



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:40 AM UTC

PDB ID : 3WQU / pdb_00003wqu
Title : Staphylococcus aureus FtsA complexed with ATP
Authors : Fujita, J.; Maeda, Y.; Miyazaki, Y.; Inoue, T.; Matsumura, H.
Deposited on : 2014-02-01
Resolution : 2.80 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

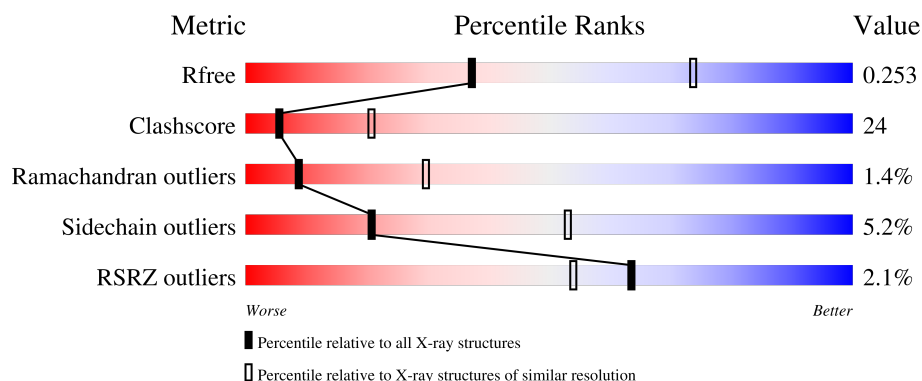
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	484	44% 30% • 24%
1	B	484	45% 29% • 23%
1	C	484	48% 25% • • 24%
1	D	484	4% 33% 39% • • 24%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11659 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cell division protein FtsA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	0	0	0
			2871	1811	458	595	7			
1	B	371	Total	C	N	O	S	0	0	0
			2880	1817	460	596	7			
1	C	370	Total	C	N	O	S	0	0	0
			2871	1811	458	595	7			
1	D	369	Total	C	N	O	S	0	0	0
			2861	1805	455	594	7			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	expression tag	UNP Q6GHQ0
A	-14	ASN	-	expression tag	UNP Q6GHQ0
A	-13	HIS	-	expression tag	UNP Q6GHQ0
A	-12	LYS	-	expression tag	UNP Q6GHQ0
A	-11	VAL	-	expression tag	UNP Q6GHQ0
A	-10	HIS	-	expression tag	UNP Q6GHQ0
A	-9	HIS	-	expression tag	UNP Q6GHQ0
A	-8	HIS	-	expression tag	UNP Q6GHQ0
A	-7	HIS	-	expression tag	UNP Q6GHQ0
A	-6	HIS	-	expression tag	UNP Q6GHQ0
A	-5	HIS	-	expression tag	UNP Q6GHQ0
A	-4	ILE	-	expression tag	UNP Q6GHQ0
A	-3	GLU	-	expression tag	UNP Q6GHQ0
A	-2	GLY	-	expression tag	UNP Q6GHQ0
A	-1	ARG	-	expression tag	UNP Q6GHQ0
A	0	HIS	-	expression tag	UNP Q6GHQ0
B	-15	MET	-	expression tag	UNP Q6GHQ0
B	-14	ASN	-	expression tag	UNP Q6GHQ0
B	-13	HIS	-	expression tag	UNP Q6GHQ0
B	-12	LYS	-	expression tag	UNP Q6GHQ0
B	-11	VAL	-	expression tag	UNP Q6GHQ0

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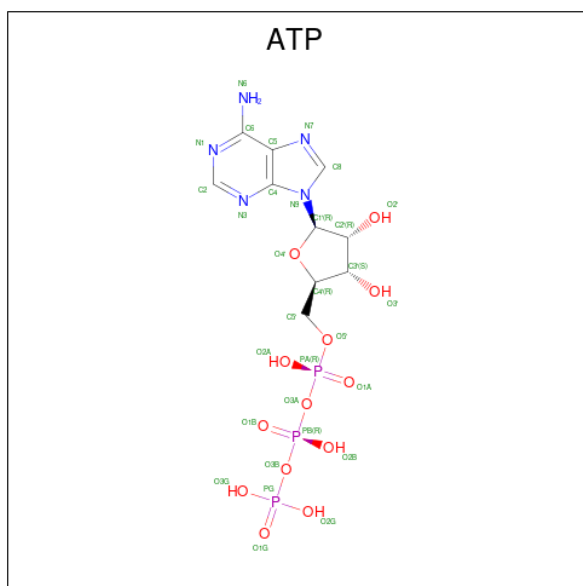
Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	HIS	-	expression tag	UNP Q6GHQ0
B	-9	HIS	-	expression tag	UNP Q6GHQ0
B	-8	HIS	-	expression tag	UNP Q6GHQ0
B	-7	HIS	-	expression tag	UNP Q6GHQ0
B	-6	HIS	-	expression tag	UNP Q6GHQ0
B	-5	HIS	-	expression tag	UNP Q6GHQ0
B	-4	ILE	-	expression tag	UNP Q6GHQ0
B	-3	GLU	-	expression tag	UNP Q6GHQ0
B	-2	GLY	-	expression tag	UNP Q6GHQ0
B	-1	ARG	-	expression tag	UNP Q6GHQ0
B	0	HIS	-	expression tag	UNP Q6GHQ0
C	-15	MET	-	expression tag	UNP Q6GHQ0
C	-14	ASN	-	expression tag	UNP Q6GHQ0
C	-13	HIS	-	expression tag	UNP Q6GHQ0
C	-12	LYS	-	expression tag	UNP Q6GHQ0
C	-11	VAL	-	expression tag	UNP Q6GHQ0
C	-10	HIS	-	expression tag	UNP Q6GHQ0
C	-9	HIS	-	expression tag	UNP Q6GHQ0
C	-8	HIS	-	expression tag	UNP Q6GHQ0
C	-7	HIS	-	expression tag	UNP Q6GHQ0
C	-6	HIS	-	expression tag	UNP Q6GHQ0
C	-5	HIS	-	expression tag	UNP Q6GHQ0
C	-4	ILE	-	expression tag	UNP Q6GHQ0
C	-3	GLU	-	expression tag	UNP Q6GHQ0
C	-2	GLY	-	expression tag	UNP Q6GHQ0
C	-1	ARG	-	expression tag	UNP Q6GHQ0
C	0	HIS	-	expression tag	UNP Q6GHQ0
D	-15	MET	-	expression tag	UNP Q6GHQ0
D	-14	ASN	-	expression tag	UNP Q6GHQ0
D	-13	HIS	-	expression tag	UNP Q6GHQ0
D	-12	LYS	-	expression tag	UNP Q6GHQ0
D	-11	VAL	-	expression tag	UNP Q6GHQ0
D	-10	HIS	-	expression tag	UNP Q6GHQ0
D	-9	HIS	-	expression tag	UNP Q6GHQ0
D	-8	HIS	-	expression tag	UNP Q6GHQ0
D	-7	HIS	-	expression tag	UNP Q6GHQ0
D	-6	HIS	-	expression tag	UNP Q6GHQ0
D	-5	HIS	-	expression tag	UNP Q6GHQ0
D	-4	ILE	-	expression tag	UNP Q6GHQ0
D	-3	GLU	-	expression tag	UNP Q6GHQ0
D	-2	GLY	-	expression tag	UNP Q6GHQ0
D	-1	ARG	-	expression tag	UNP Q6GHQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	HIS	-	expression tag	UNP Q6GHQ0

- 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		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

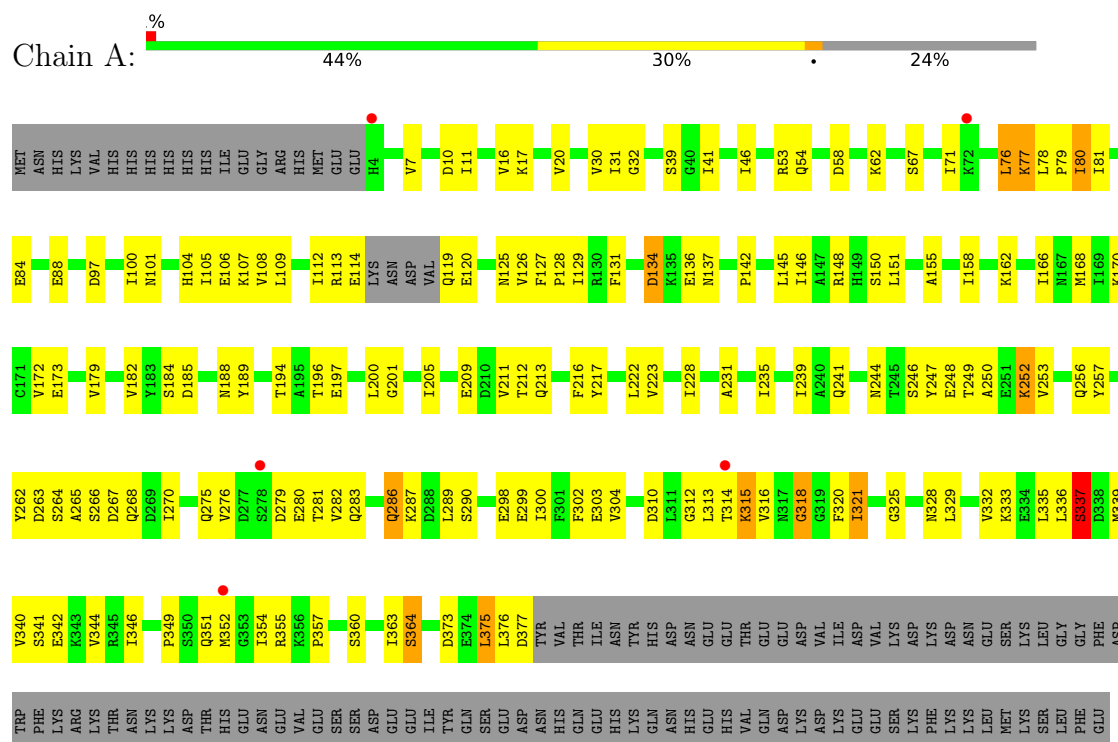
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total 13	O 13	0	0
4	B	10	Total 10	O 10	0	0
4	C	16	Total 16	O 16	0	0
4	D	9	Total 9	O 9	0	0

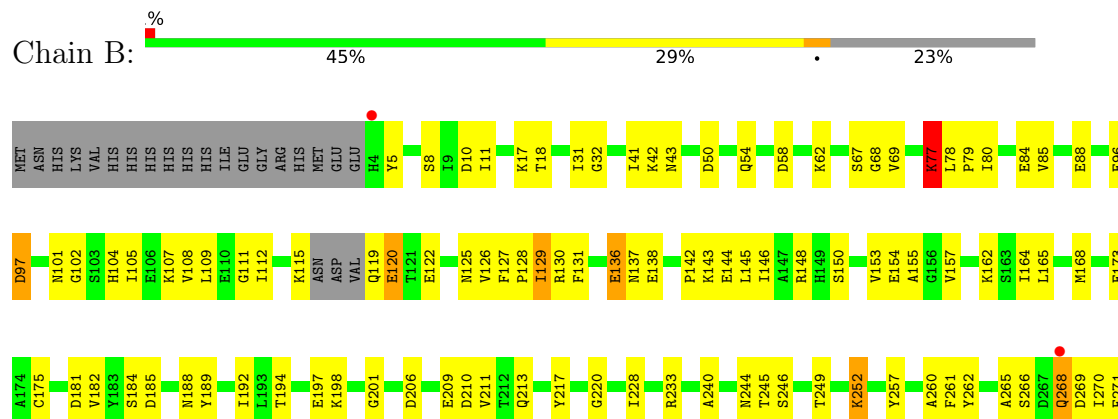
3 Residue-property plots

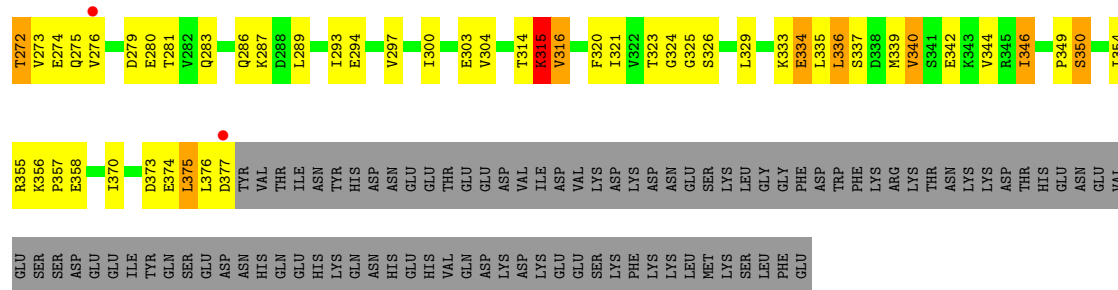
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

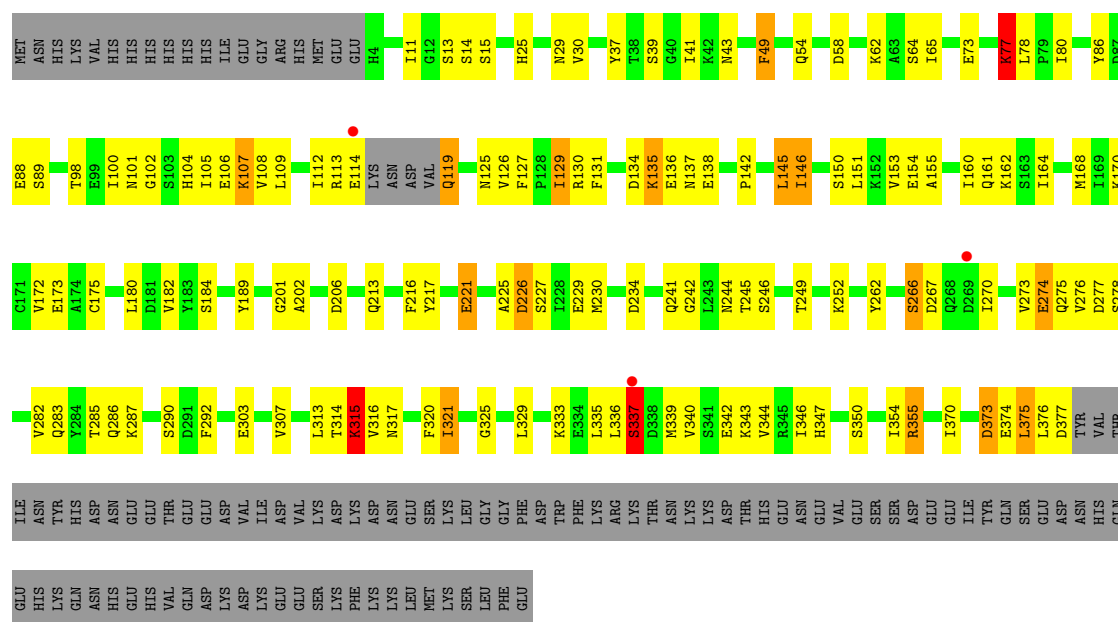


• Molecule 1: Cell division protein FtsA

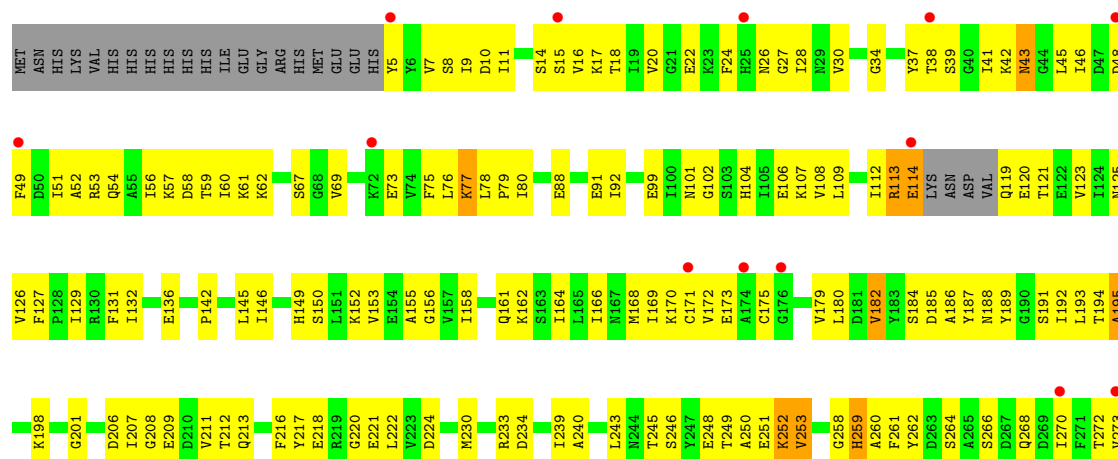




• Molecule 1: Cell division protein FtsA



• Molecule 1: Cell division protein FtsA





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.53Å 122.02Å 107.00Å 90.00° 95.66° 90.00°	Depositor
Resolution (Å)	39.65 – 2.80 39.65 – 2.80	Depositor EDS
% Data completeness (in resolution range)	88.1 (39.65-2.80) 88.1 (39.65-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.207 , 0.254 0.207 , 0.253	Depositor DCC
R_{free} test set	2393 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	48.4	Xtriage
Anisotropy	0.670	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11659	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.60	5/2910 (0.2%)	0.98	10/3935 (0.3%)
1	B	0.67	7/2919 (0.2%)	0.98	9/3946 (0.2%)
1	C	0.69	5/2910 (0.2%)	1.02	17/3935 (0.4%)
1	D	0.55	7/2899 (0.2%)	0.91	5/3920 (0.1%)
All	All	0.63	24/11638 (0.2%)	0.97	41/15736 (0.3%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	252	LYS	CA-CB	-12.58	1.33	1.53
1	B	337	SER	CA-C	-12.02	1.36	1.52
1	B	252	LYS	C-O	-11.57	1.09	1.24
1	C	252	LYS	C-O	-11.57	1.10	1.24
1	A	252	LYS	C-O	-11.14	1.08	1.23
1	A	252	LYS	CA-C	-10.58	1.40	1.52
1	B	337	SER	C-O	-10.36	1.11	1.24
1	D	252	LYS	C-O	-9.88	1.12	1.24
1	C	252	LYS	CA-C	-9.84	1.40	1.52
1	D	252	LYS	CA-C	-9.02	1.41	1.52
1	A	337	SER	CA-C	-8.05	1.41	1.52
1	A	252	LYS	CA-CB	-7.78	1.41	1.53
1	D	337	SER	CA-C	-7.33	1.42	1.52
1	B	337	SER	N-CA	-7.19	1.37	1.46
1	C	252	LYS	N-CA	-7.06	1.37	1.46
1	D	337	SER	C-O	-6.47	1.15	1.24
1	B	252	LYS	CA-C	-6.39	1.44	1.52
1	B	337	SER	CA-CB	-6.31	1.42	1.53
1	D	337	SER	N-CA	-6.17	1.38	1.46
1	C	337	SER	N-CA	-5.87	1.38	1.46
1	D	337	SER	CA-CB	-5.44	1.44	1.53
1	A	337	SER	C-O	-5.35	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	252	LYS	N-CA	-5.32	1.40	1.46
1	B	336	LEU	C-O	-5.29	1.18	1.24

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	129	ILE	N-CA-C	-11.04	102.95	111.90
1	A	129	ILE	N-CA-C	-8.40	104.34	111.56
1	C	337	SER	N-CA-CB	-7.77	98.24	110.28
1	B	120	GLU	N-CA-C	-7.12	104.22	113.12
1	A	267	ASP	N-CA-C	-7.10	104.49	113.43
1	C	129	ILE	N-CA-C	-7.09	104.93	111.67
1	C	336	LEU	CA-C-O	6.96	127.93	120.55
1	C	49	PHE	N-CA-C	6.63	119.35	111.33
1	C	267	ASP	N-CA-C	-6.57	105.79	113.88
1	D	337	SER	CA-CB-OG	-6.46	98.17	111.10
1	B	336	LEU	CA-C-O	6.30	127.23	120.55
1	B	154	GLU	N-CA-C	-6.29	98.48	108.73
1	C	252	LYS	CB-CA-C	-6.02	101.39	110.90
1	D	187	TYR	N-CA-C	-6.01	105.98	113.55
1	B	77	LYS	N-CA-C	-5.92	100.53	109.95
1	A	71	ILE	N-CA-C	5.90	117.03	109.30
1	A	16	VAL	N-CA-C	-5.90	101.19	109.21
1	A	150	SER	N-CA-C	5.87	117.44	108.52
1	C	221	GLU	N-CA-C	5.85	118.76	109.81
1	A	279	ASP	N-CA-C	-5.83	106.79	112.97
1	C	77	LYS	N-CA-C	-5.79	101.11	110.32
1	D	335	LEU	N-CA-C	5.76	118.30	111.33
1	D	211	VAL	N-CA-C	5.72	116.98	108.46
1	B	346	ILE	N-CA-C	-5.70	100.12	109.12
1	C	252	LYS	CA-C-O	-5.54	114.99	120.70
1	C	146	ILE	N-CA-C	5.52	115.81	107.80
1	C	150	SER	N-CA-C	5.42	116.52	108.60
1	B	68	GLY	N-CA-C	-5.38	108.20	115.36
1	C	337	SER	CB-CA-C	5.38	121.00	110.67
1	C	347	HIS	N-CA-C	5.36	118.28	109.76
1	A	318	GLY	N-CA-C	-5.30	108.09	114.66
1	A	11	ILE	N-CA-C	5.25	111.83	106.21
1	D	341	SER	N-CA-C	5.20	119.48	113.18
1	B	211	VAL	N-CA-C	5.18	115.94	108.48
1	A	235	ILE	N-CA-C	-5.15	105.69	110.53
1	A	39	SER	N-CA-C	-5.10	106.31	112.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	145	LEU	N-CA-C	-5.05	103.27	110.59
1	C	39	SER	N-CA-C	-5.03	106.83	113.17
1	B	150	SER	N-CA-C	5.03	116.17	108.52
1	C	86	TYR	N-CA-C	5.01	117.03	109.41
1	C	25	HIS	CB-CA-C	-5.01	110.41	117.23

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	2871	0	2813	135	0
1	B	2880	0	2826	120	0
1	C	2871	0	2813	116	0
1	D	2861	0	2806	175	0
2	A	31	0	12	2	0
2	B	31	0	12	2	0
2	C	31	0	12	5	0
2	D	31	0	12	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	13	0	0	0	0
4	B	10	0	0	0	0
4	C	16	0	0	6	0
4	D	9	0	0	3	0
All	All	11659	0	11306	541	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 24.

All (541) 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:D:358:GLU:HB3	4:D:604:HOH:O	1.52	1.06
1:B:244:ASN:HD22	1:B:275:GLN:NE2	1.59	1.00
1:D:333:LYS:O	1:D:337:SER:OG	1.84	0.96
1:A:101:ASN:H	1:A:104:HIS:HD2	1.15	0.92
1:C:189:TYR:OH	4:C:616:HOH:O	1.88	0.91
1:C:282:VAL:HG12	1:C:283:GLN:H	1.32	0.91
1:A:112:ILE:C	1:A:114:GLU:H	1.81	0.86
1:C:119:GLN:HA	1:C:119:GLN:HE21	1.41	0.85
1:D:246:SER:OG	1:D:249:THR:HG22	1.76	0.85
1:B:129:ILE:HG12	1:B:155:ALA:HA	1.60	0.83
1:B:80:ILE:H	1:B:213:GLN:NE2	1.77	0.83
1:B:270:ILE:HG21	1:B:283:GLN:HE21	1.44	0.83
1:B:101:ASN:H	1:B:104:HIS:HD2	1.28	0.80
1:D:333:LYS:HB2	1:D:346:ILE:HD11	1.65	0.78
1:A:266:SER:H	1:A:286:GLN:NE2	1.81	0.78
1:A:109:LEU:HD22	1:A:126:VAL:HG12	1.64	0.78
1:B:31:ILE:HD11	1:B:69:VAL:HG21	1.66	0.78
1:B:125:ASN:HD21	1:B:184:SER:H	1.31	0.78
1:C:101:ASN:H	1:C:104:HIS:HD2	1.33	0.78
1:A:352:MET:HA	1:A:355:ARG:HE	1.49	0.77
1:D:270:ILE:HG12	1:D:285:THR:HG22	1.66	0.77
1:A:7:VAL:HG22	1:A:20:VAL:HG13	1.65	0.77
1:A:298:GLU:HG3	1:A:339:MET:HE1	1.66	0.77
1:D:24:PHE:HB3	1:D:26:ASN:OD1	1.86	0.75
1:D:34:GLY:O	1:D:59:THR:HG23	1.86	0.75
1:D:125:ASN:HD21	1:D:184:SER:H	1.34	0.75
1:C:282:VAL:HG12	1:C:283:GLN:N	1.98	0.75
1:D:80:ILE:H	1:D:213:GLN:NE2	1.85	0.74
1:B:260:ALA:O	1:B:294:GLU:HB2	1.87	0.74
1:A:125:ASN:HD21	1:A:184:SER:H	1.36	0.74
1:C:107:LYS:HA	1:C:107:LYS:HE3	1.70	0.74
1:B:329:LEU:HD13	2:B:501:ATP:H2	1.53	0.73
1:C:316:VAL:O	1:C:342:GLU:HG2	1.89	0.73
1:D:240:ALA:HA	1:D:245:THR:HG22	1.70	0.72
1:A:53:ARG:HH22	1:A:54:GLN:HG2	1.54	0.72
1:B:244:ASN:HD22	1:B:275:GLN:HE21	1.35	0.71
1:B:228:ILE:HD13	1:B:303:GLU:HB3	1.73	0.71
1:B:101:ASN:H	1:B:104:HIS:CD2	2.08	0.71
1:C:206:ASP:CG	4:C:616:HOH:O	2.32	0.70
1:D:77:LYS:C	1:D:77:LYS:HD2	2.16	0.70
1:B:257:TYR:O	1:B:289:LEU:HD23	1.91	0.70
1:C:335:LEU:HG	1:C:339:MET:HE3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:ILE:H	1:C:213:GLN:NE2	1.89	0.70
1:C:106:GLU:HB2	1:C:376:LEU:HD22	1.74	0.70
1:C:333:LYS:O	1:C:337:SER:HB3	1.91	0.70
1:C:244:ASN:HB3	1:C:275:GLN:HE22	1.57	0.69
1:B:84:GLU:OE2	1:B:84:GLU:HA	1.91	0.69
1:A:333:LYS:HE3	1:A:344:VAL:O	1.93	0.69
1:B:273:VAL:HG12	1:B:274:GLU:O	1.94	0.68
1:C:270:ILE:HG12	1:C:285:THR:HG22	1.73	0.68
1:A:53:ARG:NH2	1:A:54:GLN:HG2	2.07	0.68
1:B:77:LYS:HD2	1:B:77:LYS:C	2.17	0.68
1:B:325:GLY:HA3	2:B:501:ATP:O5'	1.93	0.68
1:C:125:ASN:HD21	1:C:184:SER:H	1.40	0.68
1:C:206:ASP:OD1	4:C:616:HOH:O	2.11	0.68
1:A:112:ILE:C	1:A:114:GLU:N	2.52	0.67
1:B:198:LYS:HB3	1:B:220:GLY:HA2	1.76	0.67
1:D:185:ASP:HB3	1:D:189:TYR:CE2	2.30	0.67
1:D:346:ILE:HD12	1:D:346:ILE:N	2.10	0.67
1:C:206:ASP:HB3	4:C:610:HOH:O	1.95	0.66
1:B:314:THR:O	1:B:315:LYS:HB2	1.96	0.66
1:C:245:THR:OG1	1:C:249:THR:HG21	1.96	0.66
1:C:80:ILE:H	1:C:213:GLN:HE22	1.44	0.66
1:C:230:MET:HA	1:C:234:ASP:OD2	1.96	0.66
1:A:170:LYS:HD2	1:B:146:ILE:CD1	2.26	0.65
1:A:88:GLU:HG2	1:A:112:ILE:HG23	1.79	0.65
1:D:168:MET:O	1:D:172:VAL:HG23	1.97	0.65
1:D:356:LYS:HB3	1:D:358:GLU:HG2	1.79	0.65
1:D:248:GLU:O	1:D:252:LYS:HG3	1.96	0.65
1:A:127:PHE:O	1:A:155:ALA:HB1	1.95	0.65
1:C:88:GLU:HG2	1:C:112:ILE:HG23	1.79	0.65
1:C:262:TYR:HA	1:C:290:SER:OG	1.97	0.65
1:D:266:SER:O	1:D:286:GLN:HB3	1.96	0.65
1:A:106:GLU:HB2	1:A:376:LEU:HD22	1.78	0.65
1:A:325:GLY:HA3	2:A:501:ATP:O5'	1.97	0.65
1:D:56:ILE:HD12	1:D:171:CYS:HB3	1.78	0.65
1:D:185:ASP:HA	1:D:188:ASN:HB2	1.77	0.65
1:A:41:ILE:HD13	1:A:46:ILE:HA	1.79	0.65
1:C:131:PHE:CD2	1:C:142:PRO:HD3	2.32	0.65
1:D:77:LYS:HD2	1:D:78:LEU:N	2.11	0.65
1:B:335:LEU:HG	1:B:339:MET:CE	2.27	0.64
1:C:321:ILE:N	1:C:321:ILE:HD12	2.11	0.64
1:D:125:ASN:ND2	1:D:184:SER:H	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:PHE:CD2	1:D:142:PRO:HD3	2.32	0.64
1:A:320:PHE:CE2	1:A:340:VAL:HG21	2.32	0.64
1:C:244:ASN:HD22	1:C:275:GLN:NE2	1.96	0.64
1:C:226:ASP:OD1	1:C:227:SER:N	2.31	0.64
1:A:77:LYS:HD2	1:A:78:LEU:N	2.13	0.64
1:A:228:ILE:HD13	1:A:303:GLU:HB3	1.80	0.64
1:C:370:ILE:O	1:C:374:GLU:HG3	1.98	0.64
1:D:41:ILE:HD13	1:D:46:ILE:HA	1.79	0.64
1:B:270:ILE:HG22	1:B:283:GLN:HG2	1.80	0.63
1:B:111:GLY:O	1:B:115:LYS:HG3	1.99	0.63
1:A:131:PHE:CD2	1:A:142:PRO:HD3	2.33	0.63
1:B:370:ILE:O	1:B:374:GLU:HG3	1.98	0.63
1:D:300:ILE:O	1:D:304:VAL:HG23	1.99	0.63
1:B:201:GLY:HA2	1:B:217:TYR:O	1.98	0.62
1:B:275:GLN:HG2	1:B:280:GLU:O	1.99	0.62
1:D:216:PHE:CB	1:D:313:LEU:HD13	2.29	0.62
1:A:246:SER:OG	1:A:249:THR:HG23	1.99	0.62
1:B:246:SER:OG	1:B:249:THR:HG22	1.99	0.62
1:A:125:ASN:ND2	1:A:184:SER:H	1.97	0.61
1:A:321:ILE:N	1:A:321:ILE:HD12	2.15	0.61
1:D:312:GLY:O	1:D:314:THR:N	2.34	0.61
1:A:335:LEU:HG	1:A:339:MET:HE3	1.83	0.61
1:B:270:ILE:CG2	1:B:283:GLN:HG2	2.29	0.61
1:C:119:GLN:HE21	1:C:119:GLN:CA	2.07	0.61
1:A:352:MET:SD	1:A:352:MET:C	2.84	0.61
1:A:320:PHE:HE2	1:A:340:VAL:HG21	1.66	0.61
1:B:125:ASN:ND2	1:B:184:SER:H	1.97	0.61
1:D:42:LYS:O	1:D:43:ASN:HB2	2.00	0.61
1:D:56:ILE:O	1:D:60:ILE:HG13	2.00	0.61
1:B:245:THR:OG1	1:B:249:THR:HG21	2.00	0.61
1:C:225:ALA:O	1:C:226:ASP:HB2	2.01	0.61
1:A:77:LYS:HD2	1:A:77:LYS:C	2.25	0.60
1:D:314:THR:O	1:D:315:LYS:HB3	2.00	0.60
1:C:213:GLN:HB2	4:C:610:HOH:O	2.00	0.60
1:C:266:SER:H	1:C:286:GLN:NE2	2.00	0.60
1:D:127:PHE:O	1:D:155:ALA:HB1	2.01	0.60
1:A:105:ILE:HD12	1:A:131:PHE:CZ	2.37	0.59
1:C:77:LYS:HD2	1:C:77:LYS:C	2.26	0.59
1:D:7:VAL:HG22	1:D:20:VAL:HG22	1.84	0.59
1:D:132:ILE:HD12	1:D:152:LYS:HD3	1.83	0.59
1:B:10:ASP:OD1	1:B:77:LYS:HE2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:VAL:O	1:B:342:GLU:HG2	2.02	0.59
1:C:282:VAL:CG1	1:C:283:GLN:H	2.09	0.59
1:D:272:THR:HG23	1:D:282:VAL:O	2.03	0.59
1:C:333:LYS:HB2	1:C:346:ILE:HD13	1.84	0.59
1:D:189:TYR:HB2	1:D:217:TYR:OH	2.03	0.59
1:C:335:LEU:HG	1:C:339:MET:CE	2.33	0.59
1:D:80:ILE:HD12	1:D:213:GLN:HB3	1.86	0.58
1:D:189:TYR:O	1:D:192:ILE:HG12	2.03	0.58
1:D:24:PHE:HB2	1:D:27:GLY:O	2.03	0.58
1:C:170:LYS:HZ1	1:D:99:GLU:CD	2.11	0.58
1:B:189:TYR:HB2	1:B:217:TYR:OH	2.04	0.58
1:D:80:ILE:H	1:D:213:GLN:HE21	1.51	0.58
1:A:228:ILE:HD13	1:A:303:GLU:CB	2.33	0.58
1:A:329:LEU:HD13	2:A:501:ATP:H2	1.68	0.58
1:B:262:TYR:CE1	1:B:287:LYS:HG2	2.38	0.58
1:D:328:ASN:OD1	1:D:357:PRO:HD2	2.02	0.58
1:B:268:GLN:O	1:B:270:ILE:HG13	2.03	0.58
1:A:120:GLU:O	1:A:162:LYS:HB2	2.04	0.58
1:A:166:ILE:HD12	1:B:148:ARG:HD2	1.86	0.58
1:C:277:ASP:O	1:C:278:SER:HB3	2.02	0.58
1:A:216:PHE:HB3	1:A:313:LEU:HD13	1.86	0.57
1:B:131:PHE:CD2	1:B:142:PRO:HD3	2.38	0.57
1:B:245:THR:OG1	1:B:249:THR:CG2	2.52	0.57
1:D:101:ASN:H	1:D:104:HIS:HD2	1.52	0.57
1:D:250:ALA:O	1:D:253:VAL:HG22	2.03	0.57
1:B:101:ASN:N	1:B:104:HIS:HD2	2.01	0.57
1:D:102:GLY:HA3	1:D:376:LEU:O	2.04	0.57
1:B:119:GLN:HE21	1:B:119:GLN:HA	1.68	0.57
1:C:189:TYR:HB2	1:C:217:TYR:OH	2.05	0.57
1:D:259:HIS:HE1	1:D:261:PHE:HB3	1.70	0.57
1:A:101:ASN:H	1:A:104:HIS:CD2	2.08	0.57
1:A:249:THR:O	1:A:253:VAL:HG22	2.04	0.57
1:B:333:LYS:HB2	1:B:346:ILE:HD13	1.87	0.57
1:A:329:LEU:HB3	1:A:332:VAL:CG2	2.35	0.56
1:C:314:THR:O	1:C:315:LYS:HB3	2.05	0.56
1:D:28:ILE:HD13	1:D:366:ILE:HG22	1.86	0.56
1:D:164:ILE:O	1:D:168:MET:HG2	2.05	0.56
1:D:185:ASP:HA	1:D:188:ASN:HD22	1.68	0.56
1:D:273:VAL:HG12	1:D:274:GLU:N	2.20	0.56
1:A:200:LEU:HB2	1:A:318:GLY:HA2	1.88	0.56
1:D:346:ILE:HD12	1:D:346:ILE:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:SER:H	1:A:286:GLN:HE21	1.53	0.55
1:D:173:GLU:C	1:D:175:CYS:H	2.12	0.55
1:A:170:LYS:HD2	1:B:146:ILE:HD11	1.87	0.55
1:D:101:ASN:OD1	1:D:104:HIS:CD2	2.58	0.55
1:A:280:GLU:HG2	1:A:281:THR:H	1.71	0.55
1:B:80:ILE:H	1:B:213:GLN:HE22	1.52	0.55
1:C:89:SER:HB3	1:C:154:GLU:HA	1.88	0.55
1:C:246:SER:OG	1:C:249:THR:HG22	2.06	0.55
1:D:375:LEU:HD22	1:D:375:LEU:O	2.06	0.55
1:A:346:ILE:HG22	1:A:346:ILE:O	2.06	0.55
1:A:112:ILE:O	1:A:114:GLU:N	2.40	0.55
1:A:340:VAL:HG22	1:A:341:SER:H	1.70	0.55
1:A:351:GLN:O	1:A:355:ARG:HG2	2.06	0.55
1:C:129:ILE:HD13	1:C:221:GLU:HG3	1.89	0.55
1:D:363:ILE:HG23	1:D:364:SER:N	2.22	0.55
1:A:80:ILE:HD12	1:A:213:GLN:HB3	1.88	0.54
1:A:314:THR:O	1:A:315:LYS:HB3	2.08	0.54
1:B:17:LYS:HE3	1:B:358:GLU:O	2.07	0.54
1:D:79:PRO:HA	1:D:213:GLN:HE22	1.73	0.54
1:D:248:GLU:O	1:D:252:LYS:CG	2.56	0.54
1:A:162:LYS:O	1:A:166:ILE:HG13	2.08	0.54
1:D:101:ASN:H	1:D:104:HIS:CD2	2.26	0.54
1:D:106:GLU:HB2	1:D:376:LEU:HD22	1.90	0.54
1:D:88:GLU:HG2	1:D:112:ILE:HG23	1.90	0.54
1:D:321:ILE:HD12	1:D:321:ILE:N	2.23	0.54
1:A:134:ASP:CG	1:A:148:ARG:H	2.16	0.54
1:A:352:MET:CA	1:A:355:ARG:HE	2.18	0.53
1:C:201:GLY:HA2	1:C:217:TYR:O	2.08	0.53
1:D:198:LYS:HE2	1:D:220:GLY:O	2.08	0.53
1:D:216:PHE:CG	1:D:313:LEU:HD13	2.43	0.53
1:C:303:GLU:O	1:C:307:VAL:HG23	2.08	0.53
1:A:333:LYS:HB2	1:A:346:ILE:HD13	1.91	0.53
1:B:31:ILE:HG13	1:B:67:SER:HB2	1.91	0.53
1:D:303:GLU:O	1:D:307:VAL:HG23	2.09	0.53
1:A:30:VAL:HG21	1:A:354:ILE:HD13	1.91	0.53
1:A:262:TYR:O	1:A:264:SER:N	2.41	0.53
1:A:336:LEU:O	1:A:340:VAL:HG12	2.08	0.53
1:D:5:TYR:HE1	1:D:22:GLU:HB2	1.74	0.53
1:D:112:ILE:O	1:D:114:GLU:N	2.41	0.53
1:C:320:PHE:CE2	1:C:340:VAL:HG21	2.43	0.53
1:D:208:GLY:HA3	2:D:501:ATP:O2G	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:THR:O	1:D:253:VAL:HG13	2.09	0.53
1:B:373:ASP:O	1:B:377:ASP:HB2	2.09	0.53
1:D:67:SER:O	1:D:69:VAL:HG23	2.09	0.52
1:A:216:PHE:CB	1:A:313:LEU:HD13	2.39	0.52
1:B:266:SER:O	1:B:287:LYS:HB2	2.09	0.52
1:D:28:ILE:HD13	1:D:366:ILE:CG2	2.39	0.52
1:D:41:ILE:CD1	1:D:46:ILE:HG12	2.39	0.52
1:A:120:GLU:OE2	1:A:120:GLU:HA	2.09	0.52
1:A:287:LYS:O	1:A:290:SER:HB3	2.08	0.52
1:D:216:PHE:HB3	1:D:313:LEU:HD13	1.91	0.52
1:D:342:GLU:CD	1:D:342:GLU:N	2.68	0.52
1:B:105:ILE:HG21	1:B:375:LEU:HD22	1.92	0.52
1:B:88:GLU:HG2	1:B:112:ILE:HG23	1.91	0.52
1:B:257:TYR:CE2	1:B:271:PHE:HB3	2.44	0.52
1:C:266:SER:H	1:C:286:GLN:HE21	1.57	0.52
1:D:262:TYR:CE1	1:D:287:LYS:HG2	2.44	0.52
1:A:262:TYR:C	1:A:264:SER:H	2.18	0.52
1:A:270:ILE:HD13	1:A:283:GLN:HE21	1.74	0.52
1:A:315:LYS:HB2	1:A:315:LYS:NZ	2.25	0.52
1:D:285:THR:O	1:D:288:ASP:HB2	2.10	0.52
1:A:241:GLN:HG3	1:C:65:ILE:HG22	1.91	0.52
1:D:10:ASP:OD2	1:D:361:SER:HB3	2.09	0.52
1:D:24:PHE:C	1:D:26:ASN:H	2.18	0.52
1:D:146:ILE:N	1:D:146:ILE:HD12	2.24	0.52
1:D:325:GLY:HA3	2:D:501:ATP:O5'	2.09	0.52
1:A:360:SER:O	1:A:363:ILE:HG22	2.10	0.51
1:D:230:MET:HA	1:D:234:ASP:OD2	2.10	0.51
1:A:168:MET:O	1:A:172:VAL:HG23	2.10	0.51
1:B:122:GLU:HG2	1:B:165:LEU:CD2	2.40	0.51
1:C:119:GLN:HA	1:C:119:GLN:NE2	2.20	0.51
1:C:173:GLU:C	1:C:175:CYS:H	2.17	0.51
1:D:333:LYS:HE3	1:D:344:VAL:O	2.10	0.51
1:A:352:MET:HA	1:A:355:ARG:NE	2.22	0.51
1:C:11:ILE:HB	1:C:168:MET:HE1	1.92	0.51
1:C:102:GLY:HA3	1:C:376:LEU:O	2.09	0.51
1:C:168:MET:O	1:C:172:VAL:HG23	2.10	0.51
1:D:324:GLY:O	1:D:357:PRO:HB2	2.10	0.51
1:D:329:LEU:O	1:D:332:VAL:HG23	2.11	0.51
1:B:272:THR:HG22	1:B:281:THR:HB	1.91	0.51
1:D:194:THR:O	1:D:195:ALA:C	2.54	0.51
1:A:32:GLY:HA3	1:A:67:SER:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:ILE:HB	1:C:154:GLU:O	2.11	0.51
1:C:325:GLY:HA3	2:C:501:ATP:O5'	2.11	0.51
1:B:67:SER:HB2	1:B:69:VAL:HG23	1.92	0.51
1:D:335:LEU:HG	1:D:339:MET:HE3	1.91	0.51
1:A:79:PRO:O	1:A:81:ILE:N	2.43	0.51
1:A:280:GLU:HG2	1:A:281:THR:N	2.25	0.51
1:B:105:ILE:HG21	1:B:375:LEU:CD2	2.41	0.51
1:B:245:THR:HB	1:B:273:VAL:HG11	1.93	0.51
1:A:248:GLU:OE1	1:A:248:GLU:N	2.34	0.50
1:D:243:LEU:HD22	1:D:284:TYR:CE2	2.46	0.50
1:A:349:PRO:HB2	1:A:354:ILE:O	2.11	0.50
1:B:320:PHE:CE2	1:B:340:VAL:HG21	2.46	0.50
1:B:233:ARG:HG3	1:B:233:ARG:HH11	1.76	0.50
1:C:333:LYS:HE3	1:C:344:VAL:O	2.11	0.50
1:C:266:SER:O	1:C:287:LYS:HB2	2.12	0.50
1:A:352:MET:HA	1:A:355:ARG:HG3	1.92	0.50
1:D:201:GLY:CA	1:D:218:GLU:HG3	2.42	0.50
1:C:127:PHE:O	1:C:155:ALA:HB1	2.12	0.50
1:A:328:ASN:OD1	1:A:357:PRO:HD2	2.12	0.49
1:B:173:GLU:C	1:B:175:CYS:H	2.20	0.49
1:B:321:ILE:HD12	1:B:321:ILE:N	2.27	0.49
1:B:323:THR:HG23	1:B:324:GLY:N	2.26	0.49
1:C:30:VAL:HG21	1:C:354:ILE:HD13	1.94	0.49
1:D:58:ASP:O	1:D:62:LYS:HG3	2.11	0.49
1:D:262:TYR:C	1:D:264:SER:H	2.20	0.49
1:A:329:LEU:HB3	1:A:332:VAL:HG23	1.94	0.49
1:C:119:GLN:CA	1:C:119:GLN:NE2	2.73	0.49
1:D:101:ASN:OD1	1:D:104:HIS:HD2	1.95	0.49
1:A:266:SER:N	1:A:286:GLN:NE2	2.57	0.49
1:B:96:GLU:O	1:B:97:ASP:C	2.55	0.49
1:C:13:SER:HA	1:C:41:ILE:HB	1.95	0.49
1:D:239:ILE:HD13	1:D:289:LEU:HD11	1.92	0.49
1:A:109:LEU:HD22	1:A:126:VAL:CG1	2.39	0.49
1:A:119:GLN:HA	1:A:119:GLN:NE2	2.28	0.49
1:A:270:ILE:HG21	1:A:283:GLN:HE21	1.77	0.49
1:C:80:ILE:HD13	1:C:225:ALA:HB1	1.95	0.49
1:D:273:VAL:CG1	1:D:274:GLU:N	2.74	0.49
1:B:335:LEU:HG	1:B:339:MET:HE1	1.94	0.49
1:D:56:ILE:CD1	1:D:171:CYS:HB3	2.42	0.49
1:A:188:ASN:HB3	1:A:364:SER:HB2	1.93	0.49
1:A:196:THR:HG22	1:A:200:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:340:VAL:HG22	1:D:342:GLU:OE1	2.13	0.49
1:C:217:TYR:N	1:C:217:TYR:CD1	2.80	0.49
1:C:14:SER:HB3	2:C:501:ATP:O1B	2.13	0.48
1:D:315:LYS:NZ	1:D:315:LYS:HB2	2.27	0.48
1:A:266:SER:N	1:A:286:GLN:HE21	2.11	0.48
1:A:223:VAL:HG11	1:A:313:LEU:HD21	1.95	0.48
1:B:333:LYS:HB2	1:B:346:ILE:CD1	2.43	0.48
1:D:5:TYR:CE1	1:D:22:GLU:HB2	2.48	0.48
1:B:32:GLY:HA3	1:B:67:SER:HB3	1.96	0.48
1:B:240:ALA:HA	1:B:245:THR:HG22	1.94	0.48
1:A:270:ILE:HG21	1:A:283:GLN:NE2	2.29	0.48
1:C:109:LEU:HD22	1:C:126:VAL:HG12	1.94	0.48
1:D:249:THR:HA	1:D:252:LYS:HG3	1.96	0.48
1:B:194:THR:OG1	1:B:197:GLU:HG3	2.13	0.48
1:A:58:ASP:O	1:A:62:LYS:HG3	2.14	0.48
1:C:130:ARG:NH2	1:C:154:GLU:OE1	2.45	0.48
1:C:160:ILE:HG12	1:C:161:GLN:H	1.77	0.48
1:D:351:GLN:NE2	1:D:363:ILE:HD11	2.28	0.48
1:A:79:PRO:HA	1:A:213:GLN:HE22	1.79	0.48
1:A:298:GLU:HG2	1:A:302:PHE:CE2	2.49	0.48
1:B:79:PRO:HA	1:B:213:GLN:HE22	1.79	0.48
1:B:120:GLU:O	1:B:162:LYS:HB2	2.14	0.48
1:B:336:LEU:HA	1:B:339:MET:HE3	1.95	0.48
1:C:134:ASP:O	1:C:136:GLU:N	2.47	0.48
1:D:15:SER:HB3	1:D:37:TYR:CD1	2.49	0.48
1:D:77:LYS:C	1:D:77:LYS:CD	2.86	0.48
1:B:88:GLU:CG	1:B:112:ILE:HG23	2.44	0.48
1:C:11:ILE:HD12	1:C:168:MET:HE3	1.95	0.48
1:C:317:ASN:HD22	1:C:317:ASN:N	2.11	0.48
2:C:501:ATP:H1'	4:C:603:HOH:O	2.13	0.47
1:D:11:ILE:HD12	1:D:168:MET:HE3	1.95	0.47
1:D:329:LEU:HD13	2:D:501:ATP:H2	1.78	0.47
1:A:244:ASN:HD22	1:A:275:GLN:NE2	2.12	0.47
1:B:109:LEU:HD22	1:B:126:VAL:HG12	1.96	0.47
1:B:137:ASN:HD22	1:B:138:GLU:N	2.13	0.47
1:A:185:ASP:HA	1:A:188:ASN:HD22	1.79	0.47
1:C:105:ILE:O	1:C:108:VAL:HG12	2.14	0.47
1:D:109:LEU:HD22	1:D:126:VAL:HG12	1.96	0.47
1:B:122:GLU:HB2	1:B:162:LYS:HG3	1.97	0.47
1:C:108:VAL:HG22	1:C:153:VAL:HG12	1.97	0.47
1:D:38:THR:OG1	1:D:39:SER:N	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:GLN:HA	1:B:119:GLN:NE2	2.30	0.47
1:B:128:PRO:HG2	1:B:375:LEU:HD11	1.96	0.47
1:B:192:ILE:O	1:B:192:ILE:HG13	2.13	0.47
1:B:261:PHE:CD2	1:B:334:GLU:OE1	2.67	0.47
1:C:142:PRO:O	1:C:145:LEU:HB2	2.14	0.47
1:C:350:SER:O	1:C:355:ARG:HD3	2.15	0.47
1:D:41:ILE:HG23	1:D:45:LEU:O	2.14	0.47
1:A:104:HIS:O	1:A:108:VAL:HG12	2.15	0.47
1:D:14:SER:HB2	1:D:209:GLU:HB2	1.96	0.47
1:C:15:SER:HB3	1:C:37:TYR:CD1	2.50	0.46
1:C:287:LYS:O	1:C:290:SER:HB3	2.16	0.46
1:D:73:GLU:HB3	1:D:180:LEU:HG	1.98	0.46
1:B:77:LYS:HD2	1:B:78:LEU:N	2.30	0.46
1:C:101:ASN:N	1:C:104:HIS:HD2	2.06	0.46
2:D:501:ATP:PA	4:D:604:HOH:O	2.73	0.46
1:A:136:GLU:HA	1:A:136:GLU:OE1	2.15	0.46
1:B:102:GLY:HA3	1:B:376:LEU:O	2.15	0.46
1:C:160:ILE:HG12	1:C:161:GLN:N	2.30	0.46
1:A:31:ILE:HG13	1:A:67:SER:HB2	1.98	0.46
1:A:189:TYR:HB2	1:A:217:TYR:OH	2.16	0.46
1:A:30:VAL:HG21	1:A:354:ILE:CD1	2.45	0.46
1:A:146:ILE:O	1:A:146:ILE:HG22	2.16	0.46
1:C:100:ILE:HA	1:C:104:HIS:CD2	2.50	0.46
1:D:245:THR:OG1	1:D:249:THR:HG21	2.14	0.46
1:D:246:SER:H	1:D:249:THR:CG2	2.29	0.46
1:A:209:GLU:O	1:A:231:ALA:HB3	2.16	0.46
1:B:58:ASP:O	1:B:62:LYS:HG3	2.15	0.46
1:B:245:THR:HB	1:B:273:VAL:CG1	2.46	0.46
1:C:58:ASP:O	1:C:62:LYS:HG3	2.16	0.46
1:D:53:ARG:HH12	1:D:57:LYS:NZ	2.14	0.46
1:D:207:ILE:HG22	1:D:326:SER:HB2	1.98	0.46
1:D:209:GLU:HG2	1:D:233:ARG:HB2	1.96	0.46
1:C:43:ASN:HB3	1:C:229:GLU:OE2	2.16	0.46
1:C:320:PHE:C	1:C:321:ILE:HD12	2.41	0.46
1:D:53:ARG:HH12	1:D:57:LYS:HD2	1.79	0.46
1:B:293:ILE:O	1:B:297:VAL:HG23	2.16	0.46
1:C:49:PHE:CD1	1:C:49:PHE:C	2.93	0.46
1:D:243:LEU:HD22	1:D:284:TYR:CD2	2.51	0.46
1:A:262:TYR:HA	1:A:290:SER:OG	2.16	0.46
1:B:209:GLU:HG2	1:B:210:ASP:OD1	2.15	0.46
1:A:53:ARG:HH11	1:A:53:ARG:HG2	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:ASP:O	1:C:377:ASP:HB2	2.16	0.45
1:A:105:ILE:HG21	1:A:375:LEU:HD22	1.98	0.45
1:C:244:ASN:HD22	1:C:275:GLN:HE21	1.64	0.45
1:D:24:PHE:C	1:D:26:ASN:N	2.74	0.45
1:D:240:ALA:HA	1:D:245:THR:CG2	2.44	0.45
1:D:88:GLU:CG	1:D:112:ILE:HG23	2.46	0.45
1:C:270:ILE:HG21	1:C:283:GLN:NE2	2.31	0.45
1:D:8:SER:HA	1:D:75:PHE:O	2.15	0.45
1:A:100:ILE:HD12	1:A:151:LEU:HD22	1.98	0.45
1:B:125:ASN:HD21	1:B:184:SER:N	2.06	0.45
1:D:76:LEU:HD13	1:D:77:LYS:O	2.17	0.45
1:B:314:THR:O	1:C:29:ASN:OD1	2.35	0.45
1:C:321:ILE:N	1:C:321:ILE:CD1	2.80	0.45
1:C:375:LEU:O	1:C:375:LEU:HD22	2.17	0.45
1:A:119:GLN:HA	1:A:119:GLN:HE21	1.80	0.45
1:A:194:THR:HG23	1:A:197:GLU:OE1	2.17	0.45
1:A:247:TYR:O	1:A:250:ALA:HB3	2.17	0.45
1:D:258:GLY:HA3	1:D:329:LEU:HD11	1.99	0.45
1:D:275:GLN:CD	1:D:282:VAL:CG2	2.90	0.45
1:A:173:GLU:HG2	1:A:179:VAL:HG23	1.99	0.44
1:D:251:GLU:OE2	2:D:501:ATP:O2'	2.34	0.44
1:C:164:ILE:O	1:C:168:MET:HG2	2.16	0.44
1:D:16:VAL:HG12	1:D:59:THR:HG21	1.99	0.44
1:D:52:ALA:O	1:D:56:ILE:HG13	2.17	0.44
1:B:8:SER:O	1:B:18:THR:HA	2.18	0.44
1:B:108:VAL:HG22	1:B:153:VAL:HG12	1.99	0.44
1:C:329:LEU:HD13	2:C:501:ATP:C2	2.52	0.44
1:D:78:LEU:HG	1:D:182:VAL:HG22	2.00	0.44
1:D:152:LYS:HG2	1:D:153:VAL:N	2.32	0.44
1:C:100:ILE:HD12	1:C:151:LEU:HD22	1.99	0.44
1:C:317:ASN:N	1:C:317:ASN:ND2	2.64	0.44
1:D:275:GLN:OE1	1:D:275:GLN:HA	2.16	0.44
1:D:370:ILE:O	1:D:371:ALA:C	2.59	0.44
1:B:127:PHE:O	1:B:155:ALA:HB1	2.18	0.44
1:A:196:THR:HG22	1:A:200:LEU:CD1	2.48	0.44
1:D:49:PHE:C	1:D:49:PHE:CD1	2.95	0.44
1:D:169:ILE:O	1:D:173:GLU:HG3	2.18	0.44
1:A:105:ILE:HD11	1:A:142:PRO:HG2	2.00	0.44
1:D:275:GLN:CD	1:D:282:VAL:HG21	2.43	0.44
1:B:107:LYS:HB2	1:B:107:LYS:HE3	1.81	0.43
1:D:189:TYR:OH	1:D:206:ASP:OD1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:ILE:HG23	1:D:108:VAL:HG23	2.00	0.43
1:D:121:THR:HG22	1:D:161:GLN:HA	2.00	0.43
1:B:349:PRO:O	1:B:355:ARG:HA	2.18	0.43
1:C:125:ASN:ND2	1:C:184:SER:H	2.11	0.43
1:D:54:GLN:O	1:D:58:ASP:OD1	2.37	0.43
1:B:185:ASP:HA	1:B:188:ASN:HB2	1.99	0.43
1:D:169:ILE:HG23	1:D:179:VAL:HG21	1.99	0.43
1:D:298:GLU:HA	1:D:339:MET:HE1	2.00	0.43
1:D:320:PHE:CE2	1:D:340:VAL:HG21	2.53	0.43
1:A:333:LYS:O	1:A:337:SER:OG	2.35	0.43
1:C:153:VAL:O	1:C:153:VAL:HG13	2.19	0.43
1:D:186:ALA:O	1:D:222:LEU:HD22	2.19	0.43
1:A:300:ILE:O	1:A:304:VAL:HG23	2.18	0.43
1:B:244:ASN:O	1:B:244:ASN:CG	2.62	0.43
1:B:265:ALA:HB3	1:B:287:LYS:HG3	2.00	0.43
1:C:242:GLY:HA3	1:C:292:PHE:CZ	2.54	0.43
1:D:370:ILE:O	1:D:374:GLU:HG3	2.19	0.43
1:B:206:ASP:OD2	1:B:324:GLY:HA3	2.17	0.43
1:B:350:SER:O	1:B:355:ARG:HD2	2.18	0.43
1:C:80:ILE:N	1:C:213:GLN:HE22	2.12	0.43
1:A:84:GLU:O	1:A:158:ILE:HA	2.19	0.43
1:A:127:PHE:HA	1:A:128:PRO:HD3	1.86	0.43
1:A:216:PHE:HE2	1:A:316:VAL:HG22	1.84	0.43
1:B:265:ALA:HB1	1:B:287:LYS:HA	2.00	0.43
1:D:224:ASP:OD1	1:D:311:LEU:HD22	2.19	0.43
1:D:349:PRO:O	1:D:355:ARG:HA	2.18	0.43
1:B:67:SER:CB	1:B:69:VAL:HG23	2.48	0.43
1:C:270:ILE:HG21	1:C:283:GLN:HE21	1.84	0.43
1:C:273:VAL:HG12	1:C:274:GLU:O	2.18	0.43
1:B:316:VAL:HG21	1:B:320:PHE:CZ	2.53	0.43
1:C:77:LYS:HD2	1:C:78:LEU:N	2.34	0.43
1:D:49:PHE:HE2	1:D:170:LYS:HD3	1.83	0.43
1:C:101:ASN:H	1:C:104:HIS:CD2	2.23	0.42
1:C:244:ASN:ND2	1:C:276:VAL:HG12	2.33	0.42
1:A:299:GLU:O	1:A:303:GLU:HG2	2.19	0.42
1:B:354:ILE:C	1:B:356:LYS:H	2.27	0.42
1:D:9:ILE:HG12	1:D:18:THR:OG1	2.18	0.42
1:B:315:LYS:HD2	1:B:315:LYS:O	2.20	0.42
1:C:107:LYS:HE3	1:C:107:LYS:CA	2.46	0.42
1:C:146:ILE:O	1:C:146:ILE:HG22	2.20	0.42
1:D:129:ILE:CD1	1:D:221:GLU:HG3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:191:SER:HB2	1:D:364:SER:HB2	2.01	0.42
1:A:79:PRO:CG	1:A:81:ILE:HD12	2.48	0.42
1:A:194:THR:OG1	1:A:197:GLU:HG3	2.19	0.42
1:B:130:ARG:HH21	1:B:130:ARG:HG2	1.84	0.42
1:B:326:SER:O	1:B:329:LEU:HB2	2.20	0.42
1:D:260:ALA:O	1:D:294:GLU:HG3	2.20	0.42
1:B:85:VAL:HA	1:B:157:VAL:O	2.19	0.42
1:A:201:GLY:HA2	1:A:217:TYR:O	2.19	0.42
1:A:216:PHE:CG	1:A:313:LEU:HD13	2.54	0.42
1:C:216:PHE:CD1	1:C:313:LEU:HD22	2.53	0.42
1:D:41:ILE:HD11	1:D:46:ILE:HG12	2.01	0.42
1:D:76:LEU:CD2	1:D:172:VAL:HG21	2.50	0.42
1:D:119:GLN:HG3	1:D:120:GLU:N	2.34	0.42
1:A:76:LEU:HD22	1:A:77:LYS:O	2.19	0.42
1:A:205:ILE:CD1	1:A:304:VAL:HG11	2.50	0.42
1:A:211:VAL:HG12	1:A:212:THR:N	2.35	0.42
1:B:143:LYS:C	1:B:145:LEU:H	2.27	0.42
1:D:185:ASP:HA	1:D:188:ASN:ND2	2.34	0.42
1:D:282:VAL:HG12	1:D:283:GLN:N	2.35	0.42
1:A:320:PHE:C	1:A:321:ILE:HD12	2.45	0.42
1:B:11:ILE:HG22	1:B:41:ILE:HG13	2.01	0.42
1:B:233:ARG:HG3	1:B:233:ARG:NH1	2.34	0.42
1:B:266:SER:H	1:B:286:GLN:HE21	1.68	0.42
1:D:48:ASP:OD1	1:D:51:ILE:HG13	2.19	0.42
1:D:108:VAL:HG22	1:D:153:VAL:HG12	2.02	0.42
1:D:149:HIS:O	1:D:150:SER:HB3	2.19	0.42
1:A:282:VAL:HG12	1:A:283:GLN:N	2.35	0.42
1:B:42:LYS:O	1:B:43:ASN:C	2.63	0.42
1:C:162:LYS:HB2	1:C:162:LYS:HE3	1.89	0.42
1:D:91:GLU:HA	1:D:152:LYS:HA	2.02	0.42
1:D:120:GLU:O	1:D:162:LYS:HB2	2.20	0.42
1:A:239:ILE:HD13	1:A:289:LEU:HD11	2.01	0.41
1:B:130:ARG:HD3	1:B:138:GLU:CD	2.45	0.41
1:D:166:ILE:O	1:D:170:LYS:HB2	2.19	0.41
1:D:363:ILE:CG2	1:D:364:SER:N	2.82	0.41
1:C:134:ASP:O	1:C:135:LYS:C	2.64	0.41
1:D:127:PHE:CZ	1:D:156:GLY:HA3	2.55	0.41
1:D:246:SER:O	1:D:249:THR:CG2	2.69	0.41
1:D:346:ILE:N	1:D:346:ILE:CD1	2.80	0.41
1:D:125:ASN:HB2	1:D:158:ILE:HB	2.01	0.41
1:A:340:VAL:HG22	1:A:341:SER:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:HIS:O	1:B:108:VAL:HG12	2.19	0.41
1:B:261:PHE:CD1	1:B:335:LEU:HA	2.56	0.41
1:A:10:ASP:HB3	1:A:17:LYS:HB2	2.02	0.41
1:A:265:ALA:HA	1:A:286:GLN:NE2	2.35	0.41
1:A:280:GLU:CG	1:A:281:THR:H	2.33	0.41
1:B:257:TYR:CE2	1:B:271:PHE:CB	3.03	0.41
1:A:310:ASP:C	1:A:312:GLY:H	2.27	0.41
1:A:342:GLU:CD	1:A:342:GLU:N	2.79	0.41
1:B:136:GLU:OE1	1:B:136:GLU:HA	2.20	0.41
1:C:73:GLU:HB3	1:C:180:LEU:HG	2.02	0.41
1:C:173:GLU:C	1:C:175:CYS:N	2.76	0.41
1:A:249:THR:HA	1:A:252:LYS:HD3	2.02	0.41
1:C:137:ASN:HD22	1:C:138:GLU:N	2.19	0.41
1:C:329:LEU:HD13	2:C:501:ATP:H2	1.86	0.41
1:D:325:GLY:CA	4:D:604:HOH:O	2.68	0.41
1:D:354:ILE:C	1:D:356:LYS:H	2.28	0.41
1:A:342:GLU:O	1:A:344:VAL:HG23	2.20	0.41
1:B:105:ILE:HD13	1:B:375:LEU:CD2	2.50	0.41
1:B:356:LYS:HA	1:B:357:PRO:HD3	1.92	0.41
1:D:217:TYR:CD1	1:D:217:TYR:N	2.88	0.41
1:B:101:ASN:O	1:B:102:GLY:C	2.63	0.41
1:B:137:ASN:HD22	1:B:138:GLU:H	1.69	0.41
1:C:170:LYS:NZ	1:D:99:GLU:CD	2.79	0.41
1:D:17:LYS:HE3	1:D:358:GLU:O	2.21	0.41
1:D:193:LEU:HB3	1:D:198:LYS:HG3	2.02	0.41
1:D:301:PHE:O	1:D:304:VAL:HB	2.21	0.41
1:A:265:ALA:HA	1:A:286:GLN:HE22	1.86	0.41
1:A:298:GLU:HG3	1:A:339:MET:CE	2.45	0.41
1:C:245:THR:OG1	1:C:273:VAL:CG1	2.69	0.41
1:D:207:ILE:CG2	1:D:326:SER:HB2	2.51	0.41
1:A:217:TYR:CD2	1:A:222:LEU:HA	2.56	0.40
1:A:256:GLN:HE21	1:A:257:TYR:HE2	1.68	0.40
1:B:300:ILE:O	1:B:304:VAL:HG23	2.22	0.40
1:C:202:ALA:HB1	1:C:321:ILE:CD1	2.50	0.40
1:D:49:PHE:O	1:D:53:ARG:HB2	2.20	0.40
1:C:30:VAL:HG21	1:C:354:ILE:CD1	2.52	0.40
1:C:244:ASN:CG	1:C:276:VAL:HG12	2.47	0.40
1:D:258:GLY:HA3	1:D:329:LEU:CD1	2.51	0.40
1:A:145:LEU:HD23	1:A:146:ILE:N	2.35	0.40
1:D:76:LEU:O	1:D:182:VAL:HA	2.21	0.40
1:A:286:GLN:HE21	1:A:286:GLN:HB3	1.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:ILE:O	1:B:168:MET:HG2	2.20	0.40
1:C:98:THR:HG21	1:C:104:HIS:CE1	2.57	0.40
1:D:30:VAL:HG21	1:D:354:ILE:HD13	2.03	0.40
1:D:107:LYS:HE3	1:D:107:LYS:HB2	1.72	0.40
1:D:113:ARG:HG3	1:D:123:VAL:HB	2.04	0.40
1:A:321:ILE:N	1:A:321:ILE:CD1	2.83	0.40
1:B:333:LYS:HE3	1:B:344:VAL:O	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	366/484 (76%)	333 (91%)	29 (8%)	4 (1%)	11	36
1	B	367/484 (76%)	343 (94%)	21 (6%)	3 (1%)	16	44
1	C	366/484 (76%)	338 (92%)	24 (7%)	4 (1%)	11	36
1	D	365/484 (75%)	310 (85%)	45 (12%)	10 (3%)	4	15
All	All	1464/1936 (76%)	1324 (90%)	119 (8%)	21 (1%)	9	30

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	ASP
1	B	144	GLU
1	B	315	LYS
1	C	135	LYS
1	D	113	ARG
1	D	313	LEU
1	A	113	ARG
1	C	113	ARG

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Mol	Chain	Res	Type
1	A	80	ILE
1	B	97	ASP
1	D	43	ASN
1	D	61	LYS
1	D	195	ALA
1	A	134	ASP
1	C	315	LYS
1	D	259	HIS
1	D	315	LYS
1	D	355	ARG
1	D	375	LEU
1	C	226	ASP
1	D	268	GLN

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	321/432 (74%)	305 (95%)	16 (5%)	22	54
1	B	322/432 (74%)	303 (94%)	19 (6%)	18	48
1	C	321/432 (74%)	304 (95%)	17 (5%)	20	52
1	D	320/432 (74%)	305 (95%)	15 (5%)	23	57
All	All	1284/1728 (74%)	1217 (95%)	67 (5%)	21	53

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	LEU
1	A	77	LYS
1	A	97	ASP
1	A	107	LYS
1	A	137	ASN
1	A	182	VAL
1	A	268	GLN
1	A	276	VAL

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Mol	Chain	Res	Type
1	A	286	GLN
1	A	315	LYS
1	A	321	ILE
1	A	337	SER
1	A	364	SER
1	A	373	ASP
1	A	375	LEU
1	A	377	ASP
1	B	5	TYR
1	B	50	ASP
1	B	54	GLN
1	B	77	LYS
1	B	136	GLU
1	B	181	ASP
1	B	182	VAL
1	B	252	LYS
1	B	268	GLN
1	B	269	ASP
1	B	272	THR
1	B	276	VAL
1	B	279	ASP
1	B	315	LYS
1	B	316	VAL
1	B	334	GLU
1	B	340	VAL
1	B	350	SER
1	B	375	LEU
1	C	54	GLN
1	C	64	SER
1	C	77	LYS
1	C	107	LYS
1	C	114	GLU
1	C	119	GLN
1	C	182	VAL
1	C	241	GLN
1	C	266	SER
1	C	274	GLU
1	C	315	LYS
1	C	321	ILE
1	C	337	SER
1	C	343	LYS
1	C	355	ARG

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Mol	Chain	Res	Type
1	C	373	ASP
1	C	375	LEU
1	D	77	LYS
1	D	114	GLU
1	D	136	GLU
1	D	145	LEU
1	D	182	VAL
1	D	212	THR
1	D	253	VAL
1	D	309	GLN
1	D	315	LYS
1	D	337	SER
1	D	346	ILE
1	D	348	THR
1	D	352	MET
1	D	358	GLU
1	D	375	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	104	HIS
1	A	119	GLN
1	A	125	ASN
1	A	137	ASN
1	A	161	GLN
1	A	188	ASN
1	A	213	GLN
1	A	256	GLN
1	A	275	GLN
1	A	283	GLN
1	A	286	GLN
1	A	309	GLN
1	A	347	HIS
1	B	25	HIS
1	B	35	GLN
1	B	104	HIS
1	B	119	GLN
1	B	125	ASN
1	B	137	ASN
1	B	213	GLN

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Mol	Chain	Res	Type
1	B	256	GLN
1	B	268	GLN
1	B	275	GLN
1	B	283	GLN
1	B	286	GLN
1	B	317	ASN
1	C	26	ASN
1	C	90	ASN
1	C	104	HIS
1	C	119	GLN
1	C	125	ASN
1	C	137	ASN
1	C	213	GLN
1	C	256	GLN
1	C	259	HIS
1	C	275	GLN
1	C	283	GLN
1	C	286	GLN
1	C	309	GLN
1	C	317	ASN
1	D	35	GLN
1	D	90	ASN
1	D	104	HIS
1	D	119	GLN
1	D	125	ASN
1	D	137	ASN
1	D	167	ASN
1	D	188	ASN
1	D	213	GLN
1	D	244	ASN
1	D	256	GLN
1	D	283	GLN
1	D	286	GLN
1	D	309	GLN
1	D	317	ASN

5.3.3 RNA ⓘ

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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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
2	ATP	D	501	3	32,33,33	1.40	3 (9%)	48,52,52	1.83	10 (20%)
2	ATP	A	501	3	32,33,33	1.85	6 (18%)	48,52,52	1.74	7 (14%)
2	ATP	C	501	3	32,33,33	1.72	6 (18%)	48,52,52	1.83	8 (16%)
2	ATP	B	501	3	32,33,33	2.02	6 (18%)	48,52,52	1.79	9 (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
2	ATP	D	501	3	-	0/22/38/38	0/3/3/3
2	ATP	A	501	3	-	6/22/38/38	0/3/3/3
2	ATP	C	501	3	-	6/22/38/38	0/3/3/3
2	ATP	B	501	3	-	3/22/38/38	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	ATP	PA-O3A	5.72	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	ATP	PB-O3B	5.63	1.65	1.59
2	C	501	ATP	PA-O3A	5.49	1.65	1.59
2	A	501	ATP	PA-O3A	5.19	1.65	1.59
2	B	501	ATP	PB-O3A	4.77	1.64	1.59
2	A	501	ATP	PB-O3A	4.41	1.64	1.59
2	A	501	ATP	PB-O3B	4.26	1.64	1.59
2	D	501	ATP	PA-O3A	4.19	1.64	1.59
2	C	501	ATP	PB-O3A	3.94	1.63	1.59
2	C	501	ATP	PB-O3B	3.79	1.63	1.59
2	D	501	ATP	PB-O3B	3.76	1.63	1.59
2	A	501	ATP	PA-O1A	2.92	1.60	1.50
2	C	501	ATP	C5-C4	2.92	1.44	1.39
2	B	501	ATP	PA-O1A	2.54	1.59	1.50
2	C	501	ATP	PB-O1B	2.51	1.59	1.50
2	D	501	ATP	C5-C4	2.50	1.43	1.39
2	B	501	ATP	C5-C4	2.30	1.43	1.39
2	B	501	ATP	PG-O2G	2.26	1.63	1.54
2	A	501	ATP	C5-C4	2.25	1.43	1.39
2	A	501	ATP	PB-O1B	-2.14	1.43	1.50
2	C	501	ATP	PB-O2B	-2.02	1.46	1.55

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	ATP	C5-C4-N3	-6.16	118.24	126.72
2	D	501	ATP	C5-C4-N3	-5.42	119.26	126.72
2	C	501	ATP	N3-C2-N1	-5.31	120.55	128.58
2	B	501	ATP	C5-C4-N3	-5.15	119.62	126.72
2	A	501	ATP	C5-C4-N3	-5.01	119.81	126.72
2	A	501	ATP	N3-C2-N1	-4.95	121.09	128.58
2	B	501	ATP	N3-C2-N1	-4.92	121.14	128.58
2	D	501	ATP	N3-C2-N1	-4.58	121.65	128.58
2	D	501	ATP	N3-C4-N9	4.32	134.52	127.17
2	B	501	ATP	N3-C4-N9	4.28	134.45	127.17
2	A	501	ATP	N3-C4-N9	4.01	133.99	127.17
2	C	501	ATP	C4-C5-N7	-4.00	106.01	110.58
2	D	501	ATP	C5-N7-C8	3.78	109.39	103.45
2	A	501	ATP	C2-N3-C4	3.74	120.96	111.83
2	D	501	ATP	C2-N3-C4	3.72	120.92	111.83
2	A	501	ATP	C5-N7-C8	3.60	109.10	103.45
2	B	501	ATP	C2-N3-C4	3.59	120.59	111.83
2	C	501	ATP	N3-C4-N9	3.47	133.08	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	ATP	C2-N3-C4	3.43	120.21	111.83
2	C	501	ATP	N9-C8-N7	-3.42	109.08	113.94
2	D	501	ATP	C4-C5-N7	-3.38	106.72	110.58
2	A	501	ATP	C4-C5-N7	-3.30	106.81	110.58
2	C	501	ATP	C5-N7-C8	3.11	108.34	103.45
2	B	501	ATP	C5-N7-C8	3.10	108.33	103.45
2	B	501	ATP	N9-C8-N7	-3.10	109.54	113.94
2	A	501	ATP	N9-C8-N7	-2.98	109.70	113.94
2	C	501	ATP	O2G-PG-O3B	2.96	114.55	104.64
2	B	501	ATP	C4-C5-N7	-2.86	107.31	110.58
2	D	501	ATP	PA-O5'-C5'	-2.57	106.64	121.35
2	D	501	ATP	N9-C8-N7	-2.43	110.48	113.94
2	D	501	ATP	O3G-PG-O3B	2.41	112.72	104.64
2	D	501	ATP	O2B-PB-O3B	2.29	113.45	107.27
2	B	501	ATP	PA-O5'-C5'	-2.07	109.49	121.35
2	B	501	ATP	O2A-PA-O3A	2.06	112.83	107.27

There are no chirality outliers.

All (15) torsion outliers are listed below:

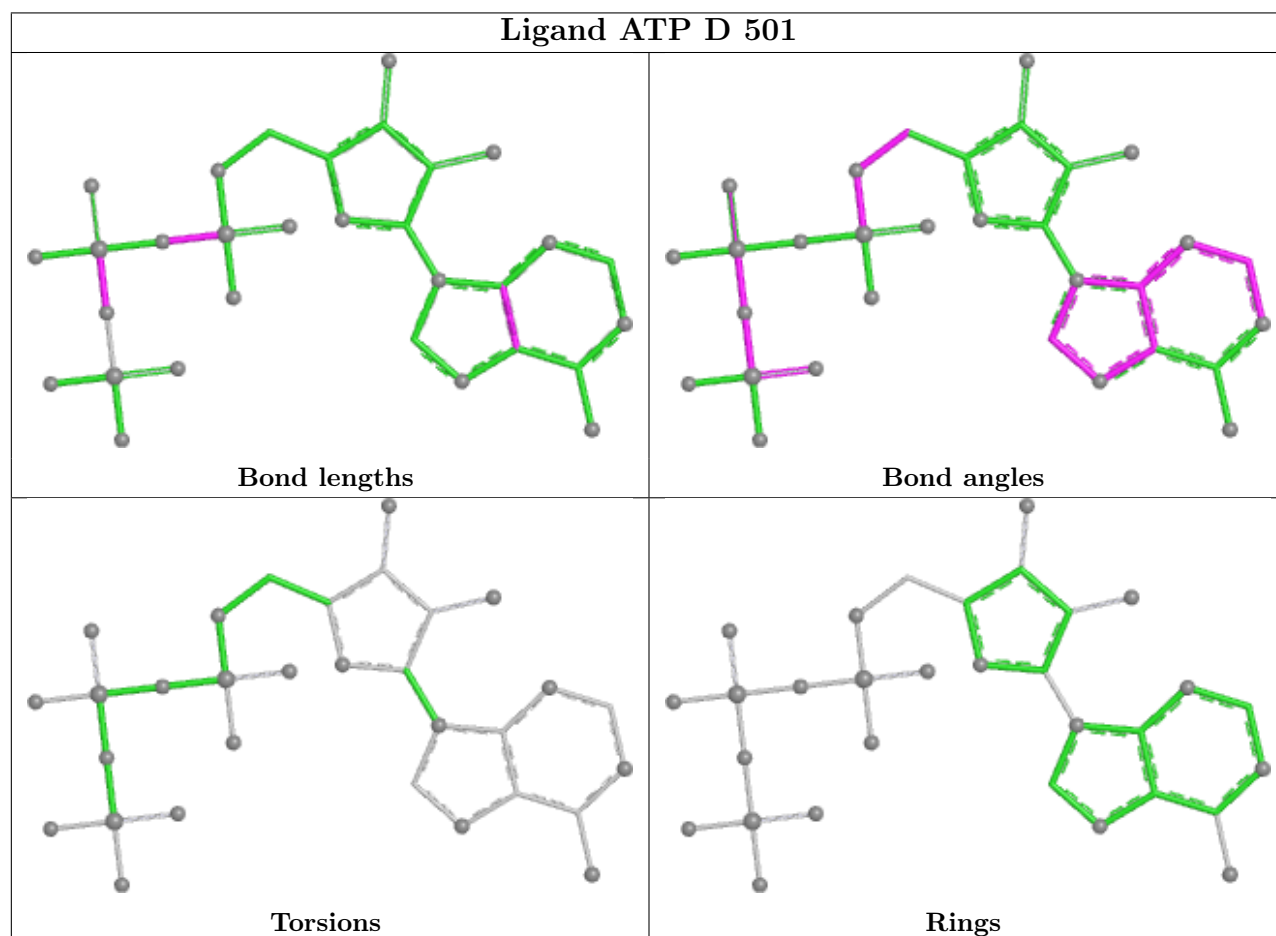
Mol	Chain	Res	Type	Atoms
2	A	501	ATP	PB-O3B-PG-O2G
2	A	501	ATP	C5'-O5'-PA-O2A
2	C	501	ATP	PB-O3B-PG-O2G
2	C	501	ATP	PB-O3B-PG-O3G
2	C	501	ATP	C5'-O5'-PA-O1A
2	C	501	ATP	C5'-O5'-PA-O3A
2	B	501	ATP	PB-O3B-PG-O1G
2	A	501	ATP	C5'-O5'-PA-O1A
2	A	501	ATP	C5'-O5'-PA-O3A
2	A	501	ATP	C3'-C4'-C5'-O5'
2	A	501	ATP	O4'-C4'-C5'-O5'
2	B	501	ATP	PB-O3B-PG-O2G
2	B	501	ATP	PB-O3B-PG-O3G
2	C	501	ATP	C3'-C4'-C5'-O5'
2	C	501	ATP	O4'-C4'-C5'-O5'

There are no ring outliers.

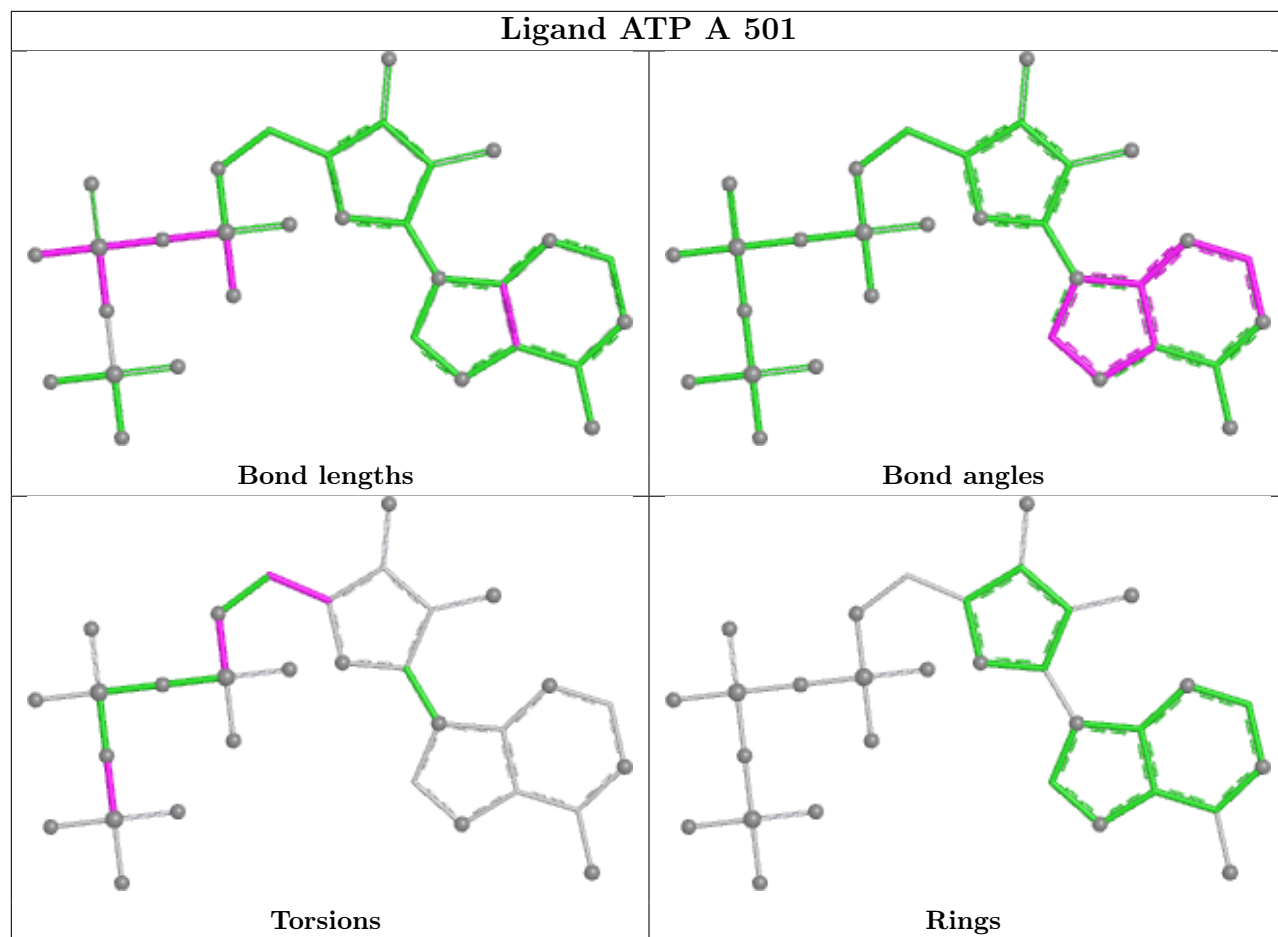
4 monomers are involved in 14 short contacts:

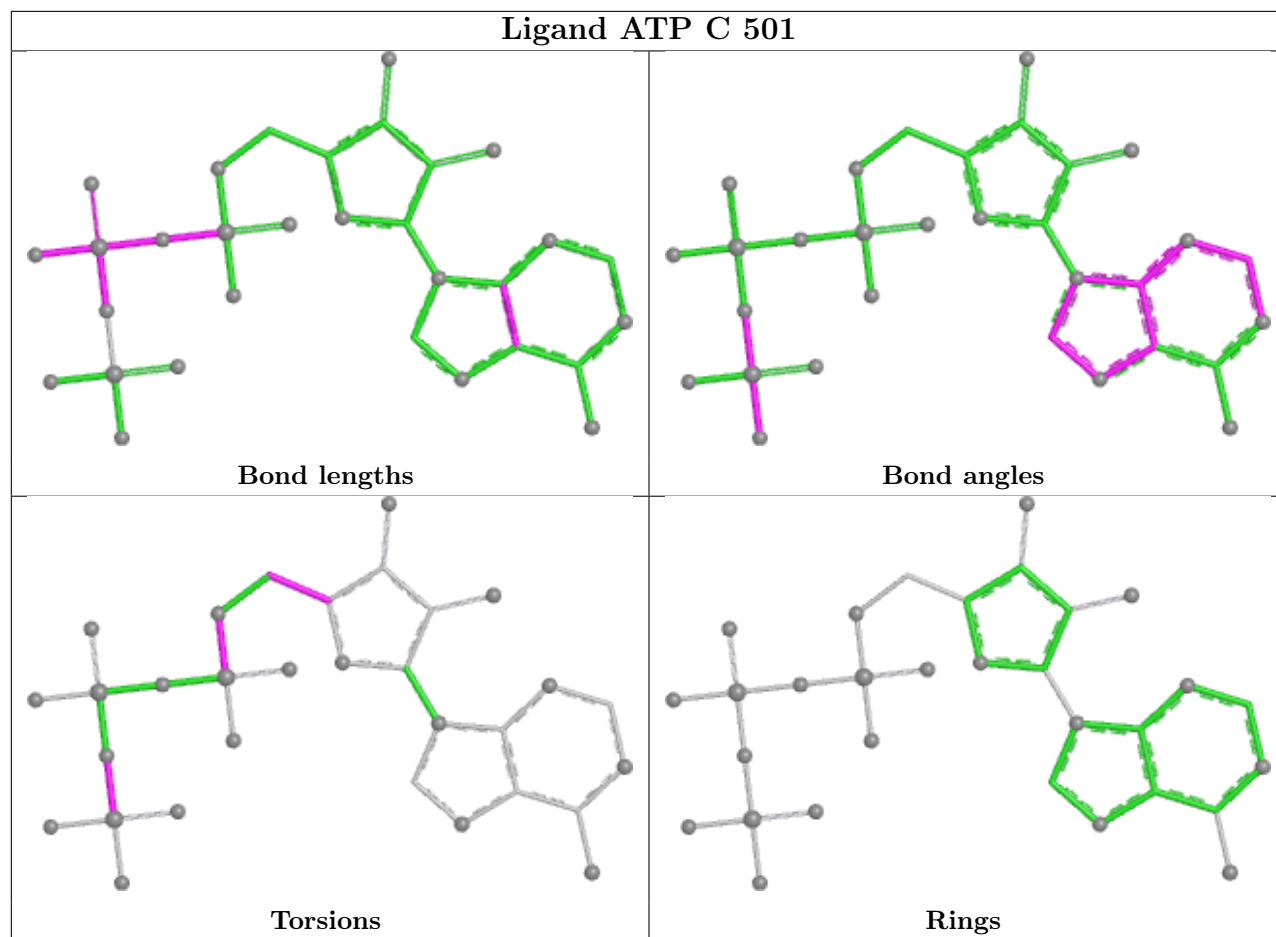
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	ATP	5	0
2	A	501	ATP	2	0
2	C	501	ATP	5	0
2	B	501	ATP	2	0

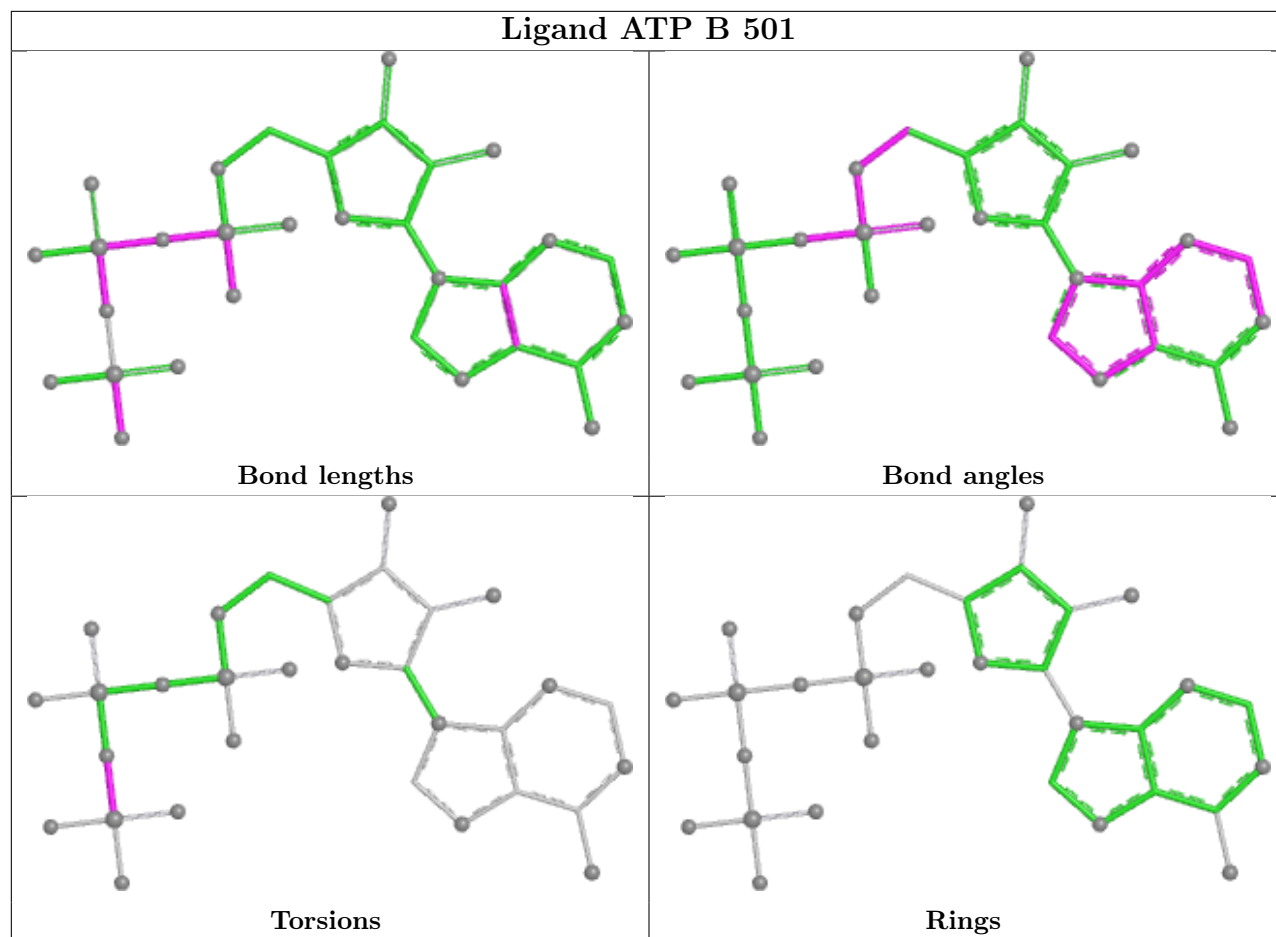
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



Ligand ATP A 501







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	370/484 (76%)	0.10	5 (1%) 73 64	35, 62, 81, 93	0
1	B	371/484 (76%)	-0.15	4 (1%) 78 70	25, 53, 75, 94	0
1	C	370/484 (76%)	-0.27	3 (0%) 82 75	30, 46, 70, 85	0
1	D	369/484 (76%)	0.73	19 (5%) 33 25	55, 82, 112, 123	0
All	All	1480/1936 (76%)	0.10	31 (2%) 63 54	25, 60, 100, 123	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	352	MET	4.5
1	D	25	HIS	3.5
1	D	48	ASP	3.2
1	A	4	HIS	3.0
1	D	280	GLU	2.9
1	D	176	GLY	2.8
1	D	273	VAL	2.7
1	D	349	PRO	2.6
1	D	38	THR	2.6
1	B	377	ASP	2.6
1	D	353	GLY	2.6
1	B	4	HIS	2.5
1	A	352	MET	2.5
1	D	270	ILE	2.5
1	D	114	GLU	2.4
1	B	268	GLN	2.4
1	C	114	GLU	2.4
1	C	337	SER	2.4
1	A	72	LYS	2.3
1	D	171	CYS	2.3
1	A	278	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	314	THR	2.2
1	D	5	TYR	2.2
1	D	330	LEU	2.2
1	D	72	LYS	2.1
1	D	15	SER	2.1
1	D	174	ALA	2.1
1	C	269	ASP	2.1
1	B	276	VAL	2.0
1	D	49	PHE	2.0
1	D	354	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

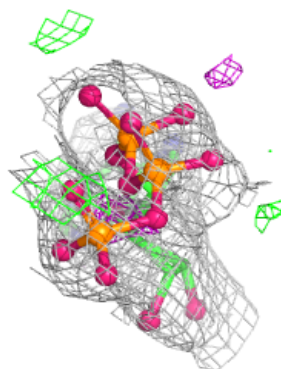
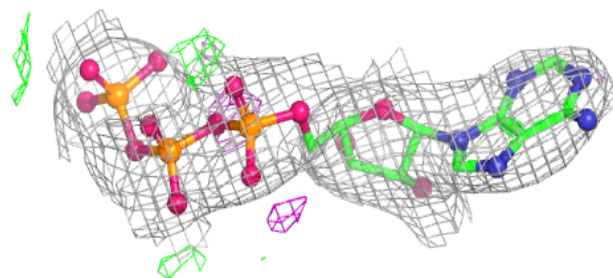
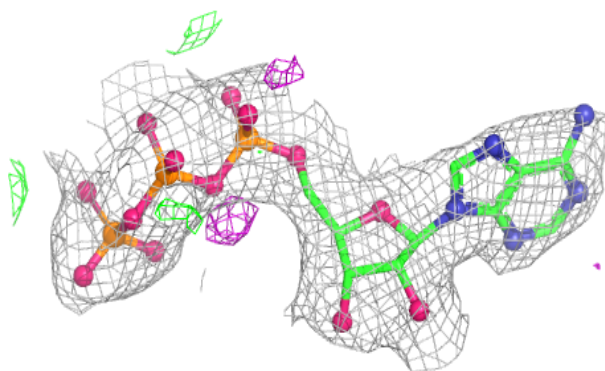
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ATP	D	501	31/31	0.95	0.10	61,69,78,79	0
3	MG	A	502	1/1	0.95	0.06	42,42,42,42	0
3	MG	D	502	1/1	0.97	0.04	61,61,61,61	0
2	ATP	B	501	31/31	0.98	0.06	30,38,40,41	0
2	ATP	A	501	31/31	0.98	0.06	32,48,55,57	0
3	MG	B	502	1/1	0.99	0.05	53,53,53,53	0
3	MG	C	502	1/1	0.99	0.04	39,39,39,39	0
2	ATP	C	501	31/31	0.99	0.04	23,31,37,39	0

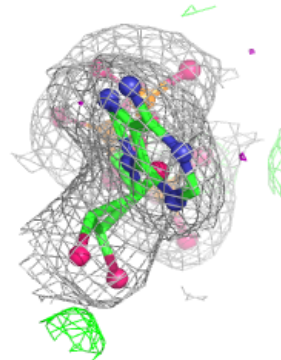
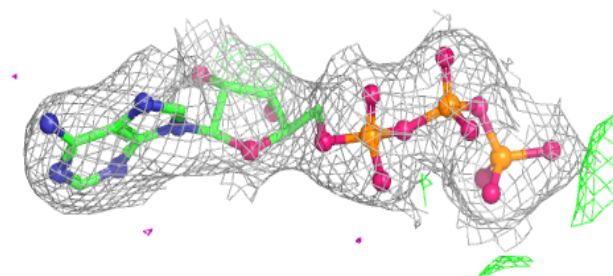
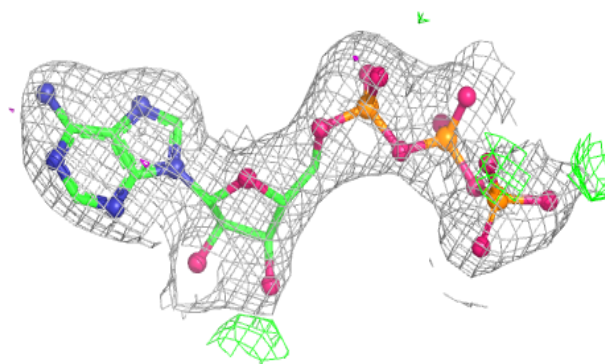
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP D 501:

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

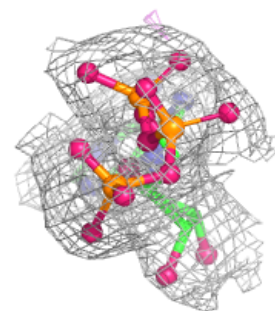
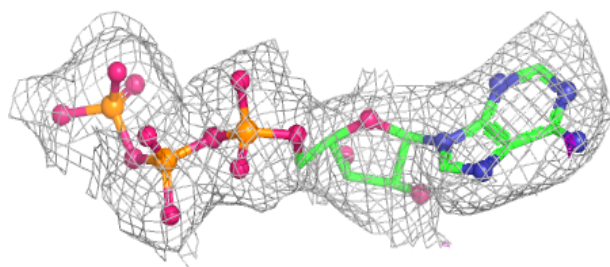
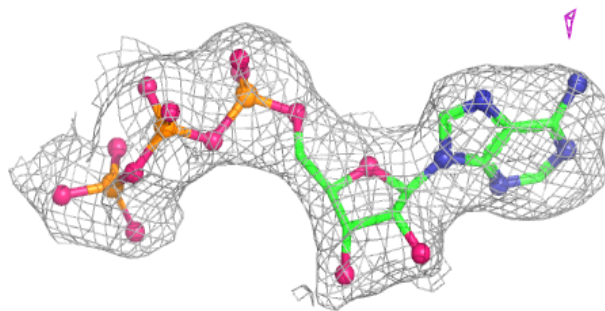
**Electron density around ATP B 501:**

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

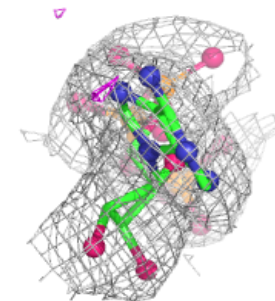
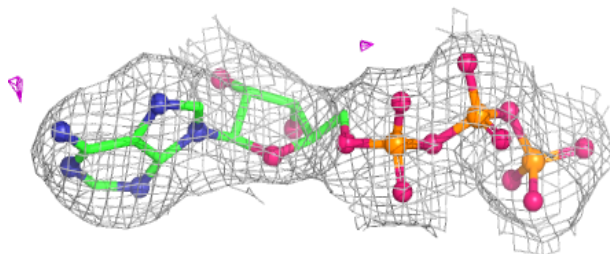
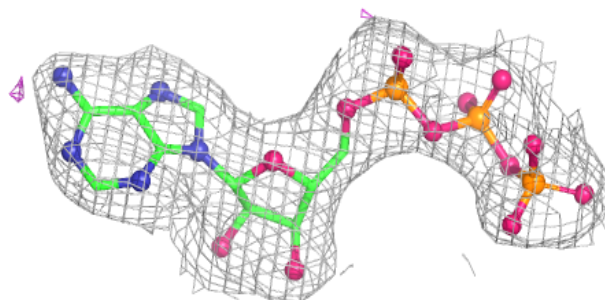


Electron density around ATP A 501:

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

**Electron density around ATP C 501:**

$2mF_o-DF_c$ (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.