



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:46 AM UTC

PDB ID : 3JUX / pdb_00003jux
Title : Structure of the translocation ATPase SecA from *Thermotoga maritima*
Authors : Zimmer, J.
Deposited on : 2009-09-15
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

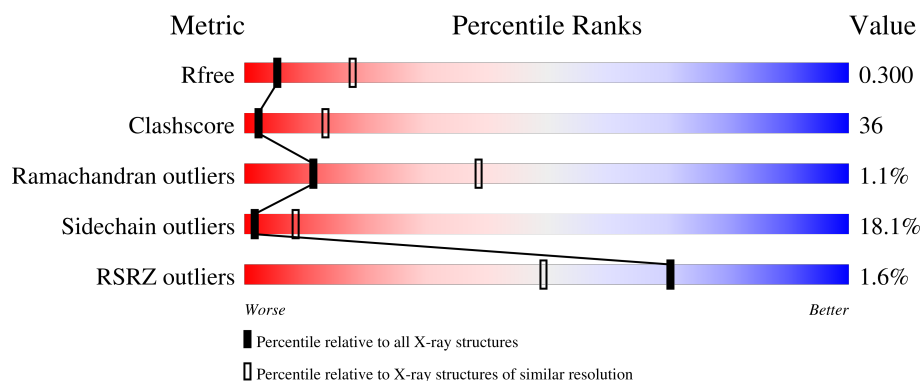
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	822	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6619 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 Protein translocase subunit secA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	813	Total	C	N	O	S	0	0	0
			6589	4198	1128	1236	27			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	817	HIS	-	expression tag	UNP Q9X1R4
A	818	HIS	-	expression tag	UNP Q9X1R4
A	819	HIS	-	expression tag	UNP Q9X1R4
A	820	HIS	-	expression tag	UNP Q9X1R4
A	821	HIS	-	expression tag	UNP Q9X1R4
A	822	HIS	-	expression tag	UNP Q9X1R4

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

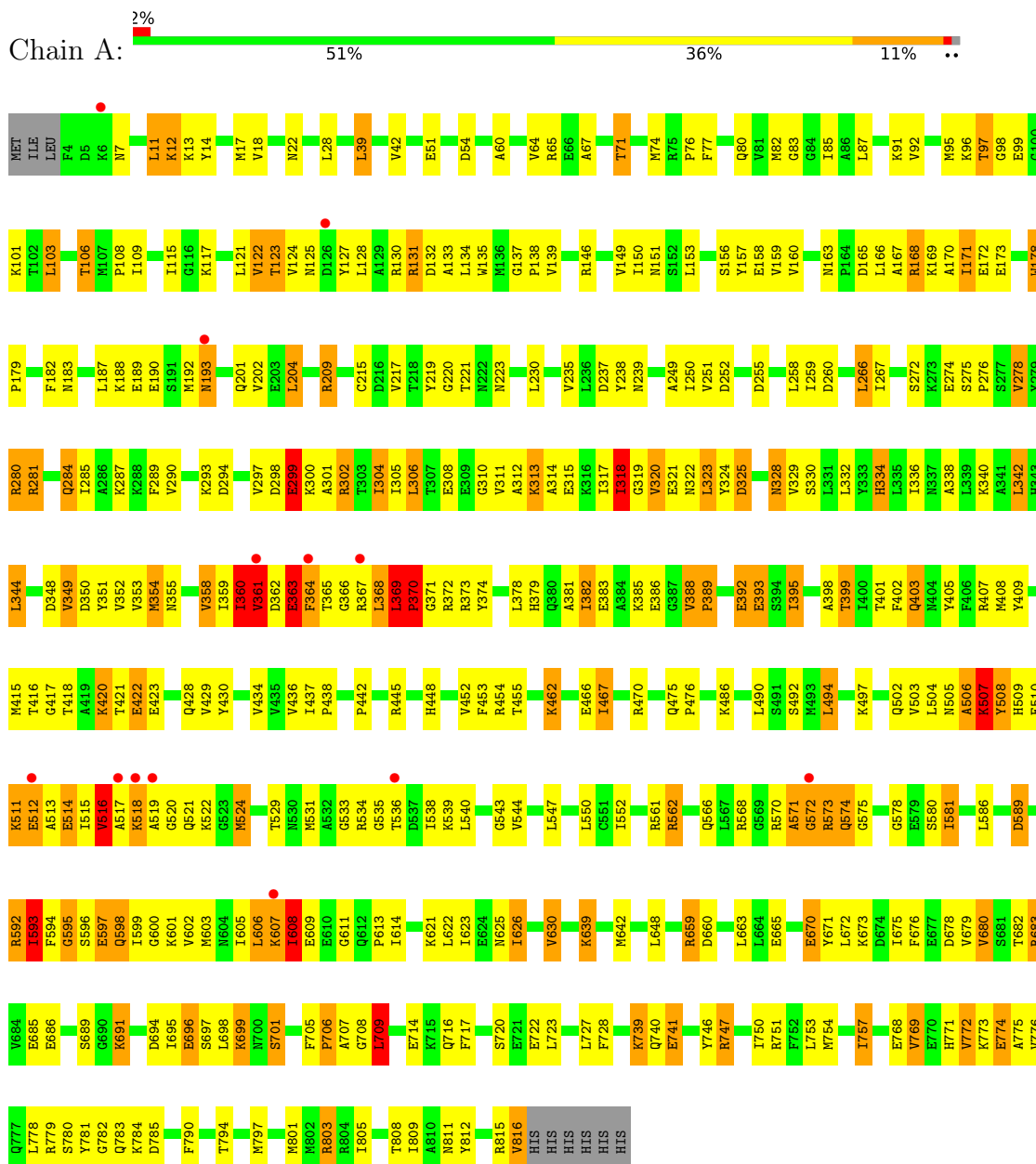
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	O	0	0
			2	2		

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: Protein translocase subunit secA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.53Å 119.40Å 120.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.10 30.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-3.10) 99.1 (30.00-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.227 , 0.303 0.223 , 0.300	Depositor DCC
R_{free} test set	1810 reflections (10.30%)	wwPDB-VP
Wilson B-factor (Å ²)	56.2	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6619	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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: MG, ADP

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	0.76	4/6706 (0.1%)	1.02	22/9016 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	706	PRO	CA-C	-6.92	1.45	1.52
1	A	511	LYS	C-O	-5.88	1.17	1.24
1	A	324	TYR	CA-C	-5.46	1.47	1.53
1	A	707	ALA	CA-C	-5.05	1.46	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	318	ILE	N-CA-C	11.75	122.58	110.72
1	A	508	TYR	N-CA-C	11.61	123.93	111.28
1	A	572	GLY	N-CA-C	-10.16	101.16	112.33
1	A	709	LEU	N-CA-C	-10.10	97.63	111.87
1	A	313	LYS	N-CA-C	-7.18	103.39	111.07
1	A	706	PRO	CB-CA-C	-7.18	103.74	111.56
1	A	372	ARG	N-CA-C	7.09	119.70	109.14
1	A	611	GLY	N-CA-C	-6.90	105.56	115.64
1	A	506	ALA	N-CA-C	6.57	124.80	110.80
1	A	360	ILE	N-CA-C	6.57	123.00	109.34
1	A	707	ALA	N-CA-C	-6.56	101.26	110.50
1	A	599	ILE	CB-CA-C	-6.19	103.68	112.22
1	A	516	VAL	CB-CA-C	-6.13	104.02	112.04
1	A	574	GLN	N-CA-C	-6.12	98.40	108.49
1	A	370	PRO	N-CA-C	-5.98	100.15	112.47
1	A	507	LYS	N-CA-C	-5.71	97.15	107.60
1	A	593	ILE	CB-CA-C	-5.37	104.90	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	598	GLN	N-CA-C	-5.27	105.53	111.28
1	A	420	LYS	N-CA-C	5.25	117.01	111.28
1	A	595	GLY	N-CA-C	5.23	122.00	114.10
1	A	571	ALA	N-CA-C	5.05	119.05	112.13
1	A	518	LYS	N-CA-C	5.03	117.54	111.40

There are no chirality outliers.

There are no planarity outliers.

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	6589	0	6655	476	0
2	A	1	0	0	0	0
3	A	27	0	12	2	0
4	A	2	0	0	1	0
All	All	6619	0	6667	476	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 36.

All (476) 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:369:LEU:C	1:A:371:GLY:HA3	1.34	1.46
1:A:368:LEU:C	1:A:370:PRO:HD3	1.40	1.42
1:A:708:GLY:C	1:A:709:LEU:HD23	1.45	1.41
1:A:515:ILE:HG21	1:A:536:THR:CG2	1.57	1.34
1:A:314:ALA:HA	1:A:317:ILE:CG2	1.68	1.24
1:A:512:GLU:CG	1:A:536:THR:HB	1.73	1.17
1:A:157:TYR:CB	1:A:204:LEU:HD12	1.77	1.15
1:A:368:LEU:C	1:A:368:LEU:HD13	1.54	1.14
1:A:314:ALA:HA	1:A:317:ILE:HG21	1.27	1.13
1:A:95:MET:O	1:A:101:LYS:HE2	1.47	1.11
1:A:299:GLU:C	1:A:301:ALA:HA	1.76	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:TYR:HB3	1:A:204:LEU:HD12	1.17	1.10
1:A:531:MET:HE2	1:A:531:MET:HA	1.34	1.08
1:A:364:PHE:C	1:A:366:GLY:HA2	1.80	1.07
1:A:373:ARG:HA	1:A:379:HIS:CD2	1.88	1.07
1:A:512:GLU:HG2	1:A:536:THR:HB	1.35	1.07
1:A:709:LEU:HD23	1:A:709:LEU:N	1.52	1.07
1:A:515:ILE:HG21	1:A:536:THR:HG21	1.15	1.06
1:A:368:LEU:C	1:A:370:PRO:CD	2.29	1.05
1:A:300:LYS:N	1:A:301:ALA:HA	1.69	1.05
1:A:301:ALA:HB1	1:A:302:ARG:CB	1.85	1.05
1:A:368:LEU:HD13	1:A:368:LEU:O	1.56	1.04
1:A:368:LEU:O	1:A:368:LEU:HD22	1.55	1.04
1:A:314:ALA:C	1:A:317:ILE:HG22	1.82	1.04
1:A:369:LEU:C	1:A:371:GLY:CA	2.30	1.03
1:A:362:ASP:HB3	1:A:369:LEU:HD21	1.40	1.03
1:A:361:VAL:HB	1:A:362:ASP:HA	1.38	1.02
1:A:470:ARG:HH11	1:A:475:GLN:HE22	1.04	1.02
1:A:365:THR:N	1:A:366:GLY:HA2	1.74	1.02
1:A:360:ILE:CG1	1:A:361:VAL:HG23	1.88	1.01
1:A:373:ARG:CA	1:A:379:HIS:HD2	1.72	1.01
1:A:359:ILE:HG21	1:A:370:PRO:HG3	1.02	1.01
1:A:301:ALA:HB1	1:A:302:ARG:HB3	1.05	1.01
1:A:515:ILE:CG2	1:A:536:THR:HG21	1.91	1.00
1:A:373:ARG:HA	1:A:379:HIS:HD2	1.20	0.99
1:A:360:ILE:HG12	1:A:361:VAL:HG23	1.01	0.99
1:A:515:ILE:CG2	1:A:536:THR:CG2	2.41	0.98
1:A:708:GLY:O	1:A:709:LEU:HD23	1.62	0.98
1:A:592:ARG:HH11	1:A:592:ARG:CG	1.76	0.98
1:A:369:LEU:N	1:A:370:PRO:HD3	1.68	0.98
1:A:369:LEU:O	1:A:371:GLY:HA3	1.64	0.97
1:A:603:MET:O	1:A:608:ILE:HG22	1.64	0.97
1:A:314:ALA:CA	1:A:317:ILE:HG22	1.93	0.97
1:A:368:LEU:C	1:A:368:LEU:CD1	2.33	0.96
1:A:360:ILE:HG12	1:A:361:VAL:CG2	1.95	0.96
1:A:368:LEU:HD12	1:A:368:LEU:N	1.77	0.96
1:A:314:ALA:CA	1:A:317:ILE:CG2	2.43	0.95
1:A:370:PRO:N	1:A:371:GLY:HA3	1.51	0.95
1:A:351:TYR:HB3	1:A:360:ILE:HG21	1.49	0.95
1:A:803:ARG:HH11	1:A:803:ARG:HG2	1.31	0.95
1:A:517:ALA:O	1:A:521:GLN:HG2	1.66	0.95
1:A:470:ARG:NH1	1:A:475:GLN:HE22	1.64	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:PRO:N	1:A:371:GLY:CA	2.30	0.94
1:A:512:GLU:HG3	1:A:536:THR:HB	1.48	0.94
1:A:533:GLY:O	1:A:536:THR:HG22	1.67	0.94
1:A:299:GLU:HA	1:A:302:ARG:HA	1.50	0.94
1:A:17:MET:HE1	1:A:85:ILE:HG21	1.49	0.93
1:A:504:LEU:O	1:A:505:ASN:ND2	2.00	0.93
1:A:189:GLU:HA	1:A:192:MET:HE2	1.50	0.93
1:A:592:ARG:HH11	1:A:592:ARG:CB	1.81	0.93
1:A:368:LEU:HD12	1:A:368:LEU:H	1.29	0.92
1:A:159:VAL:HG13	1:A:202:VAL:HG11	1.50	0.92
1:A:515:ILE:HG21	1:A:536:THR:HG23	1.47	0.92
1:A:314:ALA:O	1:A:317:ILE:HG22	1.69	0.92
1:A:267:ILE:HG22	1:A:399:THR:HG23	1.51	0.91
1:A:361:VAL:HG12	1:A:363:GLU:N	1.84	0.91
1:A:342:LEU:HD22	1:A:385:LYS:HB3	1.53	0.91
1:A:779:ARG:HA	1:A:781:TYR:CE2	2.04	0.91
1:A:77:PHE:H	1:A:80:GLN:HE21	1.18	0.91
1:A:359:ILE:CG2	1:A:370:PRO:HG3	1.97	0.91
1:A:518:LYS:HD2	1:A:524:MET:HE2	1.53	0.91
1:A:361:VAL:HG12	1:A:362:ASP:C	1.95	0.90
1:A:342:LEU:CD2	1:A:385:LYS:HB3	2.02	0.90
1:A:608:ILE:CG1	1:A:609:GLU:HA	2.01	0.90
1:A:519:ALA:HB3	1:A:538:ILE:HG21	1.53	0.90
1:A:709:LEU:N	1:A:709:LEU:CD2	2.29	0.89
1:A:708:GLY:C	1:A:709:LEU:CD2	2.41	0.89
1:A:512:GLU:HG3	1:A:536:THR:CB	2.03	0.89
1:A:159:VAL:CG1	1:A:202:VAL:HG11	2.02	0.88
1:A:168:ARG:O	1:A:172:GLU:HB2	1.74	0.88
1:A:157:TYR:CB	1:A:204:LEU:CD1	2.52	0.87
1:A:314:ALA:HA	1:A:317:ILE:HG22	1.54	0.87
1:A:512:GLU:CG	1:A:536:THR:CB	2.52	0.87
1:A:17:MET:CE	1:A:85:ILE:HG21	2.03	0.87
1:A:361:VAL:CB	1:A:362:ASP:HA	2.05	0.87
1:A:362:ASP:HB3	1:A:369:LEU:CD2	2.05	0.87
1:A:373:ARG:HB3	1:A:379:HIS:CD2	2.09	0.87
1:A:359:ILE:HG21	1:A:370:PRO:CG	1.98	0.87
1:A:592:ARG:NH1	1:A:592:ARG:HG2	1.87	0.86
1:A:608:ILE:HG12	1:A:609:GLU:HA	1.56	0.86
1:A:705:PHE:HB3	1:A:706:PRO:HD2	1.58	0.86
1:A:603:MET:CE	1:A:614:ILE:HG22	2.05	0.86
1:A:373:ARG:CA	1:A:379:HIS:CD2	2.54	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:ALA:O	1:A:317:ILE:CG2	2.25	0.84
1:A:159:VAL:HG13	1:A:202:VAL:CG1	2.08	0.84
1:A:299:GLU:O	1:A:299:GLU:HG2	1.77	0.83
1:A:368:LEU:CD1	1:A:368:LEU:N	2.40	0.83
1:A:603:MET:HE3	1:A:614:ILE:HG22	1.59	0.83
1:A:350:ASP:HB2	1:A:361:VAL:HG22	1.60	0.83
1:A:592:ARG:HH11	1:A:592:ARG:HG2	1.37	0.83
1:A:512:GLU:HG3	1:A:536:THR:CG2	2.09	0.83
1:A:603:MET:O	1:A:608:ILE:CG2	2.27	0.82
1:A:683:ARG:CD	1:A:701:SER:OG	2.27	0.82
1:A:77:PHE:H	1:A:80:GLN:NE2	1.76	0.82
1:A:351:TYR:HB3	1:A:360:ILE:CG2	2.10	0.82
1:A:593:ILE:HG22	1:A:594:PHE:N	1.94	0.82
1:A:67:ALA:O	1:A:71:THR:HB	1.80	0.81
1:A:306:LEU:HD12	1:A:306:LEU:H	1.45	0.81
1:A:470:ARG:HH11	1:A:475:GLN:NE2	1.79	0.81
1:A:351:TYR:CB	1:A:360:ILE:HG22	2.10	0.81
1:A:95:MET:O	1:A:101:LYS:CE	2.28	0.81
1:A:351:TYR:CB	1:A:360:ILE:CG2	2.58	0.80
1:A:71:THR:CG2	1:A:138:PRO:HB2	2.11	0.80
1:A:518:LYS:CD	1:A:524:MET:HE2	2.11	0.80
1:A:368:LEU:O	1:A:368:LEU:CD2	2.29	0.80
1:A:519:ALA:HB3	1:A:538:ILE:CG2	2.12	0.79
1:A:779:ARG:HA	1:A:781:TYR:HE2	1.47	0.79
1:A:373:ARG:CB	1:A:379:HIS:CD2	2.67	0.78
1:A:708:GLY:O	1:A:709:LEU:CD2	2.30	0.78
1:A:267:ILE:HG22	1:A:399:THR:CG2	2.13	0.78
1:A:515:ILE:CG2	1:A:536:THR:HG23	2.11	0.78
1:A:503:VAL:O	1:A:504:LEU:HD23	1.83	0.78
1:A:284:GLN:HA	1:A:287:LYS:HG2	1.65	0.77
1:A:676:PHE:O	1:A:680:VAL:HG22	1.85	0.76
1:A:255:ASP:OD1	1:A:416:THR:HG21	1.84	0.76
1:A:311:VAL:O	1:A:315:GLU:HG3	1.87	0.76
1:A:368:LEU:O	1:A:370:PRO:HD3	1.85	0.75
1:A:592:ARG:HH11	1:A:592:ARG:HB3	1.50	0.74
1:A:130:ARG:HH11	1:A:151:ASN:ND2	1.85	0.74
1:A:281:ARG:NH1	1:A:285:ILE:HD11	2.01	0.74
1:A:420:LYS:HG3	1:A:436:VAL:CG2	2.16	0.74
1:A:368:LEU:O	1:A:368:LEU:CD1	2.30	0.74
1:A:368:LEU:O	1:A:370:PRO:CD	2.33	0.74
1:A:131:ARG:HG2	1:A:131:ARG:HH11	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:626:ILE:O	1:A:630:VAL:HG23	1.89	0.73
1:A:595:GLY:HA2	1:A:598:GLN:NE2	2.04	0.73
1:A:803:ARG:HG2	1:A:803:ARG:NH1	1.97	0.72
1:A:157:TYR:HB2	1:A:204:LEU:CD1	2.20	0.72
1:A:314:ALA:C	1:A:317:ILE:CG2	2.61	0.72
1:A:320:VAL:HG21	1:A:328:ASN:ND2	2.05	0.71
1:A:351:TYR:HA	1:A:360:ILE:HG22	1.71	0.71
1:A:683:ARG:HD2	1:A:701:SER:OG	1.90	0.71
1:A:317:ILE:HG23	1:A:318:ILE:N	2.05	0.71
1:A:322:ASN:O	1:A:328:ASN:ND2	2.23	0.71
1:A:349:VAL:HA	1:A:350:ASP:OD1	1.91	0.71
1:A:506:ALA:N	1:A:511:LYS:HE3	2.06	0.71
1:A:365:THR:N	1:A:366:GLY:CA	2.53	0.71
1:A:670:GLU:HA	1:A:673:LYS:HE3	1.73	0.71
1:A:505:ASN:ND2	1:A:529:THR:OG1	2.23	0.71
1:A:757:ILE:HG12	1:A:808:THR:HG22	1.72	0.70
1:A:782:GLY:HA2	1:A:783:GLN:HB2	1.73	0.70
1:A:678:ASP:O	1:A:682:THR:HG23	1.91	0.70
1:A:683:ARG:HD3	1:A:701:SER:OG	1.91	0.70
1:A:299:GLU:C	1:A:301:ALA:CA	2.62	0.70
1:A:476:PRO:HG2	1:A:550:LEU:HA	1.74	0.69
1:A:342:LEU:HD22	1:A:385:LYS:HD2	1.74	0.69
1:A:369:LEU:O	1:A:371:GLY:CA	2.36	0.69
1:A:17:MET:HE3	1:A:85:ILE:HD13	1.73	0.69
1:A:502:GLN:HE21	1:A:502:GLN:HA	1.56	0.69
1:A:507:LYS:H	1:A:511:LYS:HE2	1.58	0.69
1:A:96:LYS:O	1:A:99:GLU:HB2	1.92	0.68
1:A:14:TYR:HD1	1:A:17:MET:HE2	1.57	0.68
1:A:342:LEU:HD22	1:A:385:LYS:CB	2.22	0.68
1:A:178:TRP:HZ3	1:A:182:PHE:O	1.76	0.68
1:A:531:MET:HA	1:A:531:MET:CE	2.17	0.68
1:A:130:ARG:HH11	1:A:151:ASN:HD21	1.42	0.67
1:A:512:GLU:HG3	1:A:536:THR:HG21	1.75	0.67
1:A:322:ASN:HB3	1:A:325:ASP:HB3	1.77	0.67
1:A:313:LYS:O	1:A:317:ILE:HG22	1.95	0.67
1:A:39:LEU:O	1:A:42:VAL:HG12	1.95	0.66
1:A:420:LYS:HG3	1:A:436:VAL:HG21	1.77	0.66
1:A:304:ILE:HG22	1:A:344:LEU:HD12	1.77	0.66
1:A:706:PRO:O	1:A:706:PRO:HG2	1.94	0.66
1:A:304:ILE:O	1:A:304:ILE:HG12	1.92	0.66
1:A:512:GLU:HG2	1:A:536:THR:CB	2.16	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:815:ARG:O	1:A:816:VAL:HG13	1.96	0.66
1:A:71:THR:HG23	1:A:138:PRO:HB2	1.78	0.65
1:A:131:ARG:HG2	1:A:131:ARG:NH1	2.07	0.65
1:A:534:ARG:HH21	1:A:566:GLN:NE2	1.94	0.65
1:A:351:TYR:CA	1:A:360:ILE:HG22	2.26	0.64
1:A:453:PHE:CE2	1:A:462:LYS:HG3	2.33	0.64
1:A:603:MET:HE2	1:A:614:ILE:HG22	1.78	0.64
1:A:131:ARG:HH11	1:A:131:ARG:CG	2.10	0.64
1:A:315:GLU:O	1:A:319:GLY:HA2	1.98	0.64
1:A:354:MET:O	1:A:355:ASN:HB2	1.97	0.64
1:A:543:GLY:O	1:A:547:LEU:HD12	1.99	0.63
1:A:680:VAL:HG11	1:A:727:LEU:HB3	1.80	0.63
1:A:504:LEU:C	1:A:505:ASN:ND2	2.55	0.63
1:A:416:THR:HG22	1:A:417:GLY:H	1.62	0.63
1:A:603:MET:HE3	1:A:614:ILE:CG2	2.28	0.63
1:A:255:ASP:HB2	1:A:562:ARG:NH1	2.13	0.63
1:A:255:ASP:HB2	1:A:562:ARG:HH11	1.64	0.63
1:A:362:ASP:O	1:A:363:GLU:HB2	1.99	0.63
1:A:187:LEU:HD21	1:A:192:MET:HB3	1.81	0.62
1:A:361:VAL:HG12	1:A:362:ASP:CA	2.29	0.62
1:A:300:LYS:N	1:A:301:ALA:CA	2.54	0.62
1:A:342:LEU:HD21	1:A:385:LYS:HB3	1.80	0.62
1:A:124:VAL:HG22	1:A:128:LEU:HD12	1.82	0.62
1:A:169:LYS:HE3	1:A:173:GLU:OE2	2.00	0.62
1:A:351:TYR:HA	1:A:360:ILE:CG2	2.29	0.62
1:A:368:LEU:CA	1:A:370:PRO:HD3	2.25	0.62
1:A:519:ALA:CB	1:A:538:ILE:HG21	2.26	0.62
1:A:352:VAL:HG22	1:A:359:ILE:O	1.99	0.61
1:A:315:GLU:O	1:A:319:GLY:CA	2.48	0.61
1:A:368:LEU:O	1:A:368:LEU:CG	2.48	0.61
1:A:22:ASN:ND2	1:A:65:ARG:HH12	1.97	0.61
1:A:373:ARG:CB	1:A:379:HIS:HD2	2.09	0.61
1:A:442:PRO:O	1:A:575:GLY:HA2	2.00	0.61
1:A:757:ILE:HG12	1:A:808:THR:CG2	2.31	0.60
1:A:361:VAL:CB	1:A:362:ASP:CA	2.79	0.60
1:A:281:ARG:HG3	1:A:281:ARG:HH11	1.66	0.60
1:A:423:GLU:HG3	1:A:434:VAL:HB	1.82	0.60
1:A:514:GLU:O	1:A:518:LYS:HG2	2.02	0.60
1:A:280:ARG:HH22	1:A:389:PRO:HA	1.66	0.60
1:A:168:ARG:HH11	1:A:168:ARG:CG	2.15	0.60
1:A:168:ARG:NH1	1:A:168:ARG:HG2	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:GLU:OE2	1:A:386:GLU:HA	2.02	0.59
1:A:486:LYS:O	1:A:490:LEU:HD23	2.02	0.59
1:A:784:LYS:O	1:A:785:ASP:C	2.45	0.59
1:A:407:ARG:NH1	1:A:429:VAL:O	2.35	0.59
1:A:170:ALA:O	1:A:173:GLU:O	2.21	0.59
1:A:776:VAL:O	1:A:780:SER:HB2	2.03	0.59
1:A:462:LYS:HE3	1:A:462:LYS:HA	1.83	0.58
1:A:476:PRO:HB2	1:A:519:ALA:O	2.04	0.58
1:A:369:LEU:N	1:A:370:PRO:CD	2.53	0.58
1:A:281:ARG:O	1:A:285:ILE:HG13	2.03	0.58
1:A:534:ARG:HH21	1:A:566:GLN:HE22	1.52	0.58
1:A:416:THR:HG22	1:A:417:GLY:N	2.19	0.58
1:A:536:THR:HG23	1:A:536:THR:O	2.01	0.58
1:A:381:ALA:O	1:A:385:LYS:HG2	2.03	0.57
1:A:622:LEU:O	1:A:626:ILE:HG23	2.04	0.57
1:A:342:LEU:HD22	1:A:385:LYS:CG	2.34	0.57
1:A:359:ILE:C	1:A:360:ILE:CG2	2.78	0.57
1:A:157:TYR:HB2	1:A:204:LEU:HD11	1.86	0.57
1:A:266:LEU:HD12	1:A:402:PHE:CE2	2.39	0.57
1:A:17:MET:HE3	1:A:85:ILE:HG21	1.85	0.57
1:A:178:TRP:CZ3	1:A:182:PHE:O	2.57	0.57
1:A:361:VAL:C	1:A:367:ARG:HA	2.30	0.57
1:A:534:ARG:NH2	1:A:566:GLN:HE22	2.01	0.57
1:A:445:ARG:HD3	1:A:572:GLY:H	1.70	0.57
1:A:97:THR:HA	1:A:101:LYS:NZ	2.20	0.57
1:A:351:TYR:CA	1:A:360:ILE:CG2	2.83	0.56
1:A:358:VAL:C	1:A:359:ILE:HG13	2.30	0.56
1:A:359:ILE:HD13	1:A:370:PRO:HB3	1.87	0.56
1:A:568:ARG:HG3	1:A:580:SER:OG	2.05	0.56
1:A:621:LYS:HE2	1:A:625:ASN:HD21	1.70	0.56
1:A:235:VAL:O	1:A:659:ARG:NH2	2.39	0.56
1:A:392:GLU:O	1:A:392:GLU:HG3	2.06	0.56
1:A:275:SER:O	1:A:278:VAL:HG13	2.06	0.55
1:A:507:LYS:N	1:A:511:LYS:HE2	2.21	0.55
1:A:109:ILE:HD11	1:A:121:LEU:HD12	1.88	0.55
1:A:360:ILE:HD13	1:A:360:ILE:C	2.31	0.55
1:A:17:MET:HE1	1:A:85:ILE:CG2	2.31	0.55
1:A:358:VAL:HB	1:A:379:HIS:HE1	1.71	0.55
1:A:445:ARG:HG3	1:A:578:GLY:C	2.32	0.55
1:A:503:VAL:C	1:A:504:LEU:HD23	2.32	0.55
1:A:314:ALA:O	1:A:317:ILE:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ASP:OD1	1:A:325:ASP:C	2.50	0.55
1:A:351:TYR:HA	1:A:360:ILE:CB	2.36	0.55
1:A:691:LYS:HE3	1:A:691:LYS:HA	1.89	0.55
1:A:466:GLU:OE1	1:A:466:GLU:HA	2.06	0.54
1:A:639:LYS:HA	1:A:642:MET:HE3	1.89	0.54
1:A:685:GLU:O	1:A:689:SER:OG	2.25	0.54
1:A:359:ILE:C	1:A:360:ILE:HG22	2.33	0.54
1:A:544:VAL:HA	1:A:547:LEU:HD12	1.90	0.54
1:A:351:TYR:HB2	1:A:360:ILE:HG22	1.85	0.54
1:A:706:PRO:O	1:A:706:PRO:CG	2.51	0.54
1:A:272:SER:HB3	1:A:393:GLU:H	1.72	0.54
1:A:168:ARG:HH11	1:A:168:ARG:HG2	1.72	0.54
1:A:504:LEU:HD12	1:A:515:ILE:HD13	1.90	0.53
1:A:517:ALA:O	1:A:521:GLN:CG	2.49	0.53
1:A:97:THR:HA	1:A:101:LYS:HZ2	1.72	0.53
1:A:354:MET:O	1:A:355:ASN:CB	2.57	0.53
1:A:362:ASP:CB	1:A:369:LEU:HD21	2.27	0.53
1:A:520:GLY:HA3	1:A:539:LYS:O	2.08	0.53
1:A:71:THR:HG21	1:A:139:VAL:N	2.24	0.53
1:A:153:LEU:N	1:A:153:LEU:HD12	2.24	0.53
1:A:276:PRO:O	1:A:280:ARG:HG3	2.09	0.53
1:A:342:LEU:HD22	1:A:385:LYS:CD	2.37	0.53
1:A:639:LYS:HG2	1:A:642:MET:HE3	1.91	0.53
1:A:370:PRO:HA	1:A:371:GLY:C	2.32	0.53
1:A:167:ALA:O	1:A:171:ILE:HD12	2.09	0.52
1:A:360:ILE:HD13	1:A:360:ILE:O	2.09	0.52
1:A:178:TRP:NE1	1:A:187:LEU:HB2	2.23	0.52
1:A:512:GLU:O	1:A:516:VAL:HG23	2.08	0.52
1:A:728:PHE:CD1	1:A:728:PHE:C	2.87	0.52
1:A:675:ILE:O	1:A:679:VAL:HG23	2.09	0.52
1:A:317:ILE:CG2	1:A:318:ILE:N	2.72	0.52
1:A:349:VAL:N	1:A:350:ASP:HA	2.24	0.52
1:A:470:ARG:HG2	1:A:475:GLN:NE2	2.25	0.52
1:A:608:ILE:HG12	1:A:609:GLU:CA	2.35	0.52
1:A:77:PHE:N	1:A:80:GLN:HE21	1.98	0.52
1:A:178:TRP:CD1	1:A:187:LEU:HD22	2.45	0.52
1:A:360:ILE:HG12	1:A:361:VAL:N	2.20	0.52
1:A:238:TYR:CD2	1:A:238:TYR:O	2.63	0.52
1:A:361:VAL:CG1	1:A:362:ASP:HA	2.40	0.51
1:A:14:TYR:HD1	1:A:17:MET:CE	2.22	0.51
1:A:374:TYR:H	1:A:379:HIS:CD2	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:665:GLU:O	1:A:751:ARG:NH2	2.43	0.51
1:A:753:LEU:HD13	1:A:812:TYR:HB3	1.91	0.51
1:A:11:LEU:HD11	1:A:438:PRO:HD3	1.93	0.51
1:A:445:ARG:HG3	1:A:578:GLY:O	2.10	0.51
1:A:80:GLN:HE22	3:A:873:ADP:N6	2.09	0.51
1:A:151:ASN:O	1:A:209:ARG:NH2	2.43	0.51
1:A:361:VAL:CG1	1:A:362:ASP:CA	2.89	0.50
1:A:453:PHE:CE1	1:A:613:PRO:HB3	2.45	0.50
1:A:251:VAL:HG11	1:A:258:LEU:HG	1.94	0.50
1:A:358:VAL:C	1:A:359:ILE:CG1	2.84	0.50
1:A:607:LYS:NZ	1:A:607:LYS:HB3	2.26	0.50
1:A:83:GLY:O	1:A:87:LEU:HG	2.12	0.50
1:A:274:GLU:HG2	1:A:334:HIS:HE1	1.76	0.50
1:A:595:GLY:HA2	1:A:598:GLN:CD	2.37	0.50
1:A:71:THR:HG23	1:A:138:PRO:CB	2.42	0.49
1:A:123:THR:HG21	1:A:128:LEU:HB3	1.93	0.49
1:A:401:THR:HB	1:A:403:GLN:HE21	1.77	0.49
1:A:592:ARG:CB	1:A:592:ARG:NH1	2.64	0.49
1:A:160:VAL:O	1:A:202:VAL:HG13	2.12	0.49
1:A:274:GLU:HG2	1:A:334:HIS:CE1	2.47	0.49
1:A:361:VAL:O	1:A:367:ARG:HA	2.11	0.49
1:A:510:GLU:OE2	1:A:510:GLU:O	2.30	0.49
1:A:361:VAL:O	1:A:367:ARG:CA	2.60	0.49
1:A:281:ARG:HH11	1:A:285:ILE:HD11	1.73	0.49
1:A:64:VAL:CG1	1:A:106:THR:HG23	2.42	0.49
1:A:252:ASP:OD1	1:A:415:MET:HE3	2.12	0.49
1:A:739:LYS:HE3	1:A:746:TYR:HD2	1.78	0.49
1:A:405:TYR:O	1:A:408:MET:HG3	2.13	0.49
1:A:188:LYS:HD3	1:A:190:GLU:HB2	1.95	0.49
1:A:369:LEU:O	1:A:371:GLY:C	2.56	0.49
1:A:768:GLU:HB3	1:A:797:MET:HE1	1.94	0.48
1:A:98:GLY:O	1:A:574:GLN:NE2	2.46	0.48
1:A:188:LYS:HG2	1:A:190:GLU:HG2	1.94	0.48
1:A:280:ARG:HH22	1:A:388:VAL:HA	1.78	0.48
1:A:514:GLU:O	1:A:518:LYS:CG	2.61	0.48
1:A:294:ASP:O	1:A:310:GLY:HA3	2.14	0.48
1:A:298:ASP:O	1:A:300:LYS:N	2.45	0.48
1:A:348:ASP:C	1:A:350:ASP:HA	2.39	0.48
1:A:60:ALA:O	1:A:64:VAL:HG23	2.14	0.48
1:A:403:GLN:O	1:A:407:ARG:HG3	2.13	0.47
1:A:505:ASN:C	1:A:511:LYS:HE3	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:PRO:HB2	1:A:182:PHE:CD2	2.49	0.47
1:A:505:ASN:H	1:A:511:LYS:HE3	1.79	0.47
1:A:603:MET:CE	1:A:614:ILE:CG2	2.87	0.47
1:A:448:HIS:HB2	1:A:581:ILE:HG23	1.97	0.47
1:A:805:ILE:O	1:A:809:ILE:HG13	2.14	0.47
1:A:361:VAL:O	1:A:367:ARG:HB3	2.15	0.47
1:A:281:ARG:HA	1:A:284:GLN:OE1	2.15	0.47
1:A:130:ARG:HH21	1:A:509:HIS:CE1	2.32	0.47
1:A:351:TYR:HA	1:A:360:ILE:HB	1.96	0.47
1:A:510:GLU:O	1:A:513:ALA:HB3	2.15	0.47
1:A:159:VAL:CG1	1:A:202:VAL:CG1	2.77	0.47
1:A:774:GLU:HG3	1:A:775:ALA:N	2.29	0.47
1:A:12:LYS:HA	1:A:12:LYS:HD3	1.55	0.46
1:A:230:LEU:HD22	1:A:398:ALA:HB1	1.97	0.46
1:A:680:VAL:CG1	1:A:727:LEU:HB3	2.44	0.46
1:A:304:ILE:CG2	1:A:344:LEU:HD12	2.45	0.46
1:A:714:GLU:N	1:A:714:GLU:OE1	2.48	0.46
1:A:691:LYS:O	1:A:691:LYS:HG3	2.16	0.46
1:A:76:PRO:HG3	1:A:103:LEU:HD22	1.97	0.46
1:A:360:ILE:HG21	1:A:374:TYR:OH	2.16	0.46
1:A:454:ARG:HA	1:A:586:LEU:HG	1.97	0.46
1:A:13:LYS:O	1:A:17:MET:HG3	2.16	0.46
1:A:293:LYS:HE3	1:A:293:LYS:HB2	1.60	0.46
1:A:80:GLN:HE22	3:A:873:ADP:HN61	1.63	0.46
1:A:350:ASP:C	1:A:360:ILE:HB	2.40	0.46
1:A:368:LEU:O	1:A:370:PRO:HD2	2.15	0.46
1:A:772:VAL:HG21	1:A:797:MET:SD	2.55	0.46
1:A:157:TYR:HB3	1:A:204:LEU:CD1	2.11	0.45
1:A:313:LYS:O	1:A:317:ILE:CG2	2.62	0.45
1:A:352:VAL:O	1:A:358:VAL:HA	2.16	0.45
1:A:536:THR:CG2	1:A:536:THR:O	2.64	0.45
1:A:157:TYR:CG	1:A:204:LEU:HD12	2.47	0.45
1:A:358:VAL:HG11	1:A:382:ILE:HG21	1.97	0.45
1:A:750:ILE:HG23	1:A:754:MET:HE3	1.98	0.45
1:A:237:ASP:C	1:A:239:ASN:H	2.24	0.45
1:A:600:GLY:O	1:A:603:MET:HB2	2.16	0.45
1:A:95:MET:HG2	1:A:437:ILE:HB	1.99	0.45
1:A:124:VAL:HG23	1:A:125:ASN:ND2	2.32	0.45
1:A:747:ARG:N	1:A:747:ARG:HD2	2.31	0.45
1:A:259:ILE:HD13	1:A:422:GLU:HG2	1.99	0.45
1:A:452:VAL:O	1:A:603:MET:CE	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:THR:HG22	1:A:365:THR:O	2.17	0.45
1:A:589:ASP:OD2	1:A:589:ASP:N	2.46	0.45
1:A:125:ASN:C	1:A:221:THR:HG22	2.42	0.44
1:A:323:LEU:CD2	1:A:332:LEU:HB2	2.47	0.44
1:A:467:ILE:HG21	1:A:494:LEU:HD11	1.98	0.44
1:A:694:ASP:OD2	1:A:697:SER:OG	2.34	0.44
1:A:695:ILE:O	1:A:696:GLU:C	2.59	0.44
1:A:518:LYS:O	1:A:524:MET:HB3	2.17	0.44
1:A:317:ILE:HG23	1:A:318:ILE:H	1.79	0.44
1:A:388:VAL:HG13	1:A:389:PRO:CG	2.47	0.44
1:A:109:ILE:HG13	1:A:250:ILE:HD12	1.99	0.44
1:A:369:LEU:HD13	1:A:369:LEU:HA	1.57	0.44
1:A:505:ASN:HD22	1:A:529:THR:HB	1.83	0.44
1:A:518:LYS:O	1:A:524:MET:HG2	2.18	0.44
1:A:131:ARG:NH1	1:A:132:ASP:OD1	2.51	0.44
1:A:717:PHE:HA	1:A:722:GLU:OE1	2.18	0.44
1:A:121:LEU:HD22	1:A:219:TYR:CD2	2.52	0.44
1:A:122:VAL:HG22	1:A:251:VAL:HA	1.99	0.44
1:A:362:ASP:O	1:A:363:GLU:CB	2.65	0.44
1:A:648:LEU:HD11	1:A:769:VAL:HG11	2.00	0.44
1:A:699:LYS:HZ2	1:A:699:LYS:C	2.26	0.44
1:A:133:ALA:O	1:A:137:GLY:N	2.50	0.43
1:A:504:LEU:HB3	1:A:511:LYS:HD3	2.01	0.43
1:A:149:VAL:HA	1:A:219:TYR:O	2.18	0.43
1:A:395:ILE:HD13	1:A:395:ILE:H	1.83	0.43
1:A:597:GLU:H	1:A:597:GLU:HG3	1.50	0.43
1:A:740:GLN:HB3	1:A:741:GLU:OE2	2.19	0.43
1:A:92:VAL:HB	1:A:434:VAL:HG22	1.99	0.43
1:A:150:ILE:HG12	1:A:220:GLY:HA3	2.00	0.43
1:A:266:LEU:HD12	1:A:402:PHE:CZ	2.54	0.43
1:A:753:LEU:O	1:A:757:ILE:HD12	2.18	0.43
1:A:223:ASN:HD22	1:A:223:ASN:H	1.66	0.43
1:A:320:VAL:HG23	1:A:321:GLU:N	2.33	0.43
1:A:593:ILE:O	1:A:594:PHE:CD2	2.71	0.43
1:A:750:ILE:CG2	1:A:754:MET:HE3	2.48	0.43
1:A:299:GLU:O	1:A:299:GLU:CG	2.52	0.43
1:A:801:MET:HE2	1:A:801:MET:HB3	1.91	0.43
1:A:811:ASN:OD1	1:A:815:ARG:HD2	2.18	0.43
1:A:127:TYR:CZ	1:A:131:ARG:HD3	2.53	0.43
1:A:811:ASN:O	1:A:815:ARG:HG3	2.19	0.43
1:A:7:ASN:O	1:A:11:LEU:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:VAL:HG13	1:A:304:ILE:HG22	2.01	0.42
1:A:388:VAL:HG13	1:A:389:PRO:HB3	1.99	0.42
1:A:237:ASP:C	1:A:239:ASN:N	2.76	0.42
1:A:595:GLY:HA2	1:A:598:GLN:HE22	1.79	0.42
1:A:420:LYS:CG	1:A:436:VAL:CG2	2.91	0.42
1:A:601:LYS:O	1:A:602:VAL:C	2.62	0.42
1:A:670:GLU:O	1:A:673:LYS:HG2	2.20	0.42
1:A:705:PHE:HB3	1:A:706:PRO:CD	2.38	0.42
1:A:18:VAL:HG21	1:A:82:MET:HG2	2.01	0.42
1:A:134:LEU:HD21	1:A:204:LEU:HD22	2.00	0.42
1:A:428:GLN:HE22	1:A:639:LYS:HE2	1.85	0.42
1:A:504:LEU:CD1	1:A:515:ILE:HD13	2.49	0.42
1:A:146:ARG:O	1:A:215:CYS:HB3	2.19	0.42
1:A:388:VAL:HG13	1:A:389:PRO:CB	2.50	0.42
1:A:403:GLN:HA	1:A:430:TYR:CE2	2.55	0.42
1:A:505:ASN:ND2	1:A:529:THR:CB	2.83	0.42
1:A:249:ALA:HB2	1:A:409:TYR:CE1	2.55	0.42
1:A:290:VAL:N	1:A:294:ASP:OD2	2.49	0.42
1:A:502:GLN:HA	1:A:502:GLN:NE2	2.29	0.42
1:A:514:GLU:O	1:A:518:LYS:CB	2.67	0.42
1:A:515:ILE:HD12	1:A:515:ILE:HA	1.90	0.42
1:A:519:ALA:HB3	1:A:538:ILE:HG23	1.98	0.42
1:A:370:PRO:HA	1:A:371:GLY:O	2.20	0.41
1:A:505:ASN:HD22	1:A:529:THR:CB	2.33	0.41
1:A:374:TYR:CD1	1:A:378:LEU:HD23	2.55	0.41
1:A:608:ILE:HG13	1:A:609:GLU:HA	1.97	0.41
1:A:648:LEU:HD21	1:A:790:PHE:CZ	2.55	0.41
1:A:101:LYS:HB3	1:A:415:MET:SD	2.60	0.41
1:A:312:ALA:O	1:A:313:LYS:C	2.63	0.41
1:A:361:VAL:HG12	1:A:363:GLU:H	1.76	0.41
1:A:573:ARG:HE	1:A:573:ARG:HB3	1.27	0.41
1:A:623:ILE:O	1:A:626:ILE:HG13	2.20	0.41
1:A:739:LYS:HZ1	1:A:747:ARG:HD3	1.85	0.41
1:A:535:GLY:HA2	4:A:823:HOH:O	2.20	0.41
1:A:698:LEU:HD21	1:A:727:LEU:HD11	2.03	0.41
1:A:660:ASP:O	1:A:663:LEU:HB2	2.21	0.41
1:A:168:ARG:HH11	1:A:168:ARG:CB	2.34	0.41
1:A:605:ILE:HG22	1:A:606:LEU:HD13	2.01	0.41
1:A:74:MET:HE1	1:A:135:TRP:HE1	1.86	0.41
1:A:304:ILE:HD13	1:A:340:LYS:HB2	2.03	0.41
1:A:373:ARG:HB3	1:A:379:HIS:CG	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:TYR:CZ	1:A:675:ILE:HD11	2.56	0.41
1:A:780:SER:C	1:A:783:GLN:HG3	2.46	0.41
1:A:683:ARG:HE	1:A:683:ARG:HB2	1.76	0.41
1:A:552:ILE:HG12	1:A:571:ALA:HB2	2.03	0.40
1:A:289:PHE:HD1	1:A:294:ASP:HB3	1.86	0.40
1:A:475:GLN:HG2	1:A:476:PRO:HD2	2.02	0.40
1:A:260:ASP:CG	1:A:562:ARG:HH22	2.30	0.40
1:A:671:TYR:CE2	1:A:675:ILE:HD11	2.56	0.40
1:A:138:PRO:HG3	1:A:202:VAL:HG23	2.03	0.40
1:A:360:ILE:C	1:A:360:ILE:CD1	2.89	0.40
1:A:453:PHE:CZ	1:A:613:PRO:HG3	2.56	0.40
1:A:781:TYR:HA	1:A:782:GLY:HA2	1.65	0.40
1:A:87:LEU:HD12	1:A:108:PRO:HG3	2.02	0.40
1:A:338:ALA:O	1:A:385:LYS:HE3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	811/822 (99%)	749 (92%)	53 (6%)	9 (1%)	11 39

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	363	GLU
1	A	370	PRO
1	A	193	ASN
1	A	369	LEU
1	A	608	ILE
1	A	299	GLU
1	A	364	PHE

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Mol	Chain	Res	Type
1	A	361	VAL
1	A	389	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	714/723 (99%)	585 (82%)	129 (18%)	2 8

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	12	LYS
1	A	28	LEU
1	A	39	LEU
1	A	51	GLU
1	A	54	ASP
1	A	71	THR
1	A	91	LYS
1	A	97	THR
1	A	103	LEU
1	A	106	THR
1	A	115	ILE
1	A	117	LYS
1	A	122	VAL
1	A	123	THR
1	A	131	ARG
1	A	156	SER
1	A	158	GLU
1	A	163	ASN
1	A	165	ASP
1	A	166	LEU
1	A	168	ARG
1	A	171	ILE
1	A	178	TRP

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Mol	Chain	Res	Type
1	A	183	ASN
1	A	193	ASN
1	A	201	GLN
1	A	204	LEU
1	A	209	ARG
1	A	217	VAL
1	A	266	LEU
1	A	278	VAL
1	A	280	ARG
1	A	281	ARG
1	A	284	GLN
1	A	299	GLU
1	A	302	ARG
1	A	304	ILE
1	A	305	ILE
1	A	306	LEU
1	A	308	GLU
1	A	318	ILE
1	A	320	VAL
1	A	323	LEU
1	A	325	ASP
1	A	328	ASN
1	A	329	VAL
1	A	330	SER
1	A	334	HIS
1	A	336	ILE
1	A	342	LEU
1	A	344	LEU
1	A	349	VAL
1	A	353	VAL
1	A	354	MET
1	A	358	VAL
1	A	360	ILE
1	A	361	VAL
1	A	363	GLU
1	A	368	LEU
1	A	369	LEU
1	A	382	ILE
1	A	383	GLU
1	A	388	VAL
1	A	392	GLU
1	A	393	GLU

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Mol	Chain	Res	Type
1	A	395	ILE
1	A	399	THR
1	A	403	GLN
1	A	418	THR
1	A	421	THR
1	A	422	GLU
1	A	455	THR
1	A	462	LYS
1	A	467	ILE
1	A	492	SER
1	A	494	LEU
1	A	497	LYS
1	A	507	LYS
1	A	508	TYR
1	A	512	GLU
1	A	514	GLU
1	A	516	VAL
1	A	522	LYS
1	A	524	MET
1	A	540	LEU
1	A	561	ARG
1	A	562	ARG
1	A	570	ARG
1	A	573	ARG
1	A	581	ILE
1	A	589	ASP
1	A	592	ARG
1	A	593	ILE
1	A	596	SER
1	A	597	GLU
1	A	606	LEU
1	A	607	LYS
1	A	608	ILE
1	A	626	ILE
1	A	630	VAL
1	A	639	LYS
1	A	659	ARG
1	A	670	GLU
1	A	672	LEU
1	A	680	VAL
1	A	683	ARG
1	A	686	GLU

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Mol	Chain	Res	Type
1	A	691	LYS
1	A	696	GLU
1	A	699	LYS
1	A	701	SER
1	A	709	LEU
1	A	716	GLN
1	A	720	SER
1	A	723	LEU
1	A	739	LYS
1	A	741	GLU
1	A	747	ARG
1	A	757	ILE
1	A	769	VAL
1	A	771	HIS
1	A	772	VAL
1	A	773	LYS
1	A	774	GLU
1	A	778	LEU
1	A	794	THR
1	A	803	ARG
1	A	816	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	80	GLN
1	A	120	HIS
1	A	151	ASN
1	A	193	ASN
1	A	223	ASN
1	A	379	HIS
1	A	403	GLN
1	A	428	GLN
1	A	440	HIS
1	A	475	GLN
1	A	502	GLN
1	A	505	ASN
1	A	521	GLN
1	A	558	HIS
1	A	566	GLN
1	A	598	GLN

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Mol	Chain	Res	Type
1	A	615	GLN
1	A	616	HIS
1	A	625	ASN
1	A	634	ASN
1	A	716	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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ADP	A	873	-	28,29,29	1.64	5 (17%)	43,45,45	1.86	8 (18%)

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
3	ADP	A	873	-	-	1/16/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	873	ADP	C5-C4	5.38	1.48	1.39
3	A	873	ADP	PA-O3A	3.14	1.62	1.59
3	A	873	ADP	C5-C6	2.87	1.49	1.41
3	A	873	ADP	C8-N7	2.75	1.37	1.31
3	A	873	ADP	C5-N7	-2.25	1.35	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	873	ADP	C5-C4-N3	-5.93	118.55	126.72
3	A	873	ADP	N3-C4-N9	4.77	135.28	127.17
3	A	873	ADP	C2-N3-C4	3.67	120.79	111.83
3	A	873	ADP	C4-C5-N7	-3.33	106.77	110.58
3	A	873	ADP	N3-C2-N1	-3.08	123.92	128.58
3	A	873	ADP	C5'-C4'-C3'	-2.47	106.31	115.21
3	A	873	ADP	C5-N7-C8	2.34	107.12	103.45
3	A	873	ADP	C4-N9-C8	2.33	108.18	105.74

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	873	ADP	C5'-O5'-PA-O1A

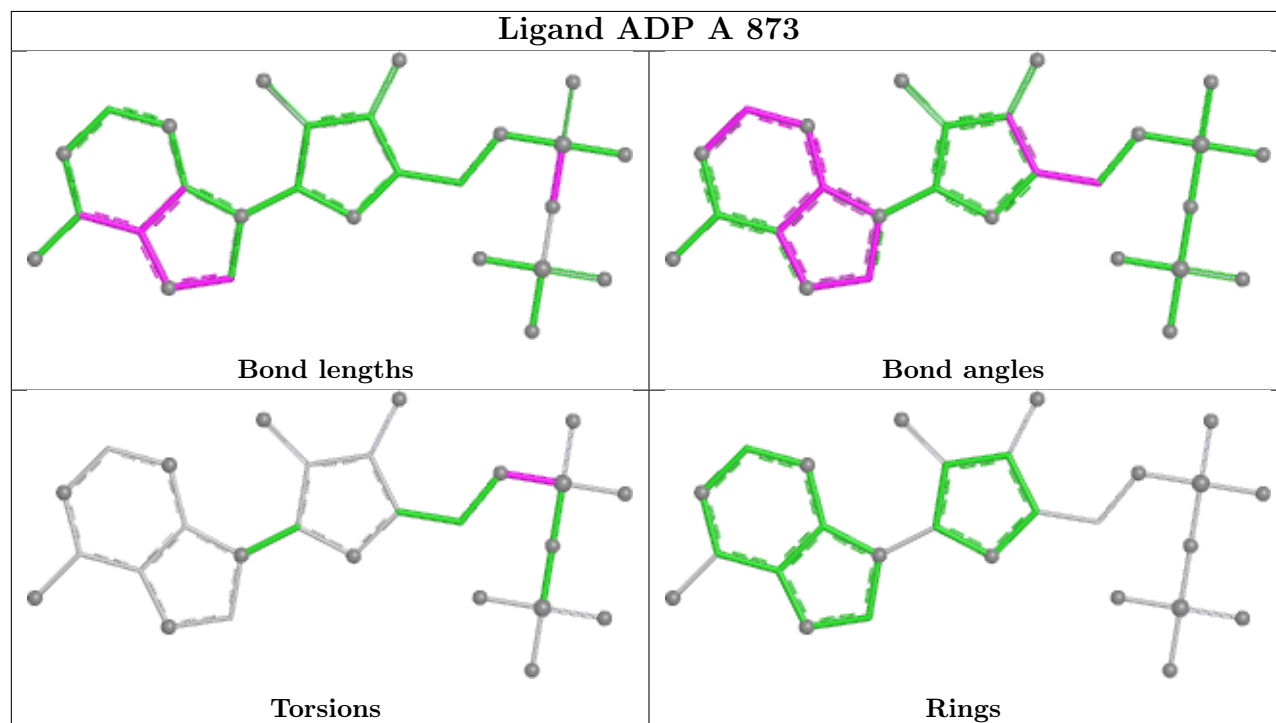
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	873	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.



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	813/822 (98%)	-0.19	13 (1%)	70 49	8, 44, 87, 131	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	519	ALA	3.3
1	A	572	GLY	2.9
1	A	518	LYS	2.8
1	A	364	PHE	2.4
1	A	517	ALA	2.4
1	A	361	VAL	2.3
1	A	536	THR	2.2
1	A	6	LYS	2.1
1	A	607	LYS	2.1
1	A	193	ASN	2.1
1	A	367	ARG	2.1
1	A	126	ASP	2.0
1	A	512	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

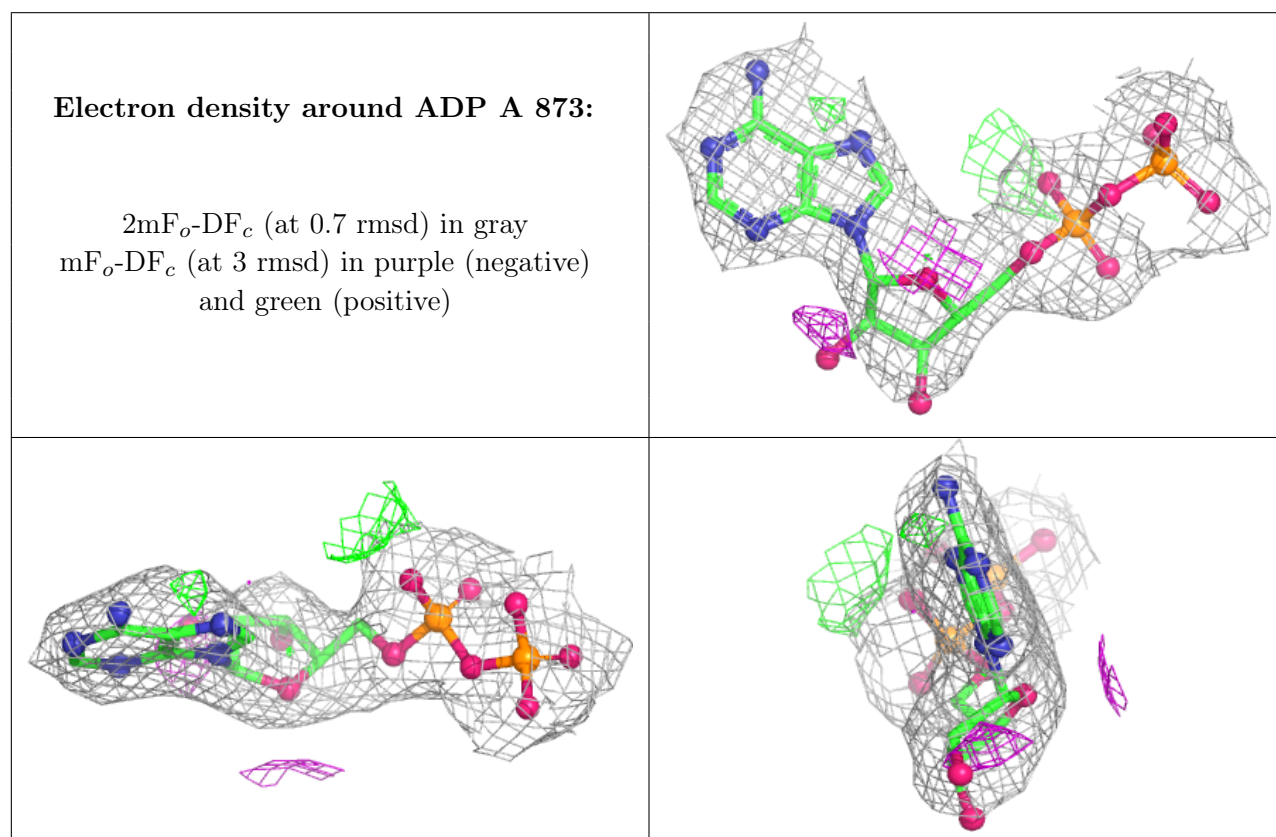
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ADP	A	873	27/27	0.90	0.13	51,52,53,54	0
2	MG	A	872	1/1	0.97	0.15	36,36,36,36	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.