG2	1:A:411:ARG:N	2.29	0.53
1:A:32:GLU:OE2	1:A:70:TYR:OH	2.20	0.53
1:A:331:VAL:O	1:A:366:TYR:OH	2.21	0.53
1:B:369:LYS:NZ	1:B:373:THR:HG21	2.23	0.53
1:B:381:GLU:O	1:B:383:LEU:N	2.41	0.53
1:A:90:LEU:HB3	1:A:98:ILE:HG22	1.89	0.53
1:A:167:HIS:CD2	1:A:169:LEU:H	2.27	0.53
1:A:289:GLU:OE1	1:A:350:HIS:CE1	2.62	0.53
1:B:63:ASN:O	1:B:64:ALA:C	2.52	0.52
1:A:172:VAL:HG22	1:A:208:TYR:CZ	2.45	0.52
1:B:235:ARG:HH11	1:B:257:ASP:CG	2.17	0.52
1:A:208:TYR:O	1:A:212:THR:HG22	2.10	0.52
1:B:56:ILE:HG23	1:B:58:ILE:HD12	1.91	0.52
1:B:236:ARG:HD2	1:B:240:PHE:CE2	2.44	0.52
1:B:374:LYS:O	1:B:376:GLU:N	2.42	0.52
1:B:381:GLU:O	1:B:384:ILE:N	2.42	0.52
1:A:22:LEU:O	1:A:26:LEU:HG	2.09	0.52
1:A:90:LEU:CD1	1:A:90:LEU:C	2.83	0.52
1:B:154:GLY:O	1:B:158:LEU:HB2	2.10	0.52
1:B:172:VAL:HG13	1:B:208:TYR:HE1	1.73	0.52
1:B:205:GLU:C	1:B:207:GLY:H	2.16	0.52
1:B:262:ASN:HD22	1:B:265:ARG:NH1	2.04	0.52
1:B:247:PHE:HB2	1:B:250:THR:HG22	1.92	0.52
1:A:10:LEU:HD11	1:A:14:ARG:CZ	2.39	0.51
1:B:382:TYR:HA	1:B:385:ARG:HB2	1.92	0.51
1:B:185:GLU:OE2	1:B:192:ILE:HG13	2.09	0.51
1:B:381:GLU:C	1:B:383:LEU:H	2.18	0.51
1:A:61:GLU:OE1	1:A:119:MET:O	2.29	0.51
1:B:177:ARG:HA	1:B:180:ARG:HB2	1.92	0.51
1:A:63:ASN:ND2	1:A:65:LEU:HB2	2.25	0.51
1:B:310:ILE:HG23	1:B:311:ASN:N	2.26	0.51
1:B:247:PHE:HB2	1:B:250:THR:CG2	2.40	0.51
1:A:38:TYR:CZ	1:A:122:ILE:HG12	2.46	0.50
1:A:175:PRO:HB2	1:A:212:THR:HG21	1.92	0.50
1:A:329:GLU:O	1:A:330:ARG:C	2.50	0.50
1:B:418:GLU:O	1:B:421:LEU:HD22	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:VAL:O	1:B:423:SER:N	2.43	0.50
1:B:91:PHE:HA	1:B:97:ARG:HB2	1.94	0.50
1:B:77:GLY:HA3	1:B:91:PHE:O	2.11	0.50
1:B:327:LEU:HD11	1:B:363:PHE:HB2	1.93	0.50
1:A:34:ASN:OD1	1:A:34:ASN:O	2.30	0.50
1:A:182:ILE:HG23	1:A:236:ARG:HG2	1.92	0.50
1:B:306:ARG:NH2	1:B:312:GLU:OE1	2.45	0.50
1:B:38:TYR:CE2	1:B:139:LYS:HG3	2.46	0.50
1:B:56:ILE:CG2	1:B:58:ILE:CD1	2.89	0.50
1:B:63:ASN:OD1	1:B:63:ASN:O	2.30	0.50
1:B:169:LEU:O	1:B:170:SER:C	2.54	0.50
1:B:388:ILE:HG23	1:B:389:THR:H	1.76	0.50
1:B:73:ARG:NH1	3:B:443:HOH:O	2.42	0.50
1:A:90:LEU:HB3	1:A:98:ILE:HG23	1.89	0.50
1:A:269:TRP:CZ2	1:A:364:LYS:HG2	2.47	0.50
1:A:272:GLU:CB	1:A:273:ASN:ND2	2.71	0.50
1:B:293:ASP:HA	1:B:314:ARG:HH12	1.77	0.50
1:A:168:THR:HG22	1:A:169:LEU:HG	1.93	0.49
1:A:166:LEU:N	1:A:166:LEU:HD23	2.26	0.49
1:A:191:ARG:HG2	1:A:191:ARG:HH21	1.77	0.49
1:A:34:ASN:O	1:A:34:ASN:CG	2.54	0.49
1:A:415:GLU:HA	1:A:418:GLU:HB2	1.94	0.49
1:B:332:PRO:HB2	1:B:407:ASP:OD1	2.12	0.49
1:B:169:LEU:O	1:B:172:VAL:N	2.45	0.49
1:B:374:LYS:O	1:B:402:LEU:HD23	2.12	0.49
1:B:174:ASP:OD1	1:B:174:ASP:O	2.30	0.49
1:B:391:GLY:O	1:B:392:LYS:HD2	2.12	0.49
1:A:139:LYS:CD	1:A:144:ASP:HB2	2.38	0.49
1:B:168:THR:HA	1:B:199:LEU:HD21	1.94	0.49
1:B:296:TRP:CD2	1:B:310:ILE:HB	2.47	0.49
1:B:421:LEU:C	1:B:423:SER:N	2.63	0.49
1:B:164:ARG:HB2	1:B:193:GLU:HG2	1.95	0.49
1:A:36:PRO:HG2	1:A:119:MET:HG2	1.94	0.49
1:A:396:GLU:O	1:A:400:LYS:HG3	2.13	0.49
1:B:165:VAL:HG22	1:B:196:THR:HG23	1.95	0.49
1:B:420:VAL:C	1:B:423:SER:H	2.21	0.49
1:A:410:THR:HB	1:A:415:GLU:HB3	1.94	0.49
1:A:172:VAL:HG22	1:A:208:TYR:CE1	2.48	0.48
1:A:270:VAL:O	1:A:271:GLU:C	2.55	0.48
1:B:203:ALA:O	1:B:208:TYR:HB2	2.13	0.48
1:B:262:ASN:HD22	1:B:265:ARG:HH22	1.59	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:502:ATP:O5'	2:B:502:ATP:H8	1.97	0.48
1:A:272:GLU:C	1:A:273:ASN:ND2	2.70	0.48
1:B:93:LYS:CD	1:B:93:LYS:N	2.73	0.48
1:B:126:LEU:HB3	1:B:152:PHE:HE2	1.78	0.48
1:B:423:SER:C	1:B:425:GLU:H	2.20	0.48
1:B:62:GLY:O	1:B:63:ASN:CB	2.62	0.48
1:A:424:LEU:C	1:A:424:LEU:HD23	2.39	0.48
1:A:36:PRO:CG	1:A:119:MET:HE2	2.43	0.48
1:A:231:LEU:HD13	1:A:235:ARG:NH2	2.29	0.48
1:A:310:ILE:O	1:A:310:ILE:HG13	2.14	0.48
1:B:141:ASN:ND2	1:B:141:ASN:H	2.11	0.48
1:B:230:PRO:HB2	1:B:264:PHE:CZ	2.49	0.48
1:B:411:ARG:HG3	1:B:413:GLU:H	1.79	0.48
1:B:183:ARG:NH2	1:B:220:GLU:OE1	2.47	0.47
1:B:409:ASP:OD1	1:B:409:ASP:O	2.31	0.47
1:B:82:HIS:HB2	1:B:87:THR:HB	1.95	0.47
1:B:411:ARG:O	1:B:412:ASP:CB	2.63	0.47
1:B:421:LEU:C	1:B:423:SER:H	2.23	0.47
1:B:285:HIS:CD2	1:B:350:HIS:HB2	2.49	0.47
1:A:193:GLU:OE2	1:A:195:THR:HB	2.15	0.47
1:B:56:ILE:HG22	1:B:58:ILE:HD12	1.97	0.47
1:B:188:PHE:HB3	1:B:190:PHE:CE2	2.50	0.47
1:A:389:THR:HB	1:A:394:ILE:CD1	2.44	0.47
1:B:382:TYR:HA	1:B:385:ARG:CB	2.44	0.47
1:B:425:GLU:O	1:B:426:THR:CB	2.62	0.47
1:A:76:PRO:O	1:A:92:LEU:HD22	2.14	0.46
1:B:54:LEU:O	1:B:55:ASP:C	2.58	0.46
1:A:331:VAL:CB	1:A:332:PRO:HD2	2.23	0.46
1:B:15:VAL:HG12	1:B:16:ASP:O	2.16	0.46
1:B:388:ILE:C	1:B:389:THR:HG23	2.37	0.46
1:A:329:GLU:O	1:A:331:VAL:HG13	2.14	0.46
1:A:377:LYS:HB2	1:A:377:LYS:NZ	2.31	0.46
1:A:49:LEU:CD2	1:A:158:LEU:HD22	2.42	0.46
1:B:421:LEU:HD23	1:B:422:ALA:N	2.31	0.46
1:A:178:ILE:HD12	1:A:209:LEU:HD13	1.98	0.45
1:B:416:ILE:O	1:B:420:VAL:HG22	2.15	0.45
1:A:28:LYS:HE3	1:B:145:PHE:CG	2.51	0.45
1:A:117:VAL:HG23	1:A:118:GLU:CG	2.47	0.45
1:A:191:ARG:HG3	1:A:191:ARG:O	2.15	0.45
1:B:280:PHE:CZ	1:B:284:LEU:HD11	2.52	0.45
1:A:36:PRO:HD2	1:A:61:GLU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ILE:CG1	1:A:98:ILE:HG12	2.47	0.45
1:A:389:THR:HB	1:A:394:ILE:HD11	1.97	0.45
1:B:129:ARG:HG2	2:B:502:ATP:H1'	1.98	0.45
1:A:217:LEU:HD12	1:A:217:LEU:HA	1.87	0.45
1:A:394:ILE:O	1:A:397:VAL:HG22	2.16	0.45
1:B:205:GLU:C	1:B:207:GLY:N	2.74	0.45
1:B:209:LEU:H	1:B:209:LEU:CD1	2.28	0.45
1:B:234:ILE:HA	1:B:237:MET:HE3	1.99	0.45
1:B:369:LYS:HZ3	1:B:373:THR:HG21	1.81	0.45
1:B:379:ASN:O	1:B:379:ASN:ND2	2.46	0.45
1:B:413:GLU:O	1:B:416:ILE:CG2	2.62	0.45
1:A:49:LEU:HB3	1:A:51:ILE:CD1	2.46	0.45
1:A:185:GLU:O	1:A:185:GLU:HG2	2.16	0.45
1:A:179:LEU:HD23	1:A:179:LEU:HA	1.76	0.45
1:A:405:LYS:O	1:A:408:GLY:O	2.35	0.45
1:A:63:ASN:OD1	1:A:86:MET:CE	2.58	0.45
1:A:285:HIS:HA	1:A:313:ILE:HG12	1.99	0.45
1:B:398:LEU:HD12	1:B:398:LEU:HA	1.84	0.45
1:B:322:ALA:O	1:B:326:MET:HG3	2.17	0.44
1:A:272:GLU:HB2	1:A:273:ASN:HD21	1.74	0.44
1:A:394:ILE:O	1:A:398:LEU:HD23	2.18	0.44
1:A:400:LYS:HD3	1:A:419:GLU:OE1	2.17	0.44
1:B:82:HIS:O	1:B:84:LYS:O	2.35	0.44
1:B:234:ILE:HA	1:B:237:MET:CE	2.47	0.44
1:A:231:LEU:HD23	1:A:231:LEU:HA	1.82	0.44
1:B:270:VAL:HG21	1:B:349:CYS:SG	2.58	0.44
1:B:325:GLU:HA	1:B:328:SER:OG	2.17	0.44
1:A:90:LEU:HD12	1:A:92:LEU:CD2	2.35	0.44
1:B:231:LEU:HD22	1:B:235:ARG:HD2	2.00	0.44
1:B:429:LYS:HE2	1:B:429:LYS:HB2	1.52	0.44
1:A:122:ILE:HD12	1:A:123:LYS:H	1.83	0.44
1:A:250:THR:OG1	1:A:287:PHE:O	2.34	0.44
1:B:369:LYS:O	1:B:373:THR:OG1	2.29	0.44
1:B:296:TRP:CH2	1:B:300:ARG:HB2	2.53	0.44
1:A:90:LEU:HD12	1:A:92:LEU:CG	2.47	0.44
1:B:285:HIS:CD2	1:B:350:HIS:HD2	2.35	0.44
1:A:410:THR:HG21	1:A:414:GLU:CB	2.46	0.43
1:B:266:ASN:HB3	1:B:352:LEU:HD13	2.01	0.43
1:B:331:VAL:HG12	1:B:332:PRO:CD	2.43	0.43
1:B:404:LYS:HB2	1:B:415:GLU:OE2	2.18	0.43
1:A:82:HIS:CB	1:A:87:THR:HG22	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:VAL:HG11	1:A:366:TYR:CD1	2.53	0.43
1:A:337:TYR:HE1	1:A:374:LYS:HZ1	1.66	0.43
1:B:352:LEU:HA	1:B:355:LEU:HD23	2.00	0.43
1:A:405:LYS:HE2	1:A:405:LYS:HB3	1.69	0.43
1:B:93:LYS:HE3	1:B:93:LYS:HB3	1.61	0.43
1:A:63:ASN:ND2	1:A:66:GLU:H	2.15	0.43
1:A:72:LYS:HA	1:A:72:LYS:HD2	1.69	0.43
1:B:5:ARG:HG2	1:B:5:ARG:NH1	2.33	0.43
1:B:20:LEU:HD23	1:B:20:LEU:HA	1.90	0.43
1:B:9:LYS:H	1:B:9:LYS:HD3	1.83	0.43
1:B:430:LEU:O	1:B:431:ALA:CB	2.67	0.43
1:A:40:VAL:HG21	1:A:59:VAL:HG23	2.00	0.43
1:B:92:LEU:HA	1:B:93:LYS:NZ	2.33	0.43
1:B:243:ILE:HG22	1:B:250:THR:CG2	2.48	0.43
1:A:323:LEU:O	1:A:324:LEU:C	2.62	0.43
1:B:90:LEU:HD12	1:B:92:LEU:HD21	2.01	0.43
1:B:337:TYR:CZ	1:B:341:LYS:HG3	2.54	0.43
1:B:378:ILE:HG21	1:B:411:ARG:NH2	2.30	0.43
1:A:82:HIS:CG	1:A:87:THR:HG22	2.53	0.43
1:A:262:ASN:HD22	1:A:265:ARG:NH2	2.06	0.43
1:A:3:ILE:O	1:A:3:ILE:HG22	2.15	0.43
1:A:336:VAL:HG11	1:A:366:TYR:CE1	2.53	0.43
1:A:352:LEU:HA	1:A:355:LEU:CD2	2.48	0.43
1:B:337:TYR:HB3	1:B:403:MET:HE1	2.01	0.43
1:A:27:GLY:HA3	1:A:140:LEU:O	2.18	0.42
1:B:175:PRO:CD	1:B:212:THR:HG21	2.45	0.42
1:A:40:VAL:CG2	1:A:59:VAL:HG23	2.48	0.42
1:A:105:LEU:HD12	1:A:105:LEU:H	1.84	0.42
1:A:341:LYS:O	1:A:342:GLY:C	2.61	0.42
1:B:285:HIS:CD2	1:B:350:HIS:CD2	3.08	0.42
1:B:391:GLY:C	1:B:393:ILE:H	2.27	0.42
1:A:302:ARG:HG2	1:A:303:TYR:CD1	2.54	0.42
1:A:308:ASN:O	1:A:312:GLU:HG3	2.19	0.42
1:A:343:VAL:HB	1:A:347:THR:HB	2.01	0.42
1:A:300:ARG:O	1:A:303:TYR:O	2.37	0.42
1:B:289:GLU:OE1	1:B:350:HIS:HE1	2.02	0.42
1:A:266:ASN:HB3	1:A:352:LEU:HD13	2.01	0.42
1:B:39:VAL:HG13	1:B:138:ILE:HB	2.00	0.42
1:B:87:THR:CG2	1:B:88:ALA:N	2.83	0.42
1:B:262:ASN:HD22	1:B:265:ARG:NH2	2.18	0.42
1:B:360:GLU:HG3	1:B:361:GLY:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:LYS:O	1:B:375:LEU:C	2.62	0.42
1:B:425:GLU:C	1:B:426:THR:CG2	2.70	0.42
1:A:260:MET:HE1	1:A:286:VAL:HB	2.02	0.42
1:A:341:LYS:H	1:A:341:LYS:HG2	1.61	0.42
1:A:120:SER:HA	1:A:122:ILE:HD11	2.01	0.42
1:A:413:GLU:O	1:A:414:GLU:C	2.58	0.42
1:B:357:GLY:O	1:B:360:GLU:HG2	2.20	0.42
1:A:163:ILE:O	1:A:163:ILE:HG22	2.20	0.42
1:A:269:TRP:CD2	1:A:364:LYS:HE2	2.55	0.42
1:B:327:LEU:CD1	1:B:363:PHE:HB2	2.50	0.42
1:A:369:LYS:HE3	1:A:406:LEU:O	2.19	0.42
1:B:84:LYS:O	1:B:85:PHE:HB2	2.20	0.41
1:A:253:THR:HB	1:A:254:PRO:CD	2.49	0.41
1:B:75:LEU:HD12	1:B:75:LEU:N	2.34	0.41
1:B:187:ARG:HD2	1:B:188:PHE:CZ	2.55	0.41
1:B:271:GLU:HA	1:B:275:GLY:O	2.19	0.41
1:B:285:HIS:HD2	1:B:350:HIS:CB	2.32	0.41
1:A:325:GLU:O	1:A:328:SER:O	2.39	0.41
1:B:178:ILE:O	1:B:182:ILE:HG13	2.20	0.41
1:B:91:PHE:CE1	1:B:97:ARG:HD2	2.55	0.41
1:A:195:THR:HG22	1:A:199:LEU:HD22	2.03	0.41
1:B:26:LEU:HD23	1:B:26:LEU:HA	1.93	0.41
1:B:169:LEU:O	1:B:171:PHE:N	2.53	0.41
1:A:36:PRO:CG	1:A:119:MET:HG2	2.50	0.41
1:A:90:LEU:CD1	1:A:92:LEU:CG	2.94	0.41
1:A:141:ASN:O	1:A:142:PRO:C	2.63	0.41
1:A:335:PHE:O	1:A:335:PHE:HD2	2.04	0.41
1:B:413:GLU:C	1:B:416:ILE:HG22	2.44	0.41
2:B:502:ATP:O3G	2:B:502:ATP:O2B	2.39	0.41
1:A:178:ILE:HD12	1:A:209:LEU:CD1	2.50	0.41
1:A:143:LYS:HE3	1:A:143:LYS:HB3	1.69	0.40
1:A:419:GLU:HA	1:A:422:ALA:HB3	2.04	0.40
1:B:209:LEU:HD12	1:B:209:LEU:N	2.28	0.40
1:B:411:ARG:O	1:B:412:ASP:HB2	2.20	0.40
1:B:424:LEU:HD12	1:B:424:LEU:HA	1.68	0.40
1:B:355:LEU:N	1:B:355:LEU:HD22	2.36	0.40
1:A:302:ARG:HG2	1:A:303:TYR:CZ	2.56	0.40
1:A:393:ILE:O	1:A:394:ILE:C	2.62	0.40
1:B:343:VAL:HB	1:B:347:THR:CB	2.52	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	411/441 (93%)	385 (94%)	23 (6%)	3 (1%)	18	35
1	B	416/441 (94%)	378 (91%)	27 (6%)	11 (3%)	4	9
All	All	827/882 (94%)	763 (92%)	50 (6%)	14 (2%)	7	16

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	412	ASP
1	B	63	ASN
1	B	389	THR
1	B	391	GLY
1	B	426	THR
1	B	429	LYS
1	B	430	LEU
1	B	431	ALA
1	A	118	GLU
1	B	412	ASP
1	A	86	MET
1	B	428	GLY
1	B	329	GLU
1	B	392	LYS

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	374/395 (95%)	312 (83%)	62 (17%)	2	4
1	B	376/395 (95%)	316 (84%)	60 (16%)	2	4
All	All	750/790 (95%)	628 (84%)	122 (16%)	2	4

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	12	VAL
1	A	20	LEU
1	A	28	LYS
1	A	56	ILE
1	A	58	ILE
1	A	63	ASN
1	A	69	GLU
1	A	72	LYS
1	A	73	ARG
1	A	75	LEU
1	A	84	LYS
1	A	85	PHE
1	A	87	THR
1	A	89	SER
1	A	90	LEU
1	A	98	ILE
1	A	104	ARG
1	A	118	GLU
1	A	119	MET
1	A	122	ILE
1	A	126	LEU
1	A	148	LEU
1	A	156	ARG
1	A	163	ILE
1	A	168	THR
1	A	176	THR
1	A	199	LEU
1	A	205	GLU
1	A	209	LEU
1	A	210	GLU
1	A	211	ARG
1	A	212	THR
1	A	217	LEU
1	A	221	LEU

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Mol	Chain	Res	Type
1	A	223	LYS
1	A	231	LEU
1	A	241	ASP
1	A	250	THR
1	A	263	LEU
1	A	273	ASN
1	A	297	LYS
1	A	299	VAL
1	A	302	ARG
1	A	306	ARG
1	A	323	LEU
1	A	324	LEU
1	A	336	VAL
1	A	340	VAL
1	A	355	LEU
1	A	367	LEU
1	A	374	LYS
1	A	383	LEU
1	A	384	ILE
1	A	389	THR
1	A	393	ILE
1	A	394	ILE
1	A	399	GLU
1	A	402	LEU
1	A	407	ASP
1	A	413	GLU
1	A	414	GLU
1	B	9	LYS
1	B	12	VAL
1	B	22	LEU
1	B	28	LYS
1	B	39	VAL
1	B	56	ILE
1	B	58	ILE
1	B	86	MET
1	B	90	LEU
1	B	93	LYS
1	B	97	ARG
1	B	104	ARG
1	B	118	GLU
1	B	122	ILE
1	B	126	LEU

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Mol	Chain	Res	Type
1	B	141	ASN
1	B	147	LEU
1	B	148	LEU
1	B	158	LEU
1	B	159	LYS
1	B	168	THR
1	B	189	ASP
1	B	210	GLU
1	B	211	ARG
1	B	213	THR
1	B	217	LEU
1	B	223	LYS
1	B	231	LEU
1	B	235	ARG
1	B	258	GLU
1	B	263	LEU
1	B	271	GLU
1	B	279	ARG
1	B	285	HIS
1	B	288	LEU
1	B	323	LEU
1	B	329	GLU
1	B	330	ARG
1	B	331	VAL
1	B	370	ILE
1	B	372	ASN
1	B	374	LYS
1	B	375	LEU
1	B	377	LYS
1	B	378	ILE
1	B	383	LEU
1	B	384	ILE
1	B	385	ARG
1	B	397	VAL
1	B	398	LEU
1	B	407	ASP
1	B	414	GLU
1	B	417	LEU
1	B	420	VAL
1	B	421	LEU
1	B	423	SER
1	B	424	LEU

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Mol	Chain	Res	Type
1	B	426	THR
1	B	429	LYS
1	B	430	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	63	ASN
1	A	82	HIS
1	A	141	ASN
1	A	167	HIS
1	A	262	ASN
1	A	273	ASN
1	A	345	ASN
1	A	350	HIS
1	B	2	GLN
1	B	141	ASN
1	B	167	HIS
1	B	219	GLN
1	B	229	ASN
1	B	262	ASN
1	B	266	ASN
1	B	285	HIS
1	B	345	ASN
1	B	350	HIS
1	B	372	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ATP	B	502	-	32,33,33	1.46	6 (18%)	48,52,52	1.78	8 (16%)
2	ATP	A	501	-	32,33,33	1.38	3 (9%)	48,52,52	1.88	12 (25%)

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
2	ATP	B	502	-	-	5/22/38/38	0/3/3/3
2	ATP	A	501	-	-	2/22/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	ATP	C5-C4	5.07	1.48	1.39
2	B	502	ATP	C5-C4	4.81	1.47	1.39
2	A	501	ATP	C8-N7	2.76	1.37	1.31
2	B	502	ATP	PB-O3B	2.68	1.62	1.59
2	B	502	ATP	C5-C6	2.67	1.48	1.41
2	A	501	ATP	C5-C6	2.57	1.48	1.41
2	B	502	ATP	C5-N7	-2.34	1.34	1.39
2	B	502	ATP	C8-N7	2.20	1.35	1.31
2	B	502	ATP	PA-O3A	2.03	1.61	1.59

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	ATP	C5-C4-N3	-6.06	118.37	126.72
2	A	501	ATP	C5-C4-N3	-5.50	119.14	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	ATP	N3-C4-N9	4.83	135.38	127.17
2	A	501	ATP	C4-C5-N7	-4.37	105.59	110.58
2	A	501	ATP	N3-C4-N9	4.19	134.29	127.17
2	B	502	ATP	C2-N3-C4	3.54	120.47	111.83
2	B	502	ATP	C4-C5-N7	-3.42	106.68	110.58
2	A	501	ATP	C4-N9-C8	3.29	109.19	105.74
2	A	501	ATP	C2-N3-C4	3.26	119.78	111.83
2	A	501	ATP	C5-N7-C8	3.23	108.53	103.45
2	B	502	ATP	N3-C2-N1	-2.87	124.23	128.58
2	A	501	ATP	N3-C2-N1	-2.84	124.28	128.58
2	A	501	ATP	O4'-C1'-N9	-2.77	102.77	108.09
2	A	501	ATP	N9-C8-N7	-2.67	110.15	113.94
2	A	501	ATP	C6-C5-N7	2.62	137.15	132.09
2	B	502	ATP	O3A-PB-O1B	-2.59	102.90	110.70
2	B	502	ATP	C4-N9-C8	2.48	108.34	105.74
2	B	502	ATP	C5-N7-C8	2.43	107.26	103.45
2	A	501	ATP	O2A-PA-O5'	2.10	117.08	107.57
2	A	501	ATP	O2G-PG-O1G	2.01	118.68	110.83

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	502	ATP	PB-O3B-PG-O2G
2	B	502	ATP	PB-O3B-PG-O3G
2	B	502	ATP	PG-O3B-PB-O1B
2	B	502	ATP	PG-O3B-PB-O2B
2	A	501	ATP	O4'-C4'-C5'-O5'
2	B	502	ATP	PB-O3B-PG-O1G
2	A	501	ATP	PG-O3B-PB-O1B

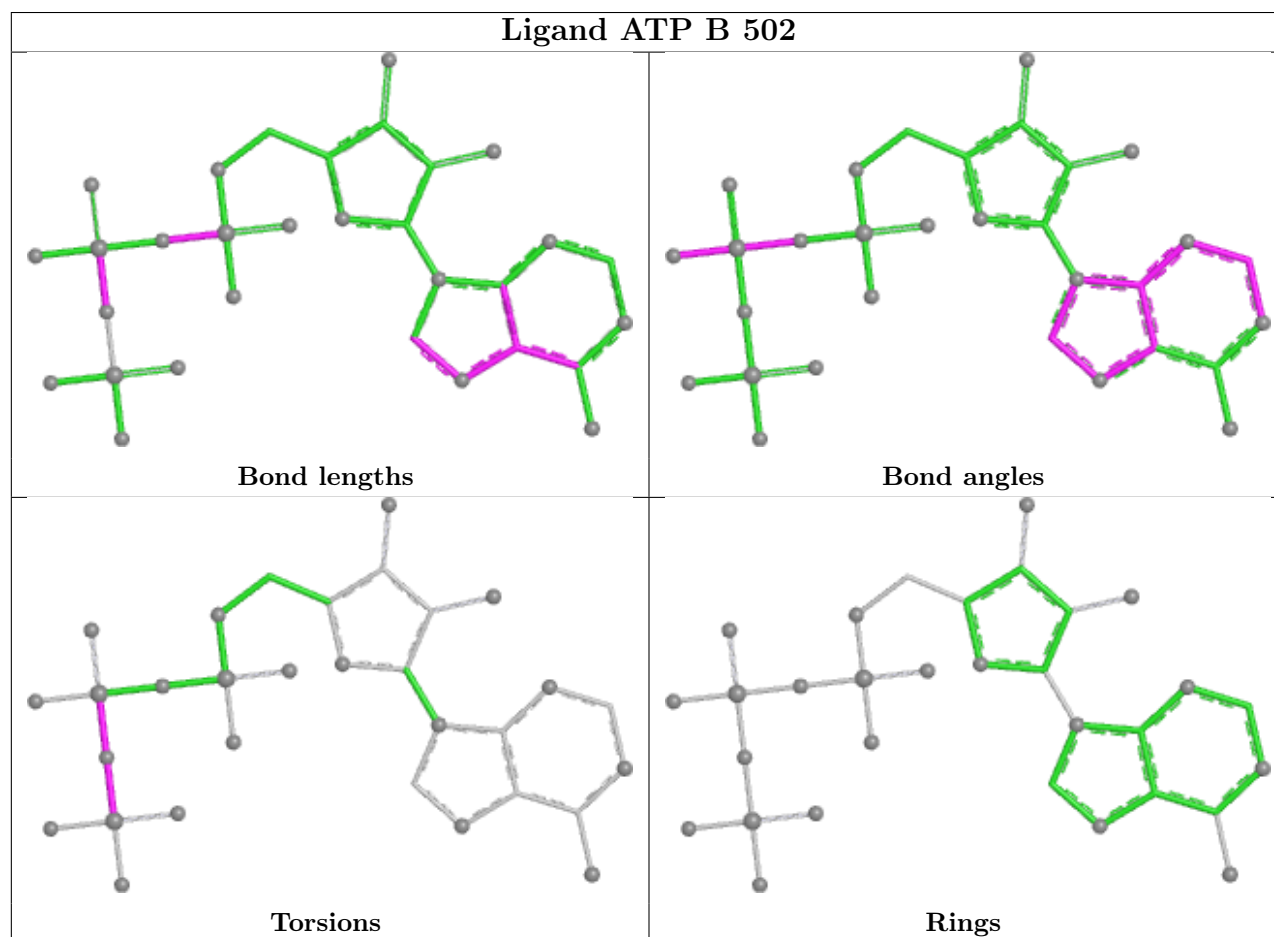
There are no ring outliers.

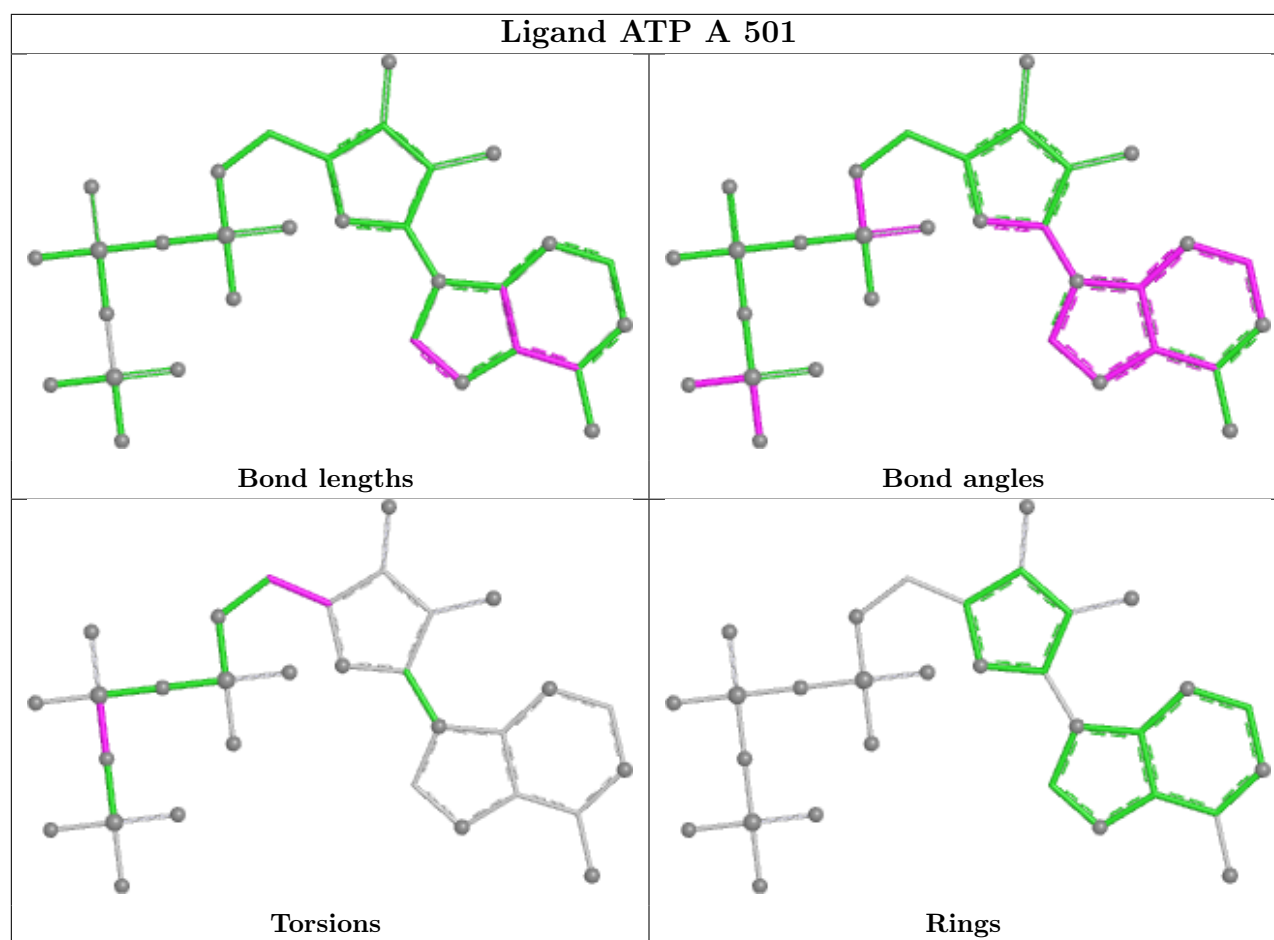
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	502	ATP	3	0
2	A	501	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 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	415/441 (94%)	-0.16	25 (6%)	27 20	30, 59, 154, 192	0
1	B	420/441 (95%)	0.31	33 (7%)	18 14	24, 95, 142, 164	0
All	All	835/882 (94%)	0.08	58 (6%)	23 17	24, 76, 148, 192	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	388	ILE	7.3
1	B	430	LEU	7.0
1	B	424	LEU	6.1
1	B	425	GLU	5.7
1	B	432	ALA	5.6
1	B	385	ARG	5.5
1	A	117	VAL	5.4
1	B	105	LEU	5.2
1	B	431	ALA	4.8
1	A	378	ILE	4.5
1	B	378	ILE	4.4
1	A	388	ILE	4.2
1	B	427	GLU	4.0
1	B	120	SER	3.5
1	B	375	LEU	3.5
1	B	384	ILE	3.4
1	B	423	SER	3.4
1	B	85	PHE	3.4
1	B	412	ASP	3.3
1	A	105	LEU	3.2
1	A	384	ILE	3.2
1	B	118	GLU	3.1
1	B	416	ILE	3.1
1	A	416	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	370	ILE	3.1
1	A	412	ASP	3.0
1	A	382	TYR	3.0
1	A	386	LYS	2.9
1	A	335	PHE	2.9
1	A	424	LEU	2.9
1	A	389	THR	2.8
1	A	421	LEU	2.8
1	B	421	LEU	2.8
1	A	375	LEU	2.8
1	B	415	GLU	2.7
1	B	429	LYS	2.7
1	B	426	THR	2.7
1	A	381	GLU	2.7
1	B	244	LYS	2.6
1	B	428	GLY	2.6
1	A	374	LYS	2.6
1	B	119	MET	2.6
1	B	392	LYS	2.6
1	A	383	LEU	2.4
1	A	385	ARG	2.4
1	A	90	LEU	2.3
1	A	417	LEU	2.3
1	A	387	GLY	2.3
1	B	335	PHE	2.3
1	A	118	GLU	2.3
1	A	119	MET	2.3
1	B	374	LYS	2.3
1	B	337	TYR	2.3
1	A	342	GLY	2.3
1	A	392	LYS	2.2
1	B	379	ASN	2.1
1	B	103	ALA	2.1
1	B	401	ILE	2.1

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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

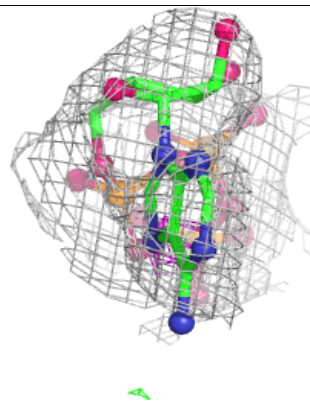
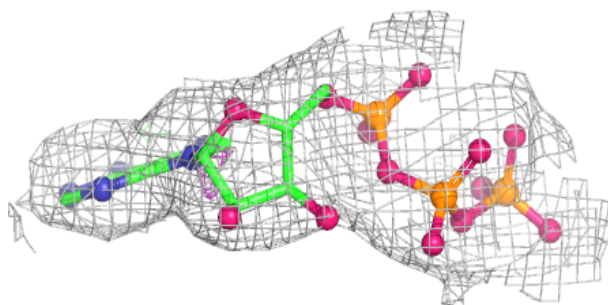
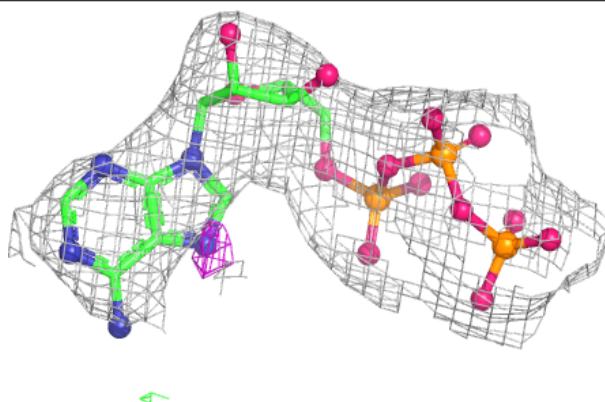
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

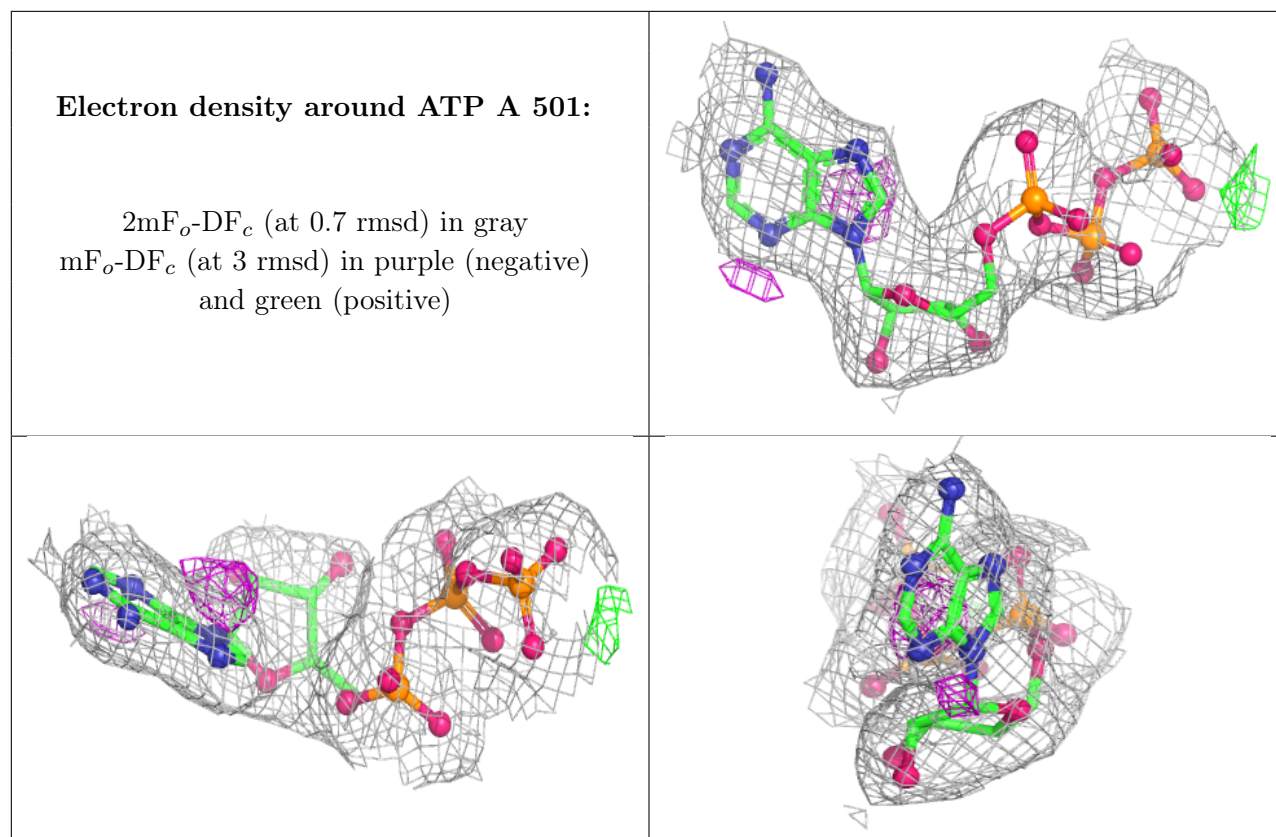
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ATP	B	502	31/31	0.95	0.09	67,99,123,134	0
2	ATP	A	501	31/31	0.98	0.06	26,43,62,102	0

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 502:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.