



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:38 PM UTC

PDB ID : 4QQX / pdb_00004qqx
Title : Crystal structure of T. fusca Cas3-ATP
Authors : Ke, A.; Huo, Y.; Nam, K.H.
Deposited on : 2014-06-30
Resolution : 3.34 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

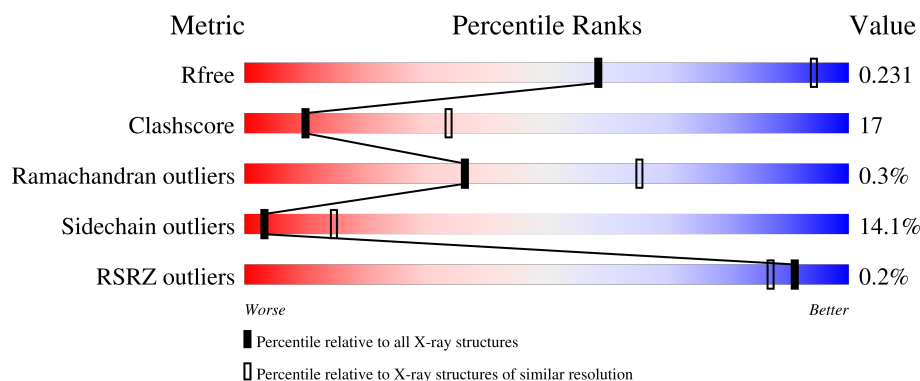
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.34 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.



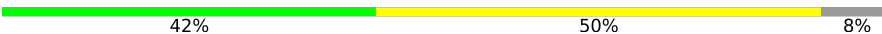
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1434 (3.38-3.30)
Clashscore	190562	1479 (3.38-3.30)
Ramachandran outliers	187476	1456 (3.38-3.30)
Sidechain outliers	187428	1455 (3.38-3.30)
RSRZ outliers	180081	1434 (3.38-3.30)

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	964	
1	C	964	
1	E	964	
1	G	964	
2	B	12	

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Mol	Chain	Length	Quality of chain
2	D	12	 50% 33% 8% 8%
2	F	12	 42% 50% 8%
2	H	12	 33% 58% 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28826 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 CRISPR-associated helicase, Cas3 family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	903	Total	C	N	O	S	0	0	0
			7028	4463	1251	1287	27			
1	C	899	Total	C	N	O	S	0	0	0
			6977	4428	1237	1285	27			
1	E	901	Total	C	N	O	S	0	0	0
			6995	4438	1242	1288	27			
1	G	887	Total	C	N	O	S	0	0	0
			6906	4390	1224	1266	26			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q47PJ0
A	-18	GLY	-	expression tag	UNP Q47PJ0
A	-17	SER	-	expression tag	UNP Q47PJ0
A	-16	SER	-	expression tag	UNP Q47PJ0
A	-15	HIS	-	expression tag	UNP Q47PJ0
A	-14	HIS	-	expression tag	UNP Q47PJ0
A	-13	HIS	-	expression tag	UNP Q47PJ0
A	-12	HIS	-	expression tag	UNP Q47PJ0
A	-11	HIS	-	expression tag	UNP Q47PJ0
A	-10	HIS	-	expression tag	UNP Q47PJ0
A	-9	SER	-	expression tag	UNP Q47PJ0
A	-8	SER	-	expression tag	UNP Q47PJ0
A	-7	GLY	-	expression tag	UNP Q47PJ0
A	-6	LEU	-	expression tag	UNP Q47PJ0
A	-5	VAL	-	expression tag	UNP Q47PJ0
A	-4	PRO	-	expression tag	UNP Q47PJ0
A	-3	ARG	-	expression tag	UNP Q47PJ0
A	-2	GLY	-	expression tag	UNP Q47PJ0
A	-1	SER	-	expression tag	UNP Q47PJ0
A	0	HIS	-	expression tag	UNP Q47PJ0
C	-19	MET	-	initiating methionine	UNP Q47PJ0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-18	GLY	-	expression tag	UNP Q47PJ0
C	-17	SER	-	expression tag	UNP Q47PJ0
C	-16	SER	-	expression tag	UNP Q47PJ0
C	-15	HIS	-	expression tag	UNP Q47PJ0
C	-14	HIS	-	expression tag	UNP Q47PJ0
C	-13	HIS	-	expression tag	UNP Q47PJ0
C	-12	HIS	-	expression tag	UNP Q47PJ0
C	-11	HIS	-	expression tag	UNP Q47PJ0
C	-10	HIS	-	expression tag	UNP Q47PJ0
C	-9	SER	-	expression tag	UNP Q47PJ0
C	-8	SER	-	expression tag	UNP Q47PJ0
C	-7	GLY	-	expression tag	UNP Q47PJ0
C	-6	LEU	-	expression tag	UNP Q47PJ0
C	-5	VAL	-	expression tag	UNP Q47PJ0
C	-4	PRO	-	expression tag	UNP Q47PJ0
C	-3	ARG	-	expression tag	UNP Q47PJ0
C	-2	GLY	-	expression tag	UNP Q47PJ0
C	-1	SER	-	expression tag	UNP Q47PJ0
C	0	HIS	-	expression tag	UNP Q47PJ0
E	-19	MET	-	initiating methionine	UNP Q47PJ0
E	-18	GLY	-	expression tag	UNP Q47PJ0
E	-17	SER	-	expression tag	UNP Q47PJ0
E	-16	SER	-	expression tag	UNP Q47PJ0
E	-15	HIS	-	expression tag	UNP Q47PJ0
E	-14	HIS	-	expression tag	UNP Q47PJ0
E	-13	HIS	-	expression tag	UNP Q47PJ0
E	-12	HIS	-	expression tag	UNP Q47PJ0
E	-11	HIS	-	expression tag	UNP Q47PJ0
E	-10	HIS	-	expression tag	UNP Q47PJ0
E	-9	SER	-	expression tag	UNP Q47PJ0
E	-8	SER	-	expression tag	UNP Q47PJ0
E	-7	GLY	-	expression tag	UNP Q47PJ0
E	-6	LEU	-	expression tag	UNP Q47PJ0
E	-5	VAL	-	expression tag	UNP Q47PJ0
E	-4	PRO	-	expression tag	UNP Q47PJ0
E	-3	ARG	-	expression tag	UNP Q47PJ0
E	-2	GLY	-	expression tag	UNP Q47PJ0
E	-1	SER	-	expression tag	UNP Q47PJ0
E	0	HIS	-	expression tag	UNP Q47PJ0
G	-19	MET	-	initiating methionine	UNP Q47PJ0
G	-18	GLY	-	expression tag	UNP Q47PJ0
G	-17	SER	-	expression tag	UNP Q47PJ0

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-16	SER	-	expression tag	UNP Q47PJ0
G	-15	HIS	-	expression tag	UNP Q47PJ0
G	-14	HIS	-	expression tag	UNP Q47PJ0
G	-13	HIS	-	expression tag	UNP Q47PJ0
G	-12	HIS	-	expression tag	UNP Q47PJ0
G	-11	HIS	-	expression tag	UNP Q47PJ0
G	-10	HIS	-	expression tag	UNP Q47PJ0
G	-9	SER	-	expression tag	UNP Q47PJ0
G	-8	SER	-	expression tag	UNP Q47PJ0
G	-7	GLY	-	expression tag	UNP Q47PJ0
G	-6	LEU	-	expression tag	UNP Q47PJ0
G	-5	VAL	-	expression tag	UNP Q47PJ0
G	-4	PRO	-	expression tag	UNP Q47PJ0
G	-3	ARG	-	expression tag	UNP Q47PJ0
G	-2	GLY	-	expression tag	UNP Q47PJ0
G	-1	SER	-	expression tag	UNP Q47PJ0
G	0	HIS	-	expression tag	UNP Q47PJ0

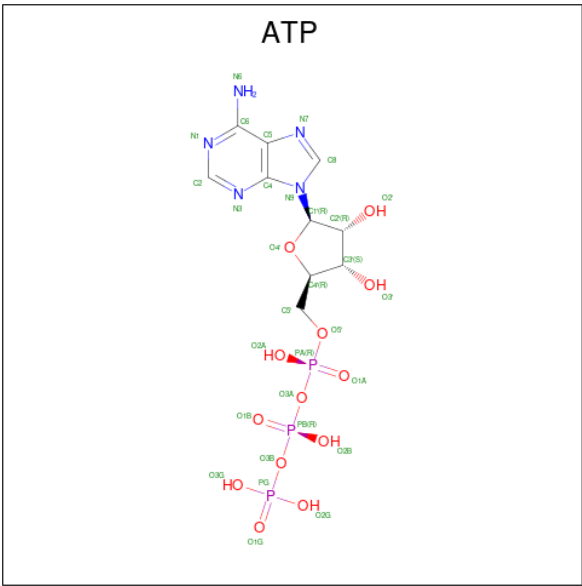
- Molecule 2 is a DNA chain called DNA (5'-D(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	11	Total	C	N	O	P	0	0	0
			197	90	45	51	11			
2	D	11	Total	C	N	O	P	0	0	0
			197	90	45	51	11			
2	F	11	Total	C	N	O	P	0	0	0
			197	90	45	51	11			
2	H	11	Total	C	N	O	P	0	0	0
			197	90	45	51	11			

- Molecule 3 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Fe	0	0
			2	2		
3	C	2	Total	Fe	0	0
			2	2		
3	E	2	Total	Fe	0	0
			2	2		
3	G	2	Total	Fe	0	0
			2	2		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

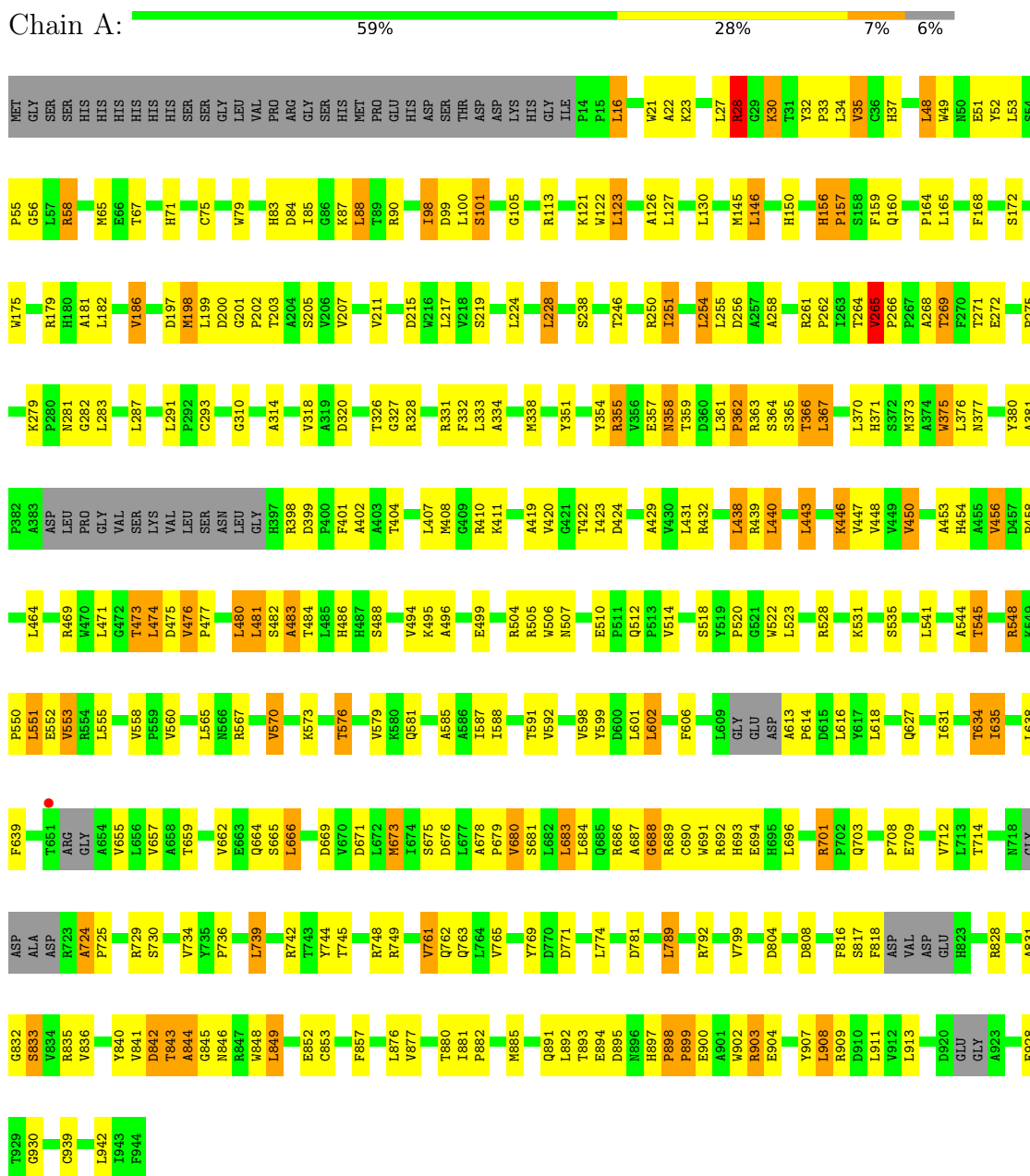


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

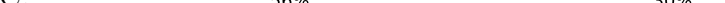
3 Residue-property plots

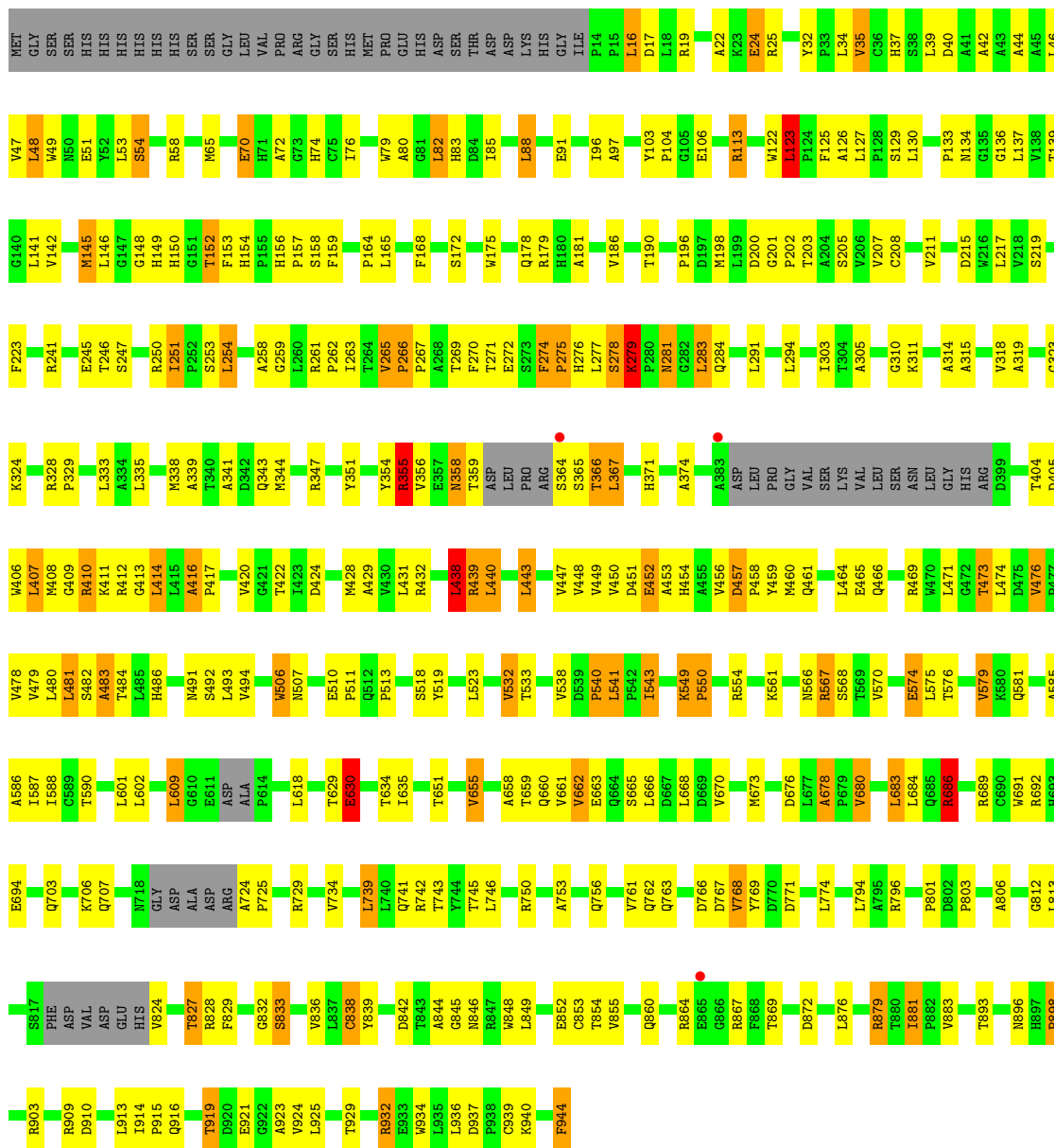
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: CRISPR-associated helicase, Cas3 family

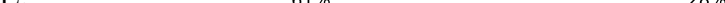


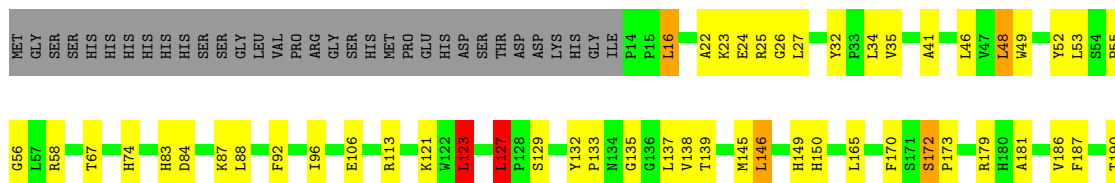
- Molecule 1: CRISPR-associated helicase, Cas3 family

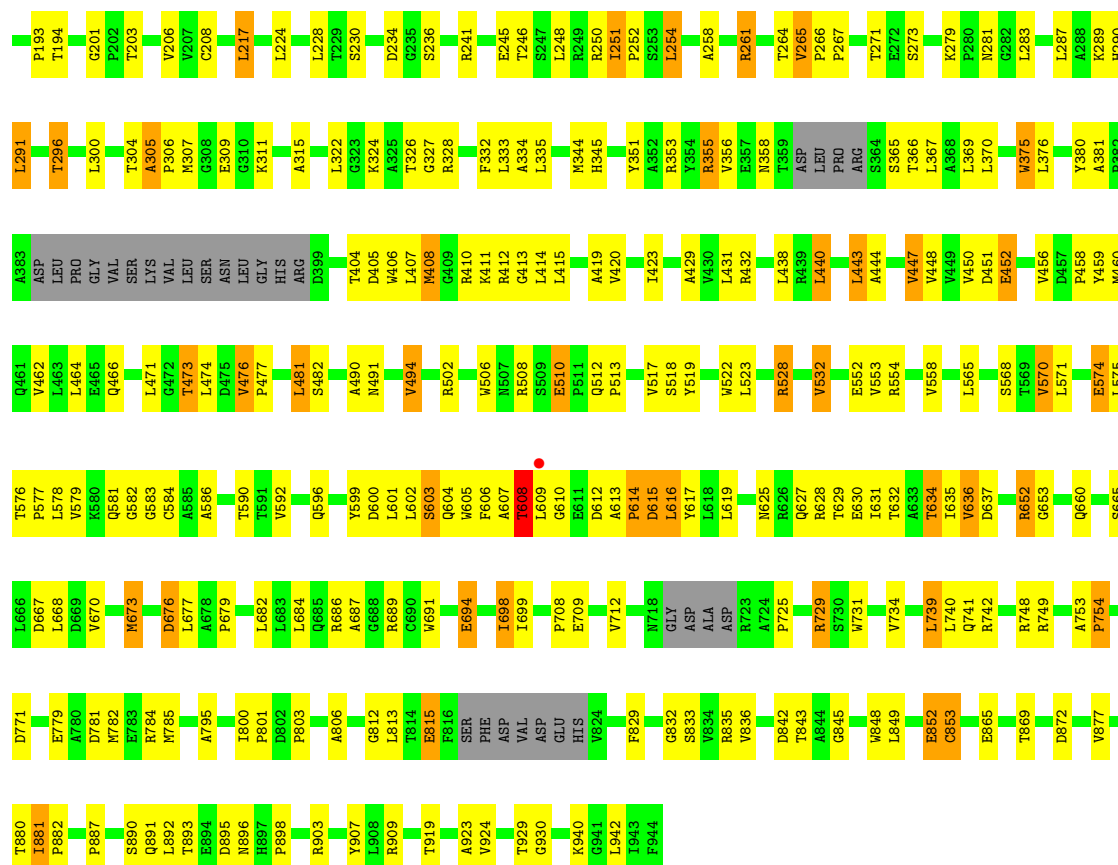
Chain C:  56% 30% 7% • 7%



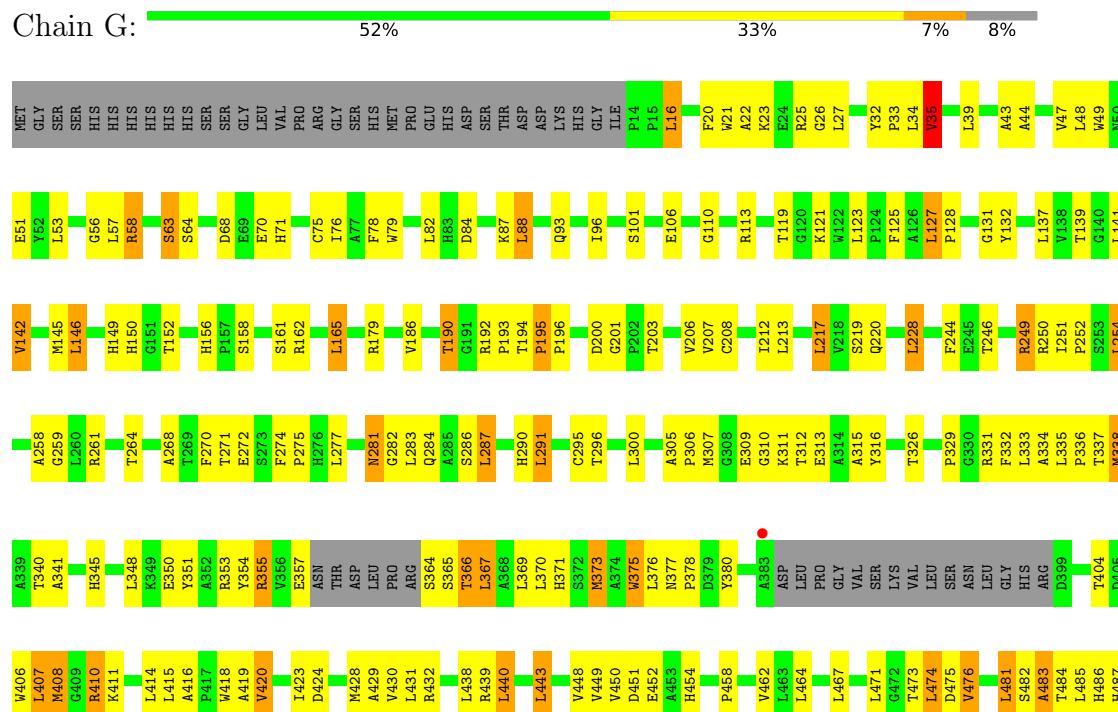
- Molecule 1: CRISPR-associated helicase, Cas3 family

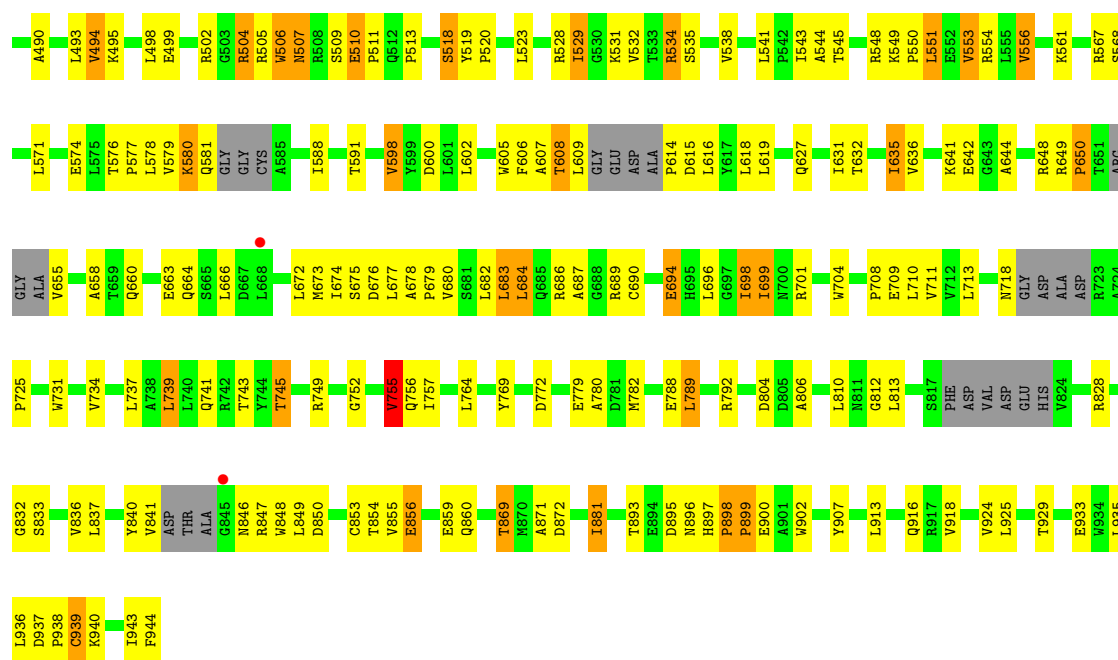
Chain E:  61% 28% 5% 7%





- Molecule 1: CRISPR-associated helicase, Cas3 family





- Molecule 2: DNA (5'-D(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain B: 42% 33% 17% 8%



- Molecule 2: DNA (5'-D(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain D: 50% 33% 8% 8%



- Molecule 2: DNA (5'-D(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain F: 42% 50% 8% 8%



- Molecule 2: DNA (5'-D(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain H: 33% 58% 8% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.25Å 222.81Å 125.09Å 90.00° 104.10° 90.00°	Depositor
Resolution (Å)	46.98 – 3.34 46.98 – 3.34	Depositor EDS
% Data completeness (in resolution range)	99.2 (46.98-3.34) 94.6 (46.98-3.34)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.172 , 0.227 0.177 , 0.231	Depositor DCC
R_{free} test set	2000 reflections (1.67%)	wwPDB-VP
Wilson B-factor (Å ²)	79.4	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 78.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	28826	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, FE

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	0.65	4/7205 (0.1%)	1.06	36/9828 (0.4%)
1	C	0.64	2/7151 (0.0%)	1.08	42/9754 (0.4%)
1	E	0.67	3/7170 (0.0%)	1.11	39/9782 (0.4%)
1	G	0.64	8/7077 (0.1%)	1.03	23/9649 (0.2%)
2	B	0.48	0/222	1.28	5/339 (1.5%)
2	D	0.46	0/222	1.24	2/339 (0.6%)
2	F	0.46	0/222	1.23	1/339 (0.3%)
2	H	0.42	0/222	1.04	1/339 (0.3%)
All	All	0.65	17/29491 (0.1%)	1.07	149/40369 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	E	0	1
1	G	0	1
All	All	0	4

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	194	THR	C-N	7.92	1.40	1.33
1	A	897	HIS	C-N	6.25	1.40	1.33
1	G	897	HIS	C-N	6.16	1.40	1.33
1	E	753	ALA	C-N	5.96	1.40	1.33
1	G	195	PRO	C-N	5.78	1.40	1.33
1	A	898	PRO	C-N	5.75	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	898	PRO	C-N	5.67	1.40	1.33
1	C	279	LYS	C-N	5.54	1.40	1.33
1	G	899	PRO	N-CD	5.53	1.55	1.47
1	G	898	PRO	N-CD	5.41	1.55	1.47
1	A	898	PRO	N-CD	5.32	1.55	1.47
1	C	275	PRO	N-CD	5.24	1.55	1.47
1	G	195	PRO	N-CD	5.23	1.55	1.47
1	G	196	PRO	N-CD	5.23	1.55	1.47
1	A	899	PRO	N-CD	5.12	1.54	1.47
1	E	614	PRO	N-CD	5.10	1.54	1.47
1	E	754	PRO	N-CD	5.03	1.54	1.47

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	852	GLU	CA-C-N	12.09	139.51	122.46
1	E	852	GLU	C-N-CA	12.09	139.51	122.46
1	E	609	LEU	N-CA-C	-11.33	86.67	110.80
1	G	608	THR	N-CA-C	10.43	133.03	110.80
1	A	483	ALA	N-CA-C	-9.82	93.10	109.80
1	E	123	LEU	CA-C-N	-9.28	110.15	120.45
1	E	123	LEU	C-N-CA	-9.28	110.15	120.45
1	E	852	GLU	CB-CA-C	8.99	127.27	110.63
1	G	194	THR	CA-C-N	-8.41	113.52	119.66
1	G	194	THR	C-N-CA	-8.41	113.52	119.66
1	A	28	ARG	N-CA-C	8.30	125.60	113.40
1	G	35	VAL	CB-CA-C	-7.85	101.92	111.97
1	C	540	PRO	N-CA-C	7.61	128.14	112.47
1	C	410	ARG	N-CA-C	7.57	119.17	111.07
1	E	853	CYS	N-CA-C	7.35	121.29	111.30
1	C	898	PRO	CA-C-N	7.26	127.29	119.89
1	C	898	PRO	C-N-CA	7.26	127.29	119.89
1	A	701	ARG	CA-C-N	7.23	127.67	119.93
1	A	701	ARG	C-N-CA	7.23	127.67	119.93
1	A	761	VAL	N-CA-C	7.14	117.24	110.53
1	G	195	PRO	CA-C-N	-7.12	113.34	120.31
1	G	195	PRO	C-N-CA	-7.12	113.34	120.31
1	C	549	LYS	CA-C-N	7.07	128.67	119.84
1	C	549	LYS	C-N-CA	7.07	128.67	119.84
1	E	753	ALA	CA-C-N	-6.91	113.54	120.31
1	E	753	ALA	C-N-CA	-6.91	113.54	120.31
1	G	195	PRO	O-C-N	6.90	124.48	121.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	650	PRO	CB-CA-C	-6.90	100.17	111.56
1	A	362	PRO	N-CA-C	-6.82	98.43	112.47
1	C	35	VAL	CB-CA-C	-6.80	102.96	112.14
1	E	335	LEU	CA-C-N	-6.78	113.22	120.47
1	E	335	LEU	C-N-CA	-6.78	113.22	120.47
1	C	438	LEU	N-CA-C	-6.76	102.30	112.04
1	G	110	GLY	N-CA-C	-6.74	105.88	114.37
1	A	897	HIS	CA-C-N	-6.72	113.45	120.38
1	A	897	HIS	C-N-CA	-6.72	113.45	120.38
1	A	799	VAL	N-CA-C	6.70	119.05	108.87
1	A	126	ALA	N-CA-C	-6.66	106.10	114.56
1	A	172	SER	CA-C-N	6.61	128.11	119.84
1	A	172	SER	C-N-CA	6.61	128.11	119.84
1	A	377	ASN	CA-C-N	6.61	126.19	119.19
1	A	377	ASN	C-N-CA	6.61	126.19	119.19
1	A	898	PRO	CA-C-N	-6.59	113.51	120.03
1	A	898	PRO	C-N-CA	-6.59	113.51	120.03
1	A	844	ALA	N-CA-C	6.58	119.05	111.02
1	E	898	PRO	CA-C-N	6.47	126.49	119.89
1	E	898	PRO	C-N-CA	6.47	126.49	119.89
1	E	322	LEU	N-CA-C	-6.45	104.25	111.28
1	G	898	PRO	CA-C-N	-6.43	114.04	120.21
1	G	898	PRO	C-N-CA	-6.43	114.04	120.21
1	C	279	LYS	CA-C-N	-6.43	113.36	119.85
1	C	279	LYS	C-N-CA	-6.43	113.36	119.85
2	H	10	DA	C1'-O4'-C4'	-6.36	100.16	109.70
1	G	483	ALA	N-CA-C	-6.32	100.33	109.31
2	D	10	DA	C1'-O4'-C4'	-6.30	100.25	109.70
1	G	897	HIS	CA-C-N	-6.30	113.89	120.38
1	G	897	HIS	C-N-CA	-6.30	113.89	120.38
1	C	328	ARG	CA-C-N	6.29	126.00	119.64
1	C	328	ARG	C-N-CA	6.29	126.00	119.64
1	E	127	LEU	CA-C-N	-6.27	113.23	119.56
1	E	127	LEU	C-N-CA	-6.27	113.23	119.56
1	C	540	PRO	CB-CA-C	-6.20	101.33	111.56
1	E	665	SER	N-CA-C	6.13	119.64	111.30
2	B	11	DA	N9-C1'-C2'	6.01	122.52	113.50
1	A	724	ALA	CA-C-N	5.99	127.33	119.84
1	A	724	ALA	C-N-CA	5.99	127.33	119.84
1	C	883	VAL	N-CA-C	5.97	116.47	107.75
1	C	767	ASP	N-CA-C	5.93	118.70	111.82
1	C	541	LEU	N-CA-C	5.92	122.89	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	608	THR	N-CA-C	5.88	121.07	111.37
1	E	447	VAL	CA-C-N	-5.81	115.61	122.93
1	E	447	VAL	C-N-CA	-5.81	115.61	122.93
1	E	699	ILE	N-CA-C	5.80	116.78	107.73
1	E	328	ARG	CA-C-N	5.80	125.48	119.56
1	E	328	ARG	C-N-CA	5.80	125.48	119.56
1	A	157	PRO	N-CA-C	-5.79	100.54	112.47
1	C	678	ALA	CA-C-N	-5.76	113.84	119.78
1	C	678	ALA	C-N-CA	-5.76	113.84	119.78
1	E	512	GLN	N-CA-C	5.76	116.23	109.60
2	B	11	DA	O5'-C5'-C4'	-5.71	102.24	110.80
1	C	154	HIS	CA-C-N	-5.70	114.10	119.85
1	C	154	HIS	C-N-CA	-5.70	114.10	119.85
1	C	686	ARG	N-CA-C	-5.66	105.11	111.28
1	G	556	VAL	N-CA-C	5.65	114.96	106.42
1	A	328	ARG	CA-C-N	5.57	125.27	119.64
1	A	328	ARG	C-N-CA	5.57	125.27	119.64
1	C	457	ASP	CA-C-N	-5.57	113.17	118.97
1	C	457	ASP	C-N-CA	-5.57	113.17	118.97
1	A	680	VAL	CB-CA-C	-5.57	104.75	112.04
1	E	852	GLU	N-CA-C	5.57	118.11	111.71
1	C	416	ALA	CA-C-N	5.55	125.02	119.24
1	C	416	ALA	C-N-CA	5.55	125.02	119.24
1	G	755	VAL	CB-CA-C	-5.53	103.33	110.84
1	E	712	VAL	N-CA-C	5.51	115.20	106.32
1	G	664	GLN	N-CA-C	5.51	119.18	107.67
1	C	274	PHE	CA-C-N	-5.50	112.95	119.05
1	C	274	PHE	C-N-CA	-5.50	112.95	119.05
1	C	278	SER	N-CA-C	5.48	117.06	111.14
1	C	630	GLU	N-CA-C	5.47	117.24	111.28
1	E	261	ARG	CA-C-N	5.46	126.67	119.84
1	E	261	ARG	C-N-CA	5.46	126.67	119.84
1	E	444	ALA	N-CA-C	5.45	117.92	111.33
1	C	82	LEU	CB-CA-C	-5.45	99.26	109.72
1	A	201	GLY	CA-C-N	-5.44	113.01	119.05
1	A	201	GLY	C-N-CA	-5.44	113.01	119.05
2	B	11	DA	C5'-C4'-O4'	-5.43	101.26	109.40
1	G	788	GLU	N-CA-C	-5.42	105.46	111.36
1	C	532	VAL	N-CA-C	5.42	112.00	106.21
1	E	41	ALA	N-CA-C	-5.41	105.28	111.07
1	C	483	ALA	N-CA-C	-5.41	101.63	109.31
1	C	896	ASN	N-CA-C	-5.38	106.64	114.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	659	THR	CB-CA-C	-5.38	102.80	113.45
1	C	367	LEU	N-CA-C	-5.36	99.37	108.26
1	C	447	VAL	N-CA-C	-5.32	100.78	108.87
1	C	123	LEU	CA-C-N	-5.31	115.42	120.83
1	C	123	LEU	C-N-CA	-5.31	115.42	120.83
1	A	269	THR	N-CA-C	-5.31	102.14	110.36
2	D	11	DA	O5'-C5'-C4'	-5.30	102.85	110.80
1	G	156	HIS	CA-C-N	5.29	126.12	119.98
1	G	156	HIS	C-N-CA	5.29	126.12	119.98
1	C	51	GLU	N-CA-C	5.29	118.89	112.23
1	E	532	VAL	CB-CA-C	-5.24	105.57	111.23
1	C	266	PRO	O-C-N	5.23	123.61	121.15
1	A	666	LEU	N-CA-C	-5.23	100.51	109.24
1	G	847	ARG	N-CA-C	5.21	117.22	109.25
1	C	658	ALA	N-CA-C	5.20	117.58	109.52
1	C	724	ALA	CA-C-N	5.20	125.20	119.90
1	C	724	ALA	C-N-CA	5.20	125.20	119.90
1	E	698	ILE	N-CA-C	5.19	119.74	113.00
2	F	2	DA	O5'-C5'-C4'	-5.17	103.05	110.80
2	B	10	DA	C1'-O4'-C4'	-5.14	101.98	109.70
1	E	365	SER	CB-CA-C	-5.14	103.93	111.23
1	A	35	VAL	CB-CA-C	-5.13	104.21	112.16
1	A	688	GLY	N-CA-C	-5.13	108.30	114.66
1	A	156	HIS	CA-C-N	5.11	126.23	119.84
1	A	156	HIS	C-N-CA	5.11	126.23	119.84
1	G	212	ILE	N-CA-C	-5.10	105.53	110.42
1	E	32	TYR	CA-C-N	5.09	125.01	119.76
1	E	32	TYR	C-N-CA	5.09	125.01	119.76
1	G	162	ARG	N-CA-C	-5.09	107.12	113.38
1	A	265	VAL	CA-C-N	5.06	125.59	120.38
1	A	265	VAL	C-N-CA	5.06	125.59	120.38
1	E	305	ALA	CA-C-N	5.06	125.53	120.52
1	E	305	ALA	C-N-CA	5.06	125.53	120.52
1	E	135	GLY	N-CA-C	-5.05	108.14	115.27
1	E	358	ASN	N-CA-C	5.03	117.33	110.24
1	A	483	ALA	CB-CA-C	-5.03	105.28	113.37
2	B	5	DA	O4'-C1'-N9	-5.02	100.87	108.40
1	A	281	ASN	N-CA-C	5.01	118.13	110.36

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	355	ARG	Sidechain
1	C	355	ARG	Sidechain
1	E	852	GLU	Peptide
1	G	355	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7028	0	6975	239	0
1	C	6977	0	6922	243	0
1	E	6995	0	6939	196	0
1	G	6906	0	6862	310	0
2	B	197	0	99	12	0
2	D	197	0	99	8	0
2	F	197	0	99	7	0
2	H	197	0	99	15	0
3	A	2	0	0	0	0
3	C	2	0	0	0	0
3	E	2	0	0	0	0
3	G	2	0	0	0	0
4	A	31	0	12	1	0
4	C	31	0	12	6	0
4	E	31	0	12	2	0
4	G	31	0	12	7	0
All	All	28826	0	28142	987	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 17.

All (987) 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:28:ARG:O	1:A:28:ARG:CD	1.95	1.14
1:A:28:ARG:HD2	1:A:30:LYS:HZ1	1.08	1.14
1:C:452:GLU:HG3	1:C:454:HIS:NE2	1.66	1.10
1:G:268:ALA:HB2	1:G:355:ARG:HH12	1.10	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:ARG:O	1:A:28:ARG:HD3	1.50	1.07
1:A:900:GLU:HG2	1:A:903:ARG:NH1	1.74	1.02
1:A:900:GLU:HG2	1:A:903:ARG:HH12	1.20	1.02
1:G:78:PHE:HB2	1:G:190:THR:HG21	1.01	1.01
1:A:265:VAL:CG1	1:A:355:ARG:NH2	2.25	0.99
1:G:268:ALA:CB	1:G:355:ARG:HH12	1.77	0.98
1:G:78:PHE:CB	1:G:190:THR:HG21	1.94	0.98
1:G:380:TYR:CE1	1:G:408:MET:HE1	1.98	0.97
1:G:78:PHE:HB2	1:G:190:THR:CG2	1.95	0.97
1:G:268:ALA:CB	1:G:355:ARG:NH1	2.30	0.95
1:A:265:VAL:CG1	1:A:355:ARG:HH21	1.78	0.95
1:A:28:ARG:CD	1:A:30:LYS:HZ1	1.79	0.94
1:C:452:GLU:HG3	1:C:454:HIS:CD2	2.03	0.93
1:A:900:GLU:CG	1:A:903:ARG:HH12	1.83	0.92
1:E:578:LEU:HD11	1:E:583:GLY:O	1.70	0.91
1:G:506:TRP:HH2	1:G:511:PRO:O	1.53	0.91
1:E:606:PHE:CE2	1:E:614:PRO:HG2	2.06	0.90
1:G:380:TYR:HE1	1:G:408:MET:HE1	1.32	0.90
1:G:606:PHE:CD2	1:G:614:PRO:HG2	2.07	0.90
1:G:268:ALA:HB2	1:G:355:ARG:NH1	1.87	0.89
1:E:613:ALA:O	1:E:652:ARG:HD3	1.73	0.89
1:A:832:GLY:HA2	2:B:5:DA:H61	1.39	0.88
1:A:28:ARG:O	1:A:28:ARG:NE	2.07	0.87
1:C:451:ASP:OD1	1:C:452:GLU:N	2.07	0.86
1:A:28:ARG:HD2	1:A:30:LYS:NZ	1.90	0.86
1:A:265:VAL:HG13	1:A:355:ARG:NH2	1.91	0.85
1:G:833:SER:H	2:H:6:DA:H61	1.25	0.85
1:C:452:GLU:CG	1:C:454:HIS:NE2	2.40	0.84
1:G:249:ARG:O	1:G:252:PRO:HD2	1.78	0.84
1:G:832:GLY:HA2	2:H:5:DA:H61	1.41	0.84
1:G:281:ASN:OD1	1:G:282:GLY:N	2.11	0.83
1:C:263:ILE:HD11	1:C:365:SER:OG	1.78	0.83
1:G:579:VAL:HG23	1:G:580:LYS:HD3	1.57	0.83
1:E:145:MET:HE3	1:E:146:LEU:HD13	1.61	0.82
1:E:429:ALA:HB1	1:E:440:LEU:HD13	1.60	0.82
1:E:578:LEU:HD12	1:E:582:GLY:C	2.05	0.82
1:G:150:HIS:CE1	2:H:11:DA:H5'	2.15	0.82
1:C:358:ASN:O	1:C:359:THR:OG1	1.96	0.81
1:E:23:LYS:NZ	2:F:12:DA:OP2	2.12	0.81
1:A:28:ARG:CD	1:A:30:LYS:NZ	2.42	0.80
1:G:268:ALA:HB3	1:G:355:ARG:NH1	1.95	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:ALA:HB2	1:C:481:LEU:HD21	1.63	0.80
1:A:665:SER:O	1:A:666:LEU:HD12	1.81	0.79
1:G:518:SER:H	1:G:534:ARG:NH2	1.80	0.79
1:G:580:LYS:HB2	1:G:581:GLN:OE1	1.81	0.79
1:A:28:ARG:HD3	1:A:30:LYS:HE3	1.65	0.79
1:G:145:MET:HE3	1:G:146:LEU:HD13	1.64	0.79
1:C:263:ILE:CD1	1:C:365:SER:OG	2.31	0.79
1:G:606:PHE:CE2	1:G:614:PRO:HG2	2.17	0.79
1:C:409:GLY:HA3	1:C:412:ARG:HD2	1.66	0.78
1:A:22:ALA:HB2	1:A:34:LEU:HA	1.65	0.78
1:C:125:PHE:HB2	1:C:165:LEU:HD13	1.63	0.78
1:C:159:PHE:CD2	1:C:164:PRO:HB3	2.20	0.77
1:E:578:LEU:HD11	1:E:583:GLY:C	2.10	0.76
1:E:150:HIS:CE1	2:F:11:DA:H5'	2.22	0.75
1:G:404:THR:CG2	1:G:407:LEU:HD23	2.16	0.75
1:G:506:TRP:CH2	1:G:511:PRO:O	2.40	0.75
1:C:246:THR:HG22	1:C:250:ARG:HH12	1.53	0.74
1:C:832:GLY:HA2	2:D:5:DA:H61	1.51	0.74
1:C:844:ALA:N	1:C:845:GLY:HA2	2.01	0.74
1:G:579:VAL:CG2	1:G:580:LYS:HE2	2.17	0.74
1:A:429:ALA:HB1	1:A:440:LEU:HD13	1.69	0.73
1:C:680:VAL:HG13	1:C:743:THR:HG23	1.70	0.73
1:A:150:HIS:CE1	2:B:11:DA:H5'	2.24	0.73
1:C:554:ARG:NH1	1:C:574:GLU:OE2	2.20	0.73
1:A:268:ALA:HB2	1:A:355:ARG:NH1	2.03	0.73
1:G:606:PHE:CE2	1:G:614:PRO:CG	2.72	0.73
1:C:277:LEU:HD23	1:C:277:LEU:C	2.14	0.73
1:G:580:LYS:HD3	1:G:580:LYS:N	2.02	0.72
1:A:908:LEU:HA	1:A:911:LEU:HD13	1.72	0.71
1:A:145:MET:HE3	1:A:146:LEU:HD13	1.71	0.71
1:C:113:ARG:NH2	1:C:168:PHE:O	2.23	0.71
1:C:429:ALA:HB1	1:C:440:LEU:HD13	1.73	0.71
1:G:406:TRP:HE3	1:G:407:LEU:HD22	1.54	0.71
1:G:414:LEU:HD22	1:G:443:LEU:HD13	1.73	0.71
1:G:506:TRP:CZ3	1:G:510:GLU:HB3	2.25	0.71
1:E:456:VAL:HA	1:E:460:MET:HE3	1.72	0.71
1:E:881:ILE:HD11	1:E:942:LEU:HB2	1.72	0.71
1:C:833:SER:H	2:D:6:DA:H61	1.37	0.70
1:A:588:ILE:HG12	1:A:662:VAL:HG11	1.72	0.70
1:A:900:GLU:HA	1:A:903:ARG:NH1	2.06	0.70
1:G:602:LEU:HB3	1:G:616:LEU:HD11	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:903:ARG:HA	1:A:909:ARG:HG2	1.74	0.70
1:G:432:ARG:NH1	1:G:812:GLY:O	2.24	0.70
1:G:27:LEU:HD13	1:G:228:LEU:HD21	1.73	0.70
1:E:612:ASP:HB3	1:E:613:ALA:HA	1.72	0.70
1:G:579:VAL:HG23	1:G:580:LYS:HE2	1.71	0.70
1:C:432:ARG:NH1	1:C:812:GLY:O	2.25	0.70
1:G:414:LEU:HD22	1:G:443:LEU:CD1	2.21	0.70
1:C:266:PRO:O	1:C:355:ARG:NH2	2.25	0.70
1:C:279:LYS:O	1:C:279:LYS:HG3	1.90	0.70
1:G:579:VAL:HG23	1:G:580:LYS:CD	2.22	0.69
1:C:864:ARG:O	1:C:867:ARG:HG2	1.92	0.69
1:E:578:LEU:HD12	1:E:582:GLY:O	1.93	0.69
1:C:277:LEU:CD1	4:C:1003:ATP:N7	2.56	0.69
1:E:123:LEU:HG	1:E:127:LEU:HD22	1.73	0.69
1:G:258:ALA:O	1:G:407:LEU:HD21	1.92	0.69
1:C:869:THR:H	1:C:872:ASP:HB2	1.57	0.69
1:C:932:ARG:HE	1:C:944:PHE:C	2.00	0.69
1:E:311:LYS:HE3	4:E:1003:ATP:O1B	1.91	0.69
1:A:551:LEU:HD23	1:A:553:VAL:HG12	1.75	0.69
1:A:742:ARG:NH1	1:A:781:ASP:OD1	2.26	0.69
1:A:376:LEU:HD21	1:A:907:TYR:CE1	2.27	0.69
1:G:333:LEU:HD22	1:G:449:VAL:HB	1.73	0.69
1:G:673:MET:HE3	1:G:710:LEU:HD13	1.75	0.68
1:E:410:ARG:O	1:E:411:LYS:CG	2.40	0.68
1:E:410:ARG:O	1:E:411:LYS:HG3	1.93	0.68
1:G:869:THR:HG23	1:G:871:ALA:H	1.57	0.68
1:E:729:ARG:NH2	1:G:101:SER:O	2.26	0.68
1:A:268:ALA:CB	1:A:355:ARG:NH1	2.56	0.68
1:E:578:LEU:CD1	1:E:583:GLY:C	2.67	0.68
1:A:666:LEU:O	1:A:689:ARG:NH1	2.26	0.68
1:A:90:ARG:NH2	1:A:105:GLY:O	2.24	0.68
1:C:678:ALA:HB3	1:C:683:LEU:HD13	1.76	0.68
1:E:612:ASP:H	1:E:613:ALA:HB2	1.58	0.68
1:E:832:GLY:HA2	2:F:5:DA:H61	1.59	0.67
1:G:338:MET:HG3	2:H:5:DA:OP1	1.93	0.67
1:E:848:TRP:CD1	1:E:853:CYS:HG	2.12	0.67
1:A:363:ARG:O	1:A:398:ARG:NH2	2.28	0.67
1:G:504:ARG:HG2	1:G:504:ARG:HH11	1.60	0.67
1:G:507:ASN:OD1	1:G:507:ASN:N	2.26	0.67
1:G:410:ARG:HH11	1:G:410:ARG:HG2	1.60	0.67
1:G:896:ASN:OD1	1:G:929:THR:HG23	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:899:PRO:HG2	1:A:902:TRP:CD1	2.30	0.67
1:C:265:VAL:O	1:C:324:LYS:NZ	2.26	0.67
1:A:265:VAL:HG11	1:A:355:ARG:HH21	1.60	0.66
1:A:771:ASP:HA	1:G:507:ASN:HD22	1.61	0.66
1:E:380:TYR:CE2	1:E:408:MET:HE1	2.29	0.66
1:A:558:VAL:HG22	1:A:570:VAL:HG21	1.77	0.66
1:A:694:GLU:HG2	1:A:701:ARG:HH21	1.61	0.66
1:G:404:THR:HG23	1:G:407:LEU:H	1.61	0.66
1:C:429:ALA:HB2	1:C:439:ARG:HG2	1.78	0.66
1:G:429:ALA:HB1	1:G:440:LEU:HD13	1.78	0.66
1:A:65:MET:HA	1:A:198:MET:O	1.95	0.66
1:E:311:LYS:HB2	4:E:1003:ATP:O1B	1.96	0.66
1:A:675:SER:OG	1:A:686:ARG:NH2	2.29	0.66
1:A:898:PRO:HA	1:A:913:LEU:HD11	1.78	0.66
1:E:345:HIS:CD2	1:E:369:LEU:HB2	2.31	0.66
1:C:742:ARG:NH2	1:C:771:ASP:O	2.29	0.65
1:G:841:VAL:HA	1:G:846:ASN:O	1.97	0.65
1:A:585:ALA:HB3	1:A:655:VAL:HG22	1.78	0.65
1:A:268:ALA:HB2	1:A:355:ARG:HH11	1.58	0.65
1:E:575:LEU:O	1:E:579:VAL:HG23	1.96	0.65
1:E:612:ASP:CB	1:E:613:ALA:HA	2.26	0.65
1:C:347:ARG:NH2	4:C:1003:ATP:O1A	2.28	0.65
1:A:447:VAL:HG22	1:A:477:PRO:HG2	1.78	0.65
1:E:578:LEU:O	1:E:582:GLY:N	2.30	0.65
1:C:471:LEU:HD22	1:C:476:VAL:HG21	1.80	0.64
1:C:449:VAL:HG13	1:C:479:VAL:HB	1.80	0.64
1:A:200:ASP:OD1	1:A:203:THR:HB	1.97	0.64
1:G:106:GLU:OE2	1:G:179:ARG:NH2	2.26	0.64
1:A:665:SER:C	1:A:666:LEU:HD12	2.22	0.64
1:G:145:MET:HG3	1:G:208:CYS:HB2	1.78	0.64
1:C:673:MET:HE1	1:C:686:ARG:HB3	1.77	0.64
1:E:842:ASP:OD1	1:E:845:GLY:HA2	1.98	0.64
1:A:197:ASP:C	1:A:198:MET:HG3	2.22	0.64
1:A:261:ARG:HD3	1:A:262:PRO:HD2	1.80	0.64
1:G:578:LEU:O	1:G:581:GLN:N	2.30	0.64
1:E:123:LEU:O	1:E:127:LEU:HB2	1.98	0.63
1:G:577:PRO:HB2	1:G:704:TRP:CG	2.33	0.63
1:G:896:ASN:OD1	1:G:929:THR:CG2	2.46	0.63
1:G:39:LEU:HD22	1:G:244:PHE:HB2	1.79	0.63
1:C:457:ASP:H	1:C:460:MET:HE3	1.63	0.63
1:E:742:ARG:NH1	1:E:781:ASP:OD1	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:THR:HG22	1:C:250:ARG:NH1	2.14	0.62
1:E:558:VAL:HG22	1:E:570:VAL:HG21	1.81	0.62
1:G:22:ALA:C	1:G:23:LYS:HG2	2.24	0.62
1:G:261:ARG:O	1:G:365:SER:CB	2.47	0.62
1:G:261:ARG:O	1:G:365:SER:HB2	1.99	0.62
1:A:507:ASN:HB2	1:A:510:GLU:HB2	1.81	0.62
1:G:579:VAL:HG23	1:G:580:LYS:CE	2.29	0.62
1:G:833:SER:N	2:H:6:DA:H61	1.95	0.62
1:E:903:ARG:HA	1:E:909:ARG:HG3	1.81	0.62
1:C:725:PRO:O	1:C:741:GLN:NE2	2.25	0.62
1:G:310:GLY:HA2	4:G:1003:ATP:O2A	1.99	0.62
1:E:252:PRO:HB3	1:E:261:ARG:HH22	1.65	0.62
1:C:568:SER:HA	1:C:601:LEU:HD21	1.82	0.62
1:G:578:LEU:O	1:G:581:GLN:C	2.42	0.61
1:G:482:SER:OG	1:G:483:ALA:O	2.14	0.61
1:C:561:LYS:HG2	1:C:566:ASN:HB2	1.82	0.61
1:E:432:ARG:NH1	1:E:812:GLY:O	2.34	0.61
1:E:84:ASP:HB3	1:E:87:LYS:HD2	1.82	0.61
1:E:296:THR:O	1:E:296:THR:OG1	2.17	0.61
1:G:287:LEU:O	1:G:291:LEU:HB2	2.01	0.61
1:G:641:LYS:HE3	1:G:696:LEU:HD21	1.82	0.61
1:A:159:PHE:CE2	1:A:164:PRO:HG3	2.36	0.61
1:C:691:TRP:HB3	1:C:694:GLU:HB2	1.83	0.61
1:G:600:ASP:OD2	1:G:940:LYS:NZ	2.27	0.60
1:A:891:GLN:O	1:A:930:GLY:HA2	2.00	0.60
1:C:507:ASN:HB2	1:C:510:GLU:HB2	1.83	0.60
1:G:312:THR:HG22	1:G:316:TYR:CE2	2.37	0.60
1:G:518:SER:H	1:G:534:ARG:HH21	1.49	0.60
1:A:265:VAL:HG12	1:A:355:ARG:NH2	2.16	0.60
1:A:469:ARG:O	1:A:473:THR:HG22	2.01	0.60
1:C:82:LEU:O	1:C:85:ILE:HG22	2.02	0.60
1:C:404:THR:O	1:C:408:MET:HG2	2.02	0.60
1:A:881:ILE:HD12	1:A:942:LEU:HD22	1.84	0.60
1:A:258:ALA:O	1:A:404:THR:HG21	2.02	0.60
1:A:358:ASN:N	1:A:358:ASN:OD1	2.32	0.60
1:G:149:HIS:CD2	1:G:150:HIS:CD2	2.90	0.60
1:G:523:LEU:HD12	1:G:534:ARG:HH11	1.67	0.60
1:G:615:ASP:O	1:G:655:VAL:N	2.35	0.60
1:G:899:PRO:HG2	1:G:902:TRP:CD1	2.36	0.60
1:C:261:ARG:O	1:C:365:SER:CB	2.50	0.60
1:C:277:LEU:HD21	1:C:279:LYS:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:746:LEU:HD22	1:C:768:VAL:HB	1.84	0.59
1:C:630:GLU:O	1:C:634:THR:HG23	2.01	0.59
1:E:606:PHE:CD2	1:E:614:PRO:HG2	2.37	0.59
1:G:506:TRP:CE3	1:G:510:GLU:HB3	2.37	0.59
1:A:23:LYS:NZ	2:B:12:DA:OP2	2.35	0.59
1:A:548:ARG:NH2	1:A:692:ARG:O	2.36	0.59
1:C:666:LEU:HB3	1:C:668:LEU:HD13	1.85	0.59
1:C:848:TRP:CD1	1:C:853:CYS:HG	2.20	0.59
1:E:600:ASP:OD1	1:E:940:LYS:NZ	2.34	0.59
1:G:745:THR:O	1:G:749:ARG:HG2	2.01	0.59
1:C:247:SER:O	1:C:251:ILE:HD12	2.01	0.59
1:C:344:MET:HA	1:C:347:ARG:HG3	1.83	0.59
1:E:432:ARG:HD3	1:E:815:GLU:O	2.02	0.59
1:A:380:TYR:CE2	1:A:408:MET:HE1	2.38	0.59
1:G:520:PRO:HG3	1:G:545:THR:HG21	1.85	0.59
1:E:266:PRO:O	1:E:355:ARG:NH2	2.34	0.59
1:A:282:GLY:HA3	1:A:544:ALA:HB3	1.85	0.59
1:C:409:GLY:CA	1:C:412:ARG:HD2	2.32	0.59
1:C:471:LEU:HB3	1:C:476:VAL:HG22	1.85	0.59
1:E:832:GLY:HA2	2:F:5:DA:N6	2.17	0.59
1:G:333:LEU:HB2	1:G:420:VAL:HB	1.83	0.58
1:C:358:ASN:N	1:C:358:ASN:HD22	2.01	0.58
1:E:304:THR:HG22	1:E:482:SER:HB3	1.85	0.58
1:C:283:LEU:HA	1:C:543:ILE:HD12	1.85	0.58
1:C:404:THR:HG22	1:C:407:LEU:HB2	1.85	0.58
1:A:404:THR:HG23	1:A:407:LEU:H	1.68	0.58
1:A:484:THR:HG23	1:A:484:THR:O	2.03	0.58
1:C:585:ALA:HB3	1:C:655:VAL:HG23	1.85	0.58
1:C:662:VAL:O	1:C:689:ARG:NH2	2.24	0.58
1:E:351:TYR:CZ	1:E:355:ARG:HD3	2.38	0.58
1:G:275:PRO:HG3	1:G:354:TYR:OH	2.04	0.58
1:G:407:LEU:HD12	1:G:416:ALA:HB2	1.85	0.58
1:A:665:SER:HA	1:A:689:ARG:HH22	1.68	0.58
1:G:380:TYR:CD1	1:G:408:MET:HE1	2.37	0.58
1:E:412:ARG:O	1:E:415:LEU:HB2	2.03	0.58
1:C:277:LEU:HD12	4:C:1003:ATP:N7	2.19	0.58
1:A:23:LYS:HD3	1:A:224:LEU:HD11	1.86	0.58
1:E:632:THR:O	1:E:636:VAL:HG13	2.03	0.58
1:A:37:HIS:CE1	1:A:215:ASP:OD1	2.56	0.58
1:A:410:ARG:HD3	1:A:410:ARG:N	2.19	0.58
1:A:587:ILE:HB	1:A:657:VAL:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:424:ASP:O	1:G:428:MET:HG3	2.04	0.57
1:C:79:TRP:O	1:C:146:LEU:HD21	2.03	0.57
1:C:750:ARG:NH1	1:C:753:ALA:O	2.37	0.57
1:C:849:LEU:HD23	1:C:879:ARG:NE	2.18	0.57
1:G:841:VAL:O	1:G:918:VAL:N	2.28	0.57
1:A:482:SER:OG	1:A:483:ALA:O	2.20	0.57
1:C:459:TYR:HE2	1:C:794:LEU:HD23	1.69	0.57
1:G:404:THR:HG21	1:G:407:LEU:HD23	1.87	0.57
1:G:642:GLU:O	1:G:648:ARG:NH2	2.37	0.57
1:C:305:ALA:O	1:C:483:ALA:HA	2.04	0.57
1:E:24:GLU:HG2	1:E:96:ILE:HG21	1.87	0.57
1:C:261:ARG:O	1:C:365:SER:HB2	2.05	0.57
1:E:568:SER:HA	1:E:601:LEU:HD21	1.85	0.57
1:G:49:TRP:CH2	1:G:58:ARG:HG2	2.39	0.57
1:A:99:ASP:OD1	1:A:101:SER:OG	2.22	0.57
1:A:602:LEU:HB3	1:A:616:LEU:HD11	1.85	0.57
1:C:274:PHE:CE1	1:C:351:TYR:HE2	2.22	0.57
1:A:49:TRP:CZ2	1:A:58:ARG:HG2	2.40	0.57
1:C:267:PRO:HG3	1:C:324:LYS:HE2	1.86	0.57
1:G:192:ARG:N	1:G:193:PRO:CD	2.68	0.57
1:A:832:GLY:HA2	2:B:5:DA:N6	2.16	0.56
1:C:201:GLY:HA3	1:C:806:ALA:O	2.05	0.56
1:A:877:VAL:O	1:A:880:THR:OG1	2.20	0.56
1:C:371:HIS:HB3	1:C:422:THR:HG23	1.86	0.56
1:G:679:PRO:HG2	1:G:682:LEU:HD12	1.86	0.56
1:C:588:ILE:HD12	1:C:662:VAL:HG11	1.86	0.56
1:E:506:TRP:CH2	1:E:513:PRO:HD3	2.39	0.56
1:A:113:ARG:NH2	1:A:168:PHE:O	2.38	0.56
1:A:606:PHE:CZ	1:A:614:PRO:HG2	2.41	0.56
1:E:490:ALA:O	1:E:494:VAL:HG13	2.04	0.56
1:G:332:PHE:HA	1:G:419:ALA:O	2.06	0.56
1:G:725:PRO:HG2	1:G:741:GLN:HG2	1.88	0.56
1:A:28:ARG:HD3	1:A:30:LYS:CE	2.34	0.56
1:E:145:MET:HG3	1:E:208:CYS:HB2	1.88	0.56
1:A:265:VAL:HG13	1:A:355:ARG:HH21	1.60	0.56
1:C:484:THR:HG23	1:C:484:THR:O	2.06	0.56
1:G:694:GLU:HG2	1:G:701:ARG:HH21	1.71	0.56
1:C:575:LEU:HD11	1:C:587:ILE:HD11	1.88	0.55
1:E:523:LEU:HD21	1:E:532:VAL:HG13	1.88	0.55
1:C:274:PHE:CE1	1:C:351:TYR:CE2	2.93	0.55
1:C:310:GLY:HA2	4:C:1003:ATP:O2A	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:335:LEU:HD13	1:C:341:ALA:HA	1.87	0.55
1:E:132:TYR:HB3	1:E:139:THR:OG1	2.06	0.55
1:G:410:ARG:NH1	2:H:9:DA:OP2	2.39	0.55
1:E:406:TRP:O	1:E:412:ARG:NH1	2.39	0.55
1:A:893:THR:OG1	1:A:895:ASP:OD1	2.22	0.55
1:C:659:THR:O	1:C:662:VAL:HG12	2.07	0.55
1:E:251:ILE:HA	1:E:254:LEU:HD22	1.88	0.55
1:E:605:TRP:CD1	1:E:605:TRP:C	2.85	0.55
1:A:599:TYR:HB2	1:A:618:LEU:HD13	1.88	0.55
1:E:833:SER:H	2:F:6:DA:H61	1.55	0.55
1:E:607:ALA:O	1:E:610:GLY:HA3	2.07	0.55
1:E:612:ASP:CB	1:E:613:ALA:CA	2.85	0.55
1:G:268:ALA:HB3	1:G:355:ARG:CZ	2.37	0.55
1:G:282:GLY:HA3	1:G:544:ALA:HB3	1.89	0.55
1:C:203:THR:O	1:C:207:VAL:HG23	2.08	0.55
1:C:270:PHE:CE2	1:C:284:GLN:HB3	2.42	0.55
1:E:676:ASP:HB3	1:E:731:TRP:CH2	2.41	0.55
1:G:25:ARG:HD2	1:G:26:GLY:H	1.72	0.55
1:G:471:LEU:HD22	1:G:476:VAL:HG21	1.88	0.55
1:G:458:PRO:O	1:G:792:ARG:NH1	2.40	0.54
1:G:859:GLU:O	1:G:860:GLN:HG2	2.07	0.54
1:A:443:LEU:HA	1:A:446:LYS:HD3	1.90	0.54
1:E:315:ALA:HB2	1:E:481:LEU:HD11	1.89	0.54
1:E:877:VAL:HA	1:E:880:THR:HG23	1.89	0.54
1:G:899:PRO:CG	1:G:902:TRP:CD1	2.90	0.54
1:E:615:ASP:OD1	1:E:615:ASP:N	2.41	0.54
1:G:313:GLU:HA	1:G:316:TYR:HD2	1.72	0.54
1:G:937:ASP:OD1	1:G:939:CYS:N	2.38	0.54
1:A:831:ALA:HB1	1:A:885:MET:HB3	1.88	0.54
1:G:201:GLY:HA3	1:G:806:ALA:O	2.06	0.54
1:E:289:LYS:HD3	1:E:290:HIS:CE1	2.43	0.54
1:E:801:PRO:HD2	1:E:813:LEU:HD12	1.89	0.54
1:G:258:ALA:O	1:G:404:THR:HG21	2.08	0.54
1:C:150:HIS:CE1	2:D:11:DA:H5'	2.42	0.54
1:G:149:HIS:NE2	1:G:150:HIS:CD2	2.76	0.54
1:G:329:PRO:O	1:G:331:ARG:NH1	2.41	0.54
1:G:404:THR:HG23	1:G:407:LEU:HD23	1.90	0.54
1:G:832:GLY:HA2	2:H:5:DA:N6	2.18	0.54
1:A:200:ASP:OD1	1:A:203:THR:CB	2.55	0.54
1:A:287:LEU:O	1:A:291:LEU:HB2	2.07	0.54
2:F:10:DA:H2''	2:F:11:DA:O4'	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:ARG:CD	1:A:30:LYS:CE	2.86	0.53
1:A:160:GLN:OE1	1:C:796:ARG:HD2	2.09	0.53
1:A:691:TRP:HE3	1:A:694:GLU:HG3	1.71	0.53
1:C:219:SER:OG	2:D:11:DA:H2"	2.08	0.53
1:C:659:THR:O	1:C:661:VAL:N	2.41	0.53
1:G:606:PHE:CD2	1:G:614:PRO:CG	2.86	0.53
1:A:552:GLU:HB2	1:A:709:GLU:HG3	1.90	0.53
1:G:23:LYS:NZ	1:G:219:SER:OG	2.40	0.53
1:C:842:ASP:OD1	1:C:846:ASN:N	2.41	0.53
1:E:725:PRO:HB2	1:E:741:GLN:HG2	1.89	0.53
1:G:551:LEU:HG	1:G:755:VAL:HG23	1.90	0.53
1:A:684:LEU:HD23	1:A:761:VAL:HG13	1.91	0.53
1:A:898:PRO:HA	1:A:913:LEU:CD1	2.38	0.53
1:E:287:LEU:O	1:E:291:LEU:HB2	2.08	0.53
1:G:335:LEU:HD13	1:G:341:ALA:HA	1.91	0.53
1:C:246:THR:CG2	1:C:250:ARG:HH12	2.20	0.53
1:A:592:VAL:HG12	2:B:2:DA:OP1	2.09	0.53
1:A:900:GLU:CG	1:A:903:ARG:NH1	2.53	0.53
1:C:279:LYS:O	4:C:1003:ATP:N6	2.42	0.53
1:G:410:ARG:H	1:G:410:ARG:HD2	1.72	0.53
1:G:678:ALA:HB3	1:G:683:LEU:HD13	1.91	0.53
1:C:133:PRO:HB2	1:C:136:GLY:HA3	1.90	0.52
1:E:26:GLY:C	1:E:27:LEU:HD12	2.35	0.52
1:E:106:GLU:HG3	1:E:172:SER:HB3	1.90	0.52
1:E:887:PRO:O	1:E:890:SER:OG	2.25	0.52
1:E:848:TRP:CE2	1:E:853:CYS:HB3	2.44	0.52
1:A:182:LEU:O	1:A:186:VAL:HG13	2.09	0.52
1:A:410:ARG:CD	1:A:410:ARG:H	2.21	0.52
1:C:270:PHE:CE1	1:C:274:PHE:HD2	2.27	0.52
1:G:44:ALA:HA	1:G:251:ILE:HD13	1.92	0.52
1:A:332:PHE:HA	1:A:419:ALA:O	2.09	0.52
1:A:357:GLU:OE1	1:A:357:GLU:N	2.34	0.52
1:A:835:ARG:NH2	1:A:882:PRO:HD3	2.24	0.52
1:C:275:PRO:HG3	1:C:354:TYR:CZ	2.45	0.52
1:C:725:PRO:HB2	1:C:741:GLN:HG2	1.90	0.52
1:E:25:ARG:O	1:E:27:LEU:HD13	2.10	0.52
1:G:430:VAL:HG11	1:G:467:LEU:HA	1.91	0.52
1:A:410:ARG:N	1:A:410:ARG:CD	2.73	0.52
1:C:37:HIS:ND1	1:C:37:HIS:O	2.42	0.52
1:C:506:TRP:HH2	1:C:511:PRO:O	1.93	0.52
1:G:380:TYR:HE1	1:G:408:MET:CE	2.14	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:484:THR:HG23	1:G:484:THR:O	2.10	0.52
1:C:663:GLU:OE2	1:C:686:ARG:NH1	2.29	0.52
1:G:404:THR:CG2	1:G:407:LEU:CD2	2.88	0.52
1:G:674:ILE:HG22	1:G:713:LEU:HD11	1.91	0.52
1:C:739:LEU:HD21	1:C:769:TYR:CE1	2.45	0.52
1:G:602:LEU:N	1:G:602:LEU:HD12	2.25	0.52
1:A:371:HIS:HB3	1:A:422:THR:HG23	1.92	0.51
1:A:669:ASP:OD2	1:A:693:HIS:N	2.28	0.51
1:C:47:VAL:HG11	1:C:251:ILE:HG22	1.92	0.51
1:C:473:THR:HG21	1:C:803:PRO:HG2	1.92	0.51
1:A:28:ARG:HB3	1:A:30:LYS:HZ2	1.74	0.51
1:A:49:TRP:CH2	1:A:58:ARG:HG2	2.45	0.51
1:C:739:LEU:HD11	1:C:769:TYR:OH	2.10	0.51
1:G:567:ARG:NH2	1:G:676:ASP:OD2	2.44	0.51
1:G:598:VAL:O	1:G:602:LEU:HD13	2.10	0.51
1:C:801:PRO:HD2	1:C:813:LEU:HD12	1.91	0.51
1:C:459:TYR:CD2	1:C:829:PHE:HB2	2.45	0.51
1:C:684:LEU:HD13	1:C:761:VAL:HG13	1.91	0.51
1:A:729:ARG:CZ	1:C:104:PRO:HG3	2.40	0.51
1:E:149:HIS:NE2	1:E:150:HIS:CD2	2.78	0.51
1:E:410:ARG:C	1:E:411:LYS:CG	2.84	0.51
1:E:451:ASP:OD1	1:E:452:GLU:N	2.43	0.51
1:G:84:ASP:HB3	1:G:87:LYS:HD2	1.93	0.51
1:A:691:TRP:CE3	1:A:694:GLU:HG3	2.45	0.51
1:G:49:TRP:CZ2	1:G:58:ARG:HG2	2.45	0.51
1:G:486:HIS:CD2	1:G:769:TYR:HD2	2.27	0.51
1:A:98:ILE:HD13	1:A:100:LEU:HD21	1.92	0.51
1:C:261:ARG:O	1:C:365:SER:HB3	2.11	0.51
1:C:414:LEU:HG	1:C:443:LEU:HD13	1.93	0.51
1:E:895:ASP:OD1	1:E:895:ASP:N	2.38	0.51
1:C:34:LEU:HD23	1:C:88:LEU:HD22	1.92	0.51
1:C:410:ARG:HD2	2:D:9:DA:H2'	1.93	0.51
1:C:519:TYR:HB3	1:C:762:GLN:HB2	1.93	0.51
1:E:625:ASN:O	1:E:629:THR:HG23	2.11	0.51
1:G:369:LEU:HB3	1:G:380:TYR:CE2	2.46	0.51
1:G:850:ASP:OD2	1:G:854:THR:OG1	2.27	0.51
1:C:241:ARG:O	1:C:245:GLU:HG2	2.11	0.51
1:G:284:GLN:CD	1:G:284:GLN:H	2.19	0.51
1:E:334:ALA:HB1	1:E:423:ILE:HA	1.93	0.50
1:E:691:TRP:HB3	1:E:694:GLU:HG2	1.91	0.50
1:G:63:SER:OG	1:G:64:SER:N	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:249:ARG:O	1:G:251:ILE:N	2.44	0.50
1:G:451:ASP:OD1	1:G:452:GLU:N	2.44	0.50
1:G:679:PRO:HB3	1:G:739:LEU:HD21	1.94	0.50
1:G:837:LEU:HB3	1:G:913:LEU:HD23	1.93	0.50
1:C:567:ARG:NH2	1:C:676:ASP:OD2	2.44	0.50
1:C:916:GLN:OE1	1:C:936:LEU:N	2.33	0.50
1:E:332:PHE:HA	1:E:419:ALA:O	2.12	0.50
1:G:131:GLY:O	1:G:195:PRO:HG2	2.12	0.50
1:C:335:LEU:HD11	1:C:344:MET:HG2	1.94	0.50
1:C:451:ASP:O	1:C:452:GLU:C	2.54	0.50
1:G:580:LYS:HD3	1:G:580:LYS:H	1.76	0.50
1:A:471:LEU:HD22	1:A:476:VAL:HG21	1.93	0.50
1:G:551:LEU:HD23	1:G:757:ILE:HD11	1.92	0.50
1:G:618:LEU:HD23	1:G:940:LYS:HA	1.92	0.50
1:C:281:ASN:HB2	1:C:284:GLN:OE1	2.10	0.50
1:E:605:TRP:HD1	1:E:605:TRP:O	1.94	0.50
1:E:848:TRP:CD2	1:E:853:CYS:HB3	2.46	0.50
1:G:282:GLY:O	1:G:543:ILE:HD11	2.11	0.50
1:A:362:PRO:HB2	1:A:365:SER:HB2	1.93	0.50
1:E:447:VAL:HG22	1:E:477:PRO:HG2	1.94	0.50
1:A:32:TYR:HD1	1:A:228:LEU:HD13	1.77	0.50
1:A:28:ARG:O	1:A:28:ARG:CG	2.58	0.50
1:G:312:THR:HG22	1:G:316:TYR:HE2	1.76	0.50
1:G:407:LEU:CD2	1:G:407:LEU:N	2.75	0.50
1:C:412:ARG:O	1:C:413:GLY:C	2.55	0.49
1:E:150:HIS:ND1	2:F:11:DA:H5'	2.27	0.49
1:E:576:THR:HB	1:E:577:PRO:HD3	1.94	0.49
1:A:483:ALA:O	1:A:484:THR:C	2.54	0.49
1:A:902:TRP:C	1:A:904:GLU:H	2.20	0.49
1:G:345:HIS:HA	1:G:420:VAL:HG11	1.93	0.49
1:G:588:ILE:HB	1:G:675:SER:HB2	1.95	0.49
1:G:649:ARG:CG	1:G:650:PRO:HD2	2.42	0.49
1:C:351:TYR:CZ	1:C:355:ARG:HD3	2.46	0.49
1:G:277:LEU:HD21	4:G:1003:ATP:C4	2.47	0.49
1:G:632:THR:O	1:G:635:ILE:HG22	2.12	0.49
1:C:16:LEU:HB3	1:C:181:ALA:HB1	1.94	0.49
1:C:65:MET:HE3	1:C:196:PRO:HG3	1.93	0.49
1:C:842:ASP:O	1:C:845:GLY:HA3	2.12	0.49
1:A:495:LYS:O	1:A:499:GLU:HG3	2.12	0.49
1:A:665:SER:C	1:A:666:LEU:CD1	2.85	0.49
1:C:844:ALA:N	1:C:845:GLY:CA	2.73	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:599:TYR:CD1	1:E:616:LEU:HD22	2.48	0.49
1:G:486:HIS:HD2	1:G:769:TYR:HD2	1.61	0.49
1:G:606:PHE:CD1	1:G:606:PHE:N	2.81	0.49
1:G:606:PHE:O	1:G:607:ALA:C	2.55	0.49
1:A:404:THR:CG2	1:A:407:LEU:H	2.26	0.49
1:A:627:GLN:HG2	1:A:631:ILE:HD11	1.94	0.49
1:C:586:ALA:HB2	1:C:670:VAL:HG11	1.95	0.49
1:E:410:ARG:C	1:E:411:LYS:HG2	2.38	0.49
1:G:43:ALA:O	1:G:47:VAL:HG23	2.13	0.49
1:A:34:LEU:HD23	1:A:88:LEU:HD22	1.94	0.49
1:C:407:LEU:HD21	1:C:416:ALA:HB2	1.95	0.49
1:C:523:LEU:HD21	1:C:532:VAL:HG13	1.94	0.49
1:E:608:THR:C	1:E:610:GLY:H	2.20	0.49
1:G:51:GLU:HB3	1:G:261:ARG:HH12	1.78	0.49
1:A:550:PRO:O	1:A:708:PRO:HG2	2.12	0.49
1:C:103:TYR:O	1:C:175:TRP:NE1	2.46	0.49
1:E:919:THR:HG22	1:E:923:ALA:H	1.77	0.49
1:G:56:GLY:HA3	1:G:326:THR:O	2.13	0.49
1:G:290:HIS:ND1	1:G:538:VAL:HB	2.28	0.49
1:C:663:GLU:OE2	1:C:686:ARG:HD2	2.13	0.49
1:E:305:ALA:HB3	1:E:311:LYS:HE2	1.94	0.49
1:G:284:GLN:NE2	1:G:309:GLU:O	2.46	0.49
1:G:404:THR:HG22	1:G:407:LEU:HG	1.94	0.49
1:G:261:ARG:O	1:G:365:SER:HB3	2.13	0.48
1:A:771:ASP:OD1	1:G:507:ASN:ND2	2.47	0.48
1:C:276:HIS:ND1	1:C:277:LEU:N	2.60	0.48
1:C:358:ASN:N	1:C:358:ASN:ND2	2.60	0.48
1:G:268:ALA:CB	1:G:355:ARG:CZ	2.89	0.48
1:G:407:LEU:HD23	1:G:407:LEU:N	2.28	0.48
1:A:471:LEU:HB3	1:A:476:VAL:HG22	1.95	0.48
1:A:366:THR:HB	1:A:402:ALA:O	2.12	0.48
1:A:555:LEU:HD23	1:A:712:VAL:HB	1.95	0.48
1:E:634:THR:O	1:E:637:ASP:HB3	2.13	0.48
1:A:678:ALA:HB3	1:A:683:LEU:HD13	1.96	0.48
1:C:404:THR:CG2	1:C:407:LEU:HB2	2.42	0.48
1:E:281:ASN:ND2	1:E:309:GLU:OE1	2.46	0.48
1:G:25:ARG:HD2	1:G:26:GLY:N	2.27	0.48
1:G:454:HIS:CD2	1:G:483:ALA:HB3	2.48	0.48
1:C:274:PHE:HE1	1:C:351:TYR:CD2	2.32	0.48
1:E:234:ASP:OD1	1:E:236:SER:OG	2.29	0.48
1:G:51:GLU:HB3	1:G:261:ARG:NH1	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:TRP:H	1:A:21:TRP:CD1	2.30	0.48
1:A:410:ARG:H	1:A:410:ARG:NE	2.12	0.48
1:A:410:ARG:C	1:A:411:LYS:CG	2.86	0.48
1:A:679:PRO:HG3	1:A:739:LEU:HD13	1.96	0.48
1:E:406:TRP:CH2	1:E:412:ARG:HD3	2.49	0.48
1:G:217:LEU:O	1:G:220:GLN:HG3	2.13	0.48
1:G:474:LEU:O	1:G:475:ASP:HB2	2.14	0.48
1:A:261:ARG:O	1:A:365:SER:OG	2.24	0.48
1:A:736:PRO:HG2	1:A:739:LEU:HB2	1.95	0.48
1:A:744:TYR:OH	1:A:748:ARG:NH1	2.46	0.48
1:A:876:LEU:HA	1:A:876:LEU:HD23	1.70	0.48
1:C:466:GLN:OE1	1:C:469:ARG:HD2	2.14	0.48
1:G:259:GLY:HA2	1:G:364:SER:O	2.13	0.48
1:A:275:PRO:HG3	1:A:354:TYR:OH	2.14	0.48
1:E:56:GLY:HA3	1:E:326:THR:O	2.14	0.48
1:E:491:ASN:OD1	1:E:513:PRO:HD2	2.13	0.48
1:E:522:TRP:HE3	1:E:523:LEU:N	2.12	0.48
1:G:125:PHE:HB2	1:G:165:LEU:HD13	1.95	0.48
1:G:606:PHE:CE2	1:G:614:PRO:HG3	2.49	0.48
1:E:22:ALA:HB2	1:E:34:LEU:HA	1.96	0.47
1:E:375:TRP:CZ3	1:E:381:ALA:HB1	2.49	0.47
1:E:586:ALA:HB3	1:E:673:MET:HG2	1.95	0.47
1:G:486:HIS:CE1	1:G:487:HIS:CD2	3.01	0.47
1:G:627:GLN:O	1:G:631:ILE:HG13	2.14	0.47
1:E:596:GLN:O	1:E:599:TYR:HB3	2.15	0.47
1:G:506:TRP:CH2	1:G:511:PRO:C	2.91	0.47
1:G:549:LYS:HB3	1:G:708:PRO:HG2	1.96	0.47
1:A:28:ARG:CG	1:A:30:LYS:NZ	2.77	0.47
1:C:198:MET:HE3	1:C:200:ASP:HB3	1.95	0.47
1:C:459:TYR:CE2	1:C:794:LEU:HD23	2.48	0.47
1:E:848:TRP:CD1	1:E:853:CYS:SG	3.07	0.47
1:G:471:LEU:HB3	1:G:476:VAL:HG22	1.96	0.47
1:A:268:ALA:HB3	1:A:355:ARG:NH1	2.29	0.47
1:A:833:SER:H	2:B:6:DA:H61	1.62	0.47
1:C:277:LEU:C	1:C:277:LEU:CD2	2.86	0.47
1:E:604:GLN:O	1:E:608:THR:HG23	2.14	0.47
1:G:274:PHE:CE2	1:G:313:GLU:HG3	2.48	0.47
1:A:739:LEU:HD23	1:A:739:LEU:HA	1.72	0.47
1:C:303:ILE:HB	1:C:481:LEU:HD13	1.96	0.47
1:C:456:VAL:HG23	1:C:456:VAL:O	2.15	0.47
1:E:267:PRO:HB3	1:E:324:LYS:HE2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:TRP:HB2	1:A:907:TYR:OH	2.14	0.47
1:C:39:LEU:O	1:C:42:ALA:N	2.46	0.47
1:C:706:LYS:HG3	1:C:707:GLN:H	1.80	0.47
1:E:55:PRO:HD2	1:E:327:GLY:O	2.14	0.47
1:E:376:LEU:HG	1:E:907:TYR:CZ	2.50	0.47
1:E:502:ARG:HH22	1:E:510:GLU:CD	2.22	0.47
1:E:893:THR:H	1:E:896:ASN:ND2	2.13	0.47
1:G:869:THR:HG22	1:G:872:ASP:CG	2.39	0.47
1:G:937:ASP:HB3	1:G:940:LYS:HB2	1.96	0.47
1:A:376:LEU:N	1:A:376:LEU:HD22	2.30	0.47
1:C:205:SER:O	1:C:208:CYS:HB3	2.15	0.47
1:E:473:THR:HG21	1:E:803:PRO:HG2	1.97	0.47
1:G:367:LEU:HD22	1:G:418:TRP:HB2	1.96	0.47
1:C:17:ASP:H	1:C:178:GLN:HE22	1.63	0.47
1:C:263:ILE:CD1	1:C:365:SER:CB	2.93	0.47
1:C:683:LEU:HD12	1:C:683:LEU:HA	1.73	0.47
1:C:691:TRP:CD1	1:C:691:TRP:N	2.83	0.47
1:E:46:LEU:HD12	1:E:46:LEU:HA	1.60	0.47
1:G:789:LEU:HD23	1:G:789:LEU:HA	1.73	0.47
1:C:276:HIS:ND1	1:C:276:HIS:C	2.73	0.46
1:E:627:GLN:O	1:E:631:ILE:HG13	2.15	0.46
1:G:213:LEU:HD22	1:G:415:LEU:HD13	1.97	0.46
1:A:84:ASP:HB3	1:A:87:LYS:HD2	1.96	0.46
1:A:310:GLY:HA2	4:A:1003:ATP:O2A	2.15	0.46
1:E:552:GLU:HB2	1:E:709:GLU:HG3	1.97	0.46
1:G:26:GLY:C	1:G:27:LEU:HD23	2.40	0.46
1:G:307:MET:HA	4:G:1003:ATP:O1B	2.15	0.46
1:G:840:TYR:OH	1:G:936:LEU:HD11	2.16	0.46
1:A:275:PRO:HG3	1:A:354:TYR:CZ	2.51	0.46
1:C:106:GLU:HG3	1:C:172:SER:CB	2.44	0.46
1:C:270:PHE:CD1	1:C:270:PHE:C	2.93	0.46
1:C:338:MET:HG2	1:C:371:HIS:HB2	1.97	0.46
1:E:201:GLY:HA3	1:E:806:ALA:O	2.15	0.46
1:E:410:ARG:O	1:E:411:LYS:HG2	2.15	0.46
1:E:606:PHE:CE2	1:E:614:PRO:CG	2.88	0.46
1:G:673:MET:HE2	1:G:673:MET:HB3	1.73	0.46
1:A:88:LEU:HG	1:A:179:ARG:HG2	1.98	0.46
1:C:407:LEU:CD2	1:C:416:ALA:HB2	2.45	0.46
1:C:486:HIS:CD2	1:C:766:ASP:HA	2.50	0.46
1:E:617:TYR:CG	1:E:635:ILE:HD11	2.50	0.46
1:E:869:THR:O	1:E:872:ASP:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:848:TRP:HB3	1:G:853:CYS:HA	1.97	0.46
1:A:849:LEU:HD13	1:A:857:PHE:HA	1.96	0.46
1:C:339:ALA:O	1:C:343:GLN:HG3	2.15	0.46
1:C:440:LEU:HD12	1:C:440:LEU:HA	1.67	0.46
1:C:493:LEU:HD23	1:C:493:LEU:HA	1.78	0.46
1:G:21:TRP:H	1:G:21:TRP:CD1	2.32	0.46
1:A:486:HIS:HE2	1:A:769:TYR:HB2	1.80	0.46
1:A:694:GLU:OE1	1:A:701:ARG:NE	2.48	0.46
1:C:122:TRP:CE3	1:C:123:LEU:HD12	2.51	0.46
1:C:319:ALA:O	1:C:323:GLY:N	2.48	0.46
1:G:22:ALA:HB2	1:G:34:LEU:HA	1.98	0.46
1:G:850:ASP:OD1	1:G:850:ASP:N	2.43	0.46
1:A:840:TYR:O	1:A:848:TRP:N	2.44	0.46
1:C:22:ALA:HB2	1:C:34:LEU:HA	1.97	0.46
1:C:364:SER:O	1:C:364:SER:OG	2.27	0.46
1:E:83:HIS:HD2	1:E:149:HIS:CD2	2.34	0.46
1:G:68:ASP:OD1	1:G:71:HIS:HB2	2.15	0.46
1:G:410:ARG:C	1:G:411:LYS:CG	2.86	0.46
1:A:207:VAL:O	1:A:211:VAL:HG23	2.16	0.46
1:C:32:TYR:OH	1:C:40:ASP:OD2	2.21	0.46
1:C:258:ALA:O	1:C:407:LEU:HD12	2.16	0.46
1:C:263:ILE:HD13	1:C:417:PRO:HB2	1.97	0.46
1:C:575:LEU:O	1:C:579:VAL:HG12	2.16	0.46
1:C:839:TYR:CZ	1:C:915:PRO:HB3	2.51	0.46
1:E:241:ARG:HD2	1:E:245:GLU:OE2	2.15	0.46
1:E:893:THR:H	1:E:896:ASN:HD22	1.63	0.46
1:G:666:LEU:O	1:G:689:ARG:NH1	2.49	0.46
1:C:148:GLY:HA2	1:C:152:THR:O	2.15	0.46
1:G:79:TRP:CE2	1:G:142:VAL:HG21	2.51	0.46
1:G:348:LEU:HD23	1:G:367:LEU:HD11	1.98	0.46
1:A:373:MET:HA	1:A:373:MET:HE2	1.98	0.45
1:A:494:VAL:HG21	1:A:514:VAL:HG23	1.97	0.45
1:A:505:ARG:HB3	1:A:506:TRP:H	1.61	0.45
1:C:150:HIS:ND1	2:D:11:DA:H5'	2.31	0.45
1:C:269:THR:OG1	1:C:272:GLU:HG3	2.16	0.45
1:E:258:ALA:O	1:E:404:THR:HG21	2.16	0.45
1:E:471:LEU:HD22	1:E:476:VAL:HG21	1.98	0.45
1:G:132:TYR:HB3	1:G:139:THR:OG1	2.16	0.45
1:G:150:HIS:ND1	2:H:11:DA:H5'	2.29	0.45
1:G:649:ARG:HG2	1:G:650:PRO:HD2	1.98	0.45
1:A:261:ARG:HB3	1:A:364:SER:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:MET:HG2	1:A:371:HIS:CG	2.51	0.45
1:A:522:TRP:O	1:A:535:SER:HB3	2.17	0.45
1:C:70:GLU:O	1:C:74:HIS:ND1	2.41	0.45
1:C:406:TRP:O	1:C:412:ARG:HD3	2.15	0.45
1:C:453:ALA:O	1:C:456:VAL:HG22	2.16	0.45
1:A:635:ILE:O	1:A:639:PHE:HD1	1.99	0.45
1:A:841:VAL:HA	1:A:846:ASN:O	2.17	0.45
1:C:261:ARG:HA	1:C:262:PRO:HD3	1.80	0.45
1:G:286:SER:HB2	1:G:543:ILE:CD1	2.46	0.45
1:G:454:HIS:HA	1:G:485:LEU:HD13	1.97	0.45
1:G:543:ILE:HD12	1:G:544:ALA:H	1.82	0.45
1:G:899:PRO:O	1:G:900:GLU:C	2.60	0.45
1:A:51:GLU:HB3	1:A:261:ARG:NH1	2.31	0.45
1:A:351:TYR:OH	1:A:355:ARG:HD3	2.17	0.45
1:C:76:ILE:HD13	1:C:207:VAL:HG13	1.99	0.45
1:E:630:GLU:O	1:E:634:THR:HG23	2.15	0.45
1:E:673:MET:HE2	1:E:673:MET:HB3	1.84	0.45
1:A:398:ARG:HG2	1:A:399:ASP:H	1.81	0.45
1:C:17:ASP:OD2	1:C:19:ARG:NE	2.43	0.45
1:C:428:MET:C	1:C:439:ARG:HD3	2.42	0.45
1:C:443:LEU:HD12	1:C:443:LEU:HA	1.73	0.45
1:E:48:LEU:HD12	1:E:52:TYR:HB3	1.98	0.45
1:E:404:THR:HG23	1:E:407:LEU:H	1.81	0.45
1:E:891:GLN:O	1:E:930:GLY:HA2	2.16	0.45
1:G:334:ALA:HB1	1:G:423:ILE:HA	1.98	0.45
1:C:898:PRO:HA	1:C:913:LEU:HD11	1.99	0.45
1:C:903:ARG:HA	1:C:909:ARG:HG3	1.99	0.45
1:G:127:LEU:HD12	1:G:127:LEU:HA	1.84	0.45
1:G:270:PHE:CE2	1:G:284:GLN:HB3	2.52	0.45
1:A:32:TYR:HA	1:A:33:PRO:HD3	1.76	0.45
1:A:664:GLN:O	1:A:689:ARG:NH2	2.50	0.45
1:C:618:LEU:HD23	1:C:940:LYS:HA	1.99	0.45
1:G:332:PHE:CE2	1:G:334:ALA:HB2	2.51	0.45
1:A:48:LEU:HD12	1:A:52:TYR:CB	2.47	0.45
1:E:217:LEU:HD12	1:E:217:LEU:HA	1.73	0.45
1:E:459:TYR:CD1	1:E:795:ALA:HB2	2.52	0.45
1:E:670:VAL:HG21	1:E:673:MET:HG3	1.99	0.45
1:E:835:ARG:NH2	1:E:882:PRO:HD3	2.32	0.45
1:G:251:ILE:O	1:G:254:LEU:HB2	2.17	0.45
1:G:451:ASP:OD2	1:G:481:LEU:HD23	2.17	0.45
1:A:56:GLY:HA3	1:A:326:THR:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:THR:HG23	1:A:250:ARG:NH1	2.32	0.45
1:A:480:LEU:C	1:A:481:LEU:HD13	2.41	0.45
1:C:506:TRP:CH2	1:C:513:PRO:HD3	2.52	0.45
1:G:410:ARG:HH11	1:G:410:ARG:CG	2.26	0.45
1:G:606:PHE:N	1:G:606:PHE:HD1	2.14	0.45
1:A:496:ALA:O	1:A:499:GLU:HB2	2.16	0.44
1:A:902:TRP:O	1:A:904:GLU:N	2.51	0.44
1:C:96:ILE:HD12	1:C:97:ALA:H	1.81	0.44
1:C:294:LEU:HD21	1:C:533:THR:HG21	1.99	0.44
1:A:28:ARG:CD	1:A:30:LYS:HE3	2.39	0.44
1:A:373:MET:HE2	1:A:376:LEU:HD23	1.99	0.44
1:G:451:ASP:HA	1:G:481:LEU:HB2	1.99	0.44
1:A:251:ILE:O	1:A:254:LEU:HB2	2.17	0.44
1:C:74:HIS:HD2	1:C:190:THR:O	2.00	0.44
1:C:291:LEU:HD23	1:C:291:LEU:HA	1.74	0.44
1:E:74:HIS:HD2	1:E:190:THR:O	2.00	0.44
1:E:619:LEU:HA	1:E:619:LEU:HD12	1.80	0.44
1:G:350:GLU:HA	1:G:353:ARG:HB3	1.99	0.44
1:G:357:GLU:N	1:G:357:GLU:OE1	2.50	0.44
1:A:683:LEU:HD12	1:A:683:LEU:HA	1.71	0.44
1:A:902:TRP:CD1	1:A:902:TRP:N	2.85	0.44
1:C:49:TRP:CZ2	1:C:58:ARG:HG2	2.52	0.44
1:G:84:ASP:OD2	1:G:87:LYS:NZ	2.49	0.44
1:G:504:ARG:HH11	1:G:504:ARG:CG	2.27	0.44
1:G:848:TRP:CE3	1:G:856:GLU:HA	2.52	0.44
1:G:893:THR:O	1:G:896:ASN:HB2	2.17	0.44
1:A:376:LEU:HD21	1:A:907:TYR:CD1	2.52	0.44
1:C:665:SER:O	1:C:665:SER:OG	2.29	0.44
1:E:599:TYR:HD1	1:E:616:LEU:HD22	1.82	0.44
1:G:373:MET:HE1	1:G:376:LEU:HD12	1.99	0.44
1:A:613:ALA:HA	1:A:614:PRO:HA	1.84	0.44
1:A:844:ALA:N	1:A:845:GLY:HA2	2.33	0.44
1:C:80:ALA:HB2	1:C:211:VAL:HG22	2.00	0.44
1:C:344:MET:HE2	1:C:344:MET:HB2	1.92	0.44
1:E:24:GLU:C	1:E:24:GLU:CD	2.85	0.44
1:G:605:TRP:O	1:G:605:TRP:CD1	2.70	0.44
4:G:1003:ATP:H5'1	4:G:1003:ATP:H8	1.83	0.44
1:A:65:MET:HG2	1:A:199:LEU:HD13	2.00	0.44
1:E:502:ARG:NH2	1:E:510:GLU:OE2	2.45	0.44
1:G:51:GLU:OE1	1:G:261:ARG:NH2	2.48	0.44
1:G:141:LEU:HA	1:G:141:LEU:HD23	1.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:561:LYS:HE3	1:G:561:LYS:HB2	1.82	0.44
1:A:265:VAL:HA	1:A:266:PRO:HD3	1.84	0.44
1:A:424:ASP:OD1	1:A:424:ASP:N	2.51	0.44
1:E:146:LEU:HD12	1:E:146:LEU:HA	1.78	0.44
1:E:592:VAL:O	1:E:596:GLN:HG3	2.18	0.44
1:E:691:TRP:CZ3	1:E:708:PRO:HD3	2.53	0.44
1:A:808:ASP:OD1	1:A:808:ASP:N	2.51	0.44
1:C:16:LEU:O	1:C:16:LEU:HD12	2.17	0.44
1:C:24:GLU:C	1:C:24:GLU:CD	2.85	0.44
1:C:44:ALA:O	1:C:48:LEU:HD22	2.17	0.44
1:E:459:TYR:CB	1:E:829:PHE:HB2	2.47	0.44
1:E:667:ASP:O	1:E:668:LEU:HD23	2.18	0.44
1:G:258:ALA:O	1:G:407:LEU:CD2	2.63	0.44
1:G:295:CYS:O	1:G:295:CYS:SG	2.75	0.44
1:G:462:VAL:HG23	1:G:792:ARG:HH11	1.82	0.44
1:G:490:ALA:O	1:G:494:VAL:HG13	2.17	0.44
1:G:520:PRO:HG3	1:G:545:THR:CG2	2.48	0.44
1:G:608:THR:O	1:G:609:LEU:C	2.61	0.44
1:A:16:LEU:HB3	1:A:181:ALA:HB1	2.00	0.43
1:A:269:THR:OG1	1:A:272:GLU:HG3	2.17	0.43
1:A:902:TRP:C	1:A:904:GLU:N	2.76	0.43
1:G:315:ALA:HB2	1:G:481:LEU:HD11	1.99	0.43
1:G:673:MET:HE1	1:G:687:ALA:HA	2.00	0.43
1:G:677:LEU:HD11	1:G:743:THR:HG22	1.99	0.43
1:G:933:GLU:O	1:G:944:PHE:HA	2.18	0.43
1:A:156:HIS:HA	1:A:157:PRO:HD3	1.91	0.43
1:A:573:LYS:O	1:A:576:THR:OG1	2.35	0.43
1:C:549:LYS:HA	1:C:550:PRO:HD2	1.56	0.43
1:E:590:THR:HG21	1:E:731:TRP:HA	2.00	0.43
1:E:637:ASP:C	1:E:637:ASP:OD1	2.60	0.43
1:E:682:LEU:HD23	1:E:682:LEU:HA	1.69	0.43
1:E:691:TRP:HB3	1:E:694:GLU:CG	2.48	0.43
1:C:277:LEU:HD11	4:C:1003:ATP:N7	2.33	0.43
1:C:354:TYR:CD2	1:C:355:ARG:HG2	2.54	0.43
1:C:852:GLU:O	1:C:854:THR:HG23	2.18	0.43
1:E:87:LYS:HG2	1:E:92:PHE:CZ	2.53	0.43
1:A:638:LEU:HB2	1:A:639:PHE:CD1	2.53	0.43
1:C:929:THR:HB	1:C:934:TRP:CD1	2.53	0.43
1:G:128:PRO:HA	1:G:132:TYR:O	2.19	0.43
1:G:375:TRP:CE2	1:G:408:MET:HG3	2.53	0.43
1:G:443:LEU:HA	1:G:443:LEU:HD12	1.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:306:PRO:HG3	1:E:519:TYR:CZ	2.53	0.43
1:E:554:ARG:NH1	1:E:574:GLU:OE2	2.48	0.43
1:E:599:TYR:O	1:E:603:SER:HB2	2.18	0.43
1:A:495:LYS:NZ	1:A:512:GLN:OE1	2.49	0.43
1:E:558:VAL:HG11	1:E:565:LEU:HB3	2.00	0.43
1:E:605:TRP:CD1	1:E:605:TRP:O	2.70	0.43
1:E:679:PRO:CG	1:E:739:LEU:HD13	2.48	0.43
1:G:506:TRP:CZ2	1:G:513:PRO:HD3	2.54	0.43
1:G:520:PRO:HG2	1:G:543:ILE:CG2	2.49	0.43
1:G:534:ARG:HG3	1:G:535:SER:N	2.34	0.43
1:A:200:ASP:OD2	1:A:202:PRO:HD2	2.18	0.43
1:A:320:ASP:HA	1:A:331:ARG:NH2	2.34	0.43
1:A:531:LYS:HD2	1:E:133:PRO:HB3	2.01	0.43
1:C:281:ASN:HB2	1:C:284:GLN:CD	2.43	0.43
1:G:936:LEU:HG	1:G:936:LEU:O	2.19	0.43
1:A:634:THR:O	1:A:638:LEU:HG	2.18	0.43
1:C:72:ALA:O	1:C:76:ILE:HG13	2.18	0.43
1:C:405:ASP:O	1:C:408:MET:N	2.40	0.43
1:C:635:ILE:HD13	1:C:635:ILE:HA	1.93	0.43
1:G:309:GLU:CD	1:G:545:THR:HG22	2.44	0.43
1:A:833:SER:N	2:B:6:DA:H61	2.17	0.43
1:A:842:ASP:HB2	1:A:843:THR:H	1.70	0.43
1:C:165:LEU:HD12	1:C:165:LEU:HA	1.67	0.43
1:E:300:LEU:HD23	1:E:300:LEU:C	2.44	0.43
1:E:440:LEU:HD12	1:E:440:LEU:HA	1.89	0.43
1:E:677:LEU:HD23	1:E:740:LEU:HD22	2.00	0.43
1:G:493:LEU:HD23	1:G:493:LEU:HA	1.89	0.43
1:G:694:GLU:HG2	1:G:701:ARG:NH2	2.33	0.43
1:G:916:GLN:OE1	1:G:935:LEU:HA	2.18	0.43
1:A:55:PRO:HD2	1:A:327:GLY:O	2.19	0.43
1:A:202:PRO:O	1:A:205:SER:OG	2.27	0.43
1:A:367:LEU:HB3	1:A:401:PHE:HB3	2.01	0.43
1:A:908:LEU:O	1:A:911:LEU:HB2	2.19	0.43
1:C:223:PHE:CD1	1:C:254:LEU:HD21	2.54	0.43
1:C:263:ILE:HD11	1:C:365:SER:CB	2.49	0.43
1:E:48:LEU:HD12	1:E:52:TYR:CB	2.48	0.43
1:E:333:LEU:HD12	1:E:344:MET:HG3	2.01	0.43
1:E:528:ARG:HH21	1:E:528:ARG:HB3	1.84	0.43
1:E:571:LEU:HD13	1:E:602:LEU:HD21	2.00	0.43
1:C:270:PHE:C	1:C:270:PHE:HD1	2.27	0.42
1:C:550:PRO:HG3	1:C:756:GLN:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:739:LEU:HD23	1:C:739:LEU:HA	1.77	0.42
1:C:842:ASP:OD1	1:C:845:GLY:HA2	2.19	0.42
1:E:458:PRO:O	1:E:462:VAL:HG23	2.19	0.42
1:E:785:MET:HE3	1:E:785:MET:HB2	1.77	0.42
1:G:495:LYS:O	1:G:499:GLU:HG3	2.18	0.42
1:G:571:LEU:HD11	1:G:598:VAL:HG22	2.01	0.42
1:A:145:MET:CE	1:A:146:LEU:HD13	2.46	0.42
1:A:438:LEU:HD23	1:A:438:LEU:HA	1.80	0.42
1:A:456:VAL:O	1:A:456:VAL:HG23	2.20	0.42
1:C:49:TRP:HA	1:C:53:LEU:HD13	2.01	0.42
1:C:54:SER:HB3	1:C:329:PRO:HD2	2.00	0.42
1:C:126:ALA:O	1:C:129:SER:HB2	2.18	0.42
1:C:141:LEU:HA	1:C:141:LEU:HD23	1.63	0.42
1:C:828:ARG:HG3	2:D:5:DA:N3	2.34	0.42
1:G:556:VAL:HG21	1:G:711:VAL:HG13	2.01	0.42
1:G:828:ARG:HB2	2:H:5:DA:C2	2.53	0.42
1:A:635:ILE:HD13	1:A:635:ILE:HA	1.91	0.42
1:C:827:THR:C	1:C:828:ARG:HG2	2.44	0.42
1:E:170:PHE:HB3	1:E:179:ARG:NH2	2.34	0.42
1:E:466:GLN:NE2	1:E:800:ILE:O	2.46	0.42
1:G:32:TYR:HA	1:G:33:PRO:HD3	1.74	0.42
1:G:336:PRO:HG3	1:G:452:GLU:HG3	2.00	0.42
1:G:605:TRP:CE3	1:G:606:PHE:HE1	2.37	0.42
1:A:591:THR:HG22	2:B:2:DA:H5"	2.02	0.42
1:A:686:ARG:C	1:A:688:GLY:H	2.26	0.42
1:A:724:ALA:HA	1:A:725:PRO:HD3	1.82	0.42
1:A:789:LEU:HD23	1:A:789:LEU:HA	1.84	0.42
1:A:848:TRP:CD1	1:A:853:CYS:HB3	2.54	0.42
1:C:836:VAL:HB	1:C:914:ILE:HG12	2.01	0.42
1:C:919:THR:OG1	1:C:923:ALA:N	2.39	0.42
1:E:415:LEU:HA	1:E:415:LEU:HD23	1.79	0.42
1:G:554:ARG:NH1	1:G:574:GLU:OE2	2.42	0.42
1:G:828:ARG:HG3	2:H:5:DA:N3	2.35	0.42
1:A:314:ALA:O	1:A:318:VAL:HG23	2.20	0.42
1:C:438:LEU:HD23	1:C:438:LEU:HA	1.86	0.42
1:E:311:LYS:HE3	1:E:311:LYS:HB2	1.86	0.42
1:E:552:GLU:CD	1:E:754:PRO:HB3	2.43	0.42
1:G:588:ILE:HA	1:G:658:ALA:O	2.19	0.42
1:G:674:ILE:CG2	1:G:713:LEU:HD11	2.49	0.42
1:A:598:VAL:HG12	1:A:657:VAL:HG21	2.02	0.42
1:A:762:GLN:O	1:A:763:GLN:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:579:VAL:HG23	1:C:609:LEU:HD11	2.02	0.42
1:C:848:TRP:CG	1:C:853:CYS:HA	2.54	0.42
1:E:87:LYS:HE2	1:E:92:PHE:CZ	2.55	0.42
1:E:251:ILE:O	1:E:254:LEU:HB2	2.20	0.42
1:G:203:THR:O	1:G:207:VAL:HG23	2.20	0.42
1:G:439:ARG:NH1	1:G:439:ARG:HG3	2.35	0.42
1:G:676:ASP:HB3	1:G:731:TRP:CH2	2.54	0.42
1:A:256:ASP:HA	1:A:364:SER:HB2	2.02	0.42
1:A:398:ARG:HG2	1:A:399:ASP:N	2.35	0.42
1:A:828:ARG:HB2	2:B:5:DA:C2	2.54	0.42
1:A:840:TYR:N	1:A:848:TRP:O	2.46	0.42
1:C:46:LEU:O	1:C:49:TRP:HB3	2.19	0.42
1:E:691:TRP:CG	1:E:708:PRO:HB3	2.55	0.42
1:G:146:LEU:HD12	1:G:146:LEU:HA	1.93	0.42
1:A:453:ALA:O	1:A:456:VAL:HG13	2.20	0.42
1:A:567:ARG:HH21	1:A:676:ASP:CG	2.28	0.42
1:A:627:GLN:O	1:A:631:ILE:HG13	2.19	0.42
1:C:881:ILE:HD13	1:C:881:ILE:HG21	1.86	0.42
1:E:49:TRP:HA	1:E:53:LEU:HD13	2.01	0.42
1:G:259:GLY:HA3	1:G:366:THR:HG23	2.02	0.42
1:G:313:GLU:OE2	4:G:1003:ATP:H2'	2.20	0.42
1:G:410:ARG:C	1:G:411:LYS:HG3	2.45	0.42
1:A:27:LEU:O	1:A:28:ARG:HB3	2.19	0.42
1:A:75:CYS:O	1:A:79:TRP:N	2.48	0.42
1:A:83:HIS:CG	1:A:84:ASP:N	2.88	0.42
1:E:613:ALA:C	1:E:652:ARG:HD3	2.42	0.42
1:E:635:ILE:HG22	1:E:668:LEU:HD21	2.01	0.42
1:E:749:ARG:NH1	1:E:771:ASP:OD2	2.48	0.42
1:E:779:GLU:O	1:E:782:MET:N	2.53	0.42
1:C:358:ASN:C	1:C:359:THR:HG1	2.09	0.42
1:E:842:ASP:OD1	1:E:845:GLY:CA	2.65	0.42
1:G:228:LEU:HD13	1:G:228:LEU:HA	1.86	0.42
1:G:309:GLU:OE1	1:G:545:THR:HG22	2.20	0.42
1:G:338:MET:HE2	1:G:371:HIS:ND1	2.35	0.42
1:G:338:MET:HE3	2:H:6:DA:OP2	2.20	0.42
1:G:523:LEU:HD21	1:G:532:VAL:HG13	2.01	0.42
1:G:529:ILE:HD11	1:G:531:LYS:HB2	2.02	0.42
1:G:810:LEU:O	1:G:813:LEU:HB2	2.19	0.42
1:A:219:SER:OG	2:B:11:DA:H2''	2.20	0.41
1:C:266:PRO:HA	1:C:267:PRO:HD3	1.95	0.41
1:E:49:TRP:CZ2	1:E:58:ARG:HG2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:679:PRO:HG3	1:E:739:LEU:HD13	2.00	0.41
1:G:576:THR:O	1:G:579:VAL:HG22	2.20	0.41
1:G:644:ALA:C	1:G:698:ILE:HD11	2.45	0.41
1:A:691:TRP:CZ2	1:A:701:ARG:HD2	2.54	0.41
1:C:79:TRP:CE3	1:C:145:MET:HE1	2.54	0.41
1:C:457:ASP:HB2	1:C:458:PRO:CD	2.50	0.41
1:C:666:LEU:HD23	1:C:666:LEU:HA	1.86	0.41
1:C:836:VAL:HG22	1:C:881:ILE:O	2.20	0.41
1:E:676:ASP:OD1	1:E:676:ASP:N	2.53	0.41
1:E:748:ARG:HA	1:E:748:ARG:HD3	1.84	0.41
1:G:87:LYS:HZ1	2:H:12:DA:P	2.43	0.41
1:G:305:ALA:C	1:G:519:TYR:HE1	2.28	0.41
1:G:310:GLY:HA3	4:G:1003:ATP:N7	2.35	0.41
1:G:376:LEU:HG	1:G:907:TYR:CZ	2.55	0.41
1:G:406:TRP:CE3	1:G:407:LEU:HD22	2.44	0.41
1:G:498:LEU:HD23	1:G:498:LEU:HA	1.95	0.41
1:G:576:THR:HB	1:G:577:PRO:HD3	2.02	0.41
1:A:100:LEU:HD13	1:A:175:TRP:CH2	2.56	0.41
1:A:745:THR:HG21	1:A:774:LEU:HA	2.03	0.41
1:C:482:SER:OG	1:C:483:ALA:N	2.52	0.41
1:G:337:THR:HG22	2:H:4:DA:O3'	2.20	0.41
1:A:269:THR:HG23	1:A:272:GLU:OE1	2.20	0.41
1:A:671:ASP:OD1	1:A:701:ARG:HD3	2.21	0.41
1:C:83:HIS:HD2	1:C:149:HIS:CD2	2.38	0.41
1:C:461:GLN:O	1:C:465:GLU:HG3	2.20	0.41
1:E:16:LEU:HB2	1:E:181:ALA:HB1	2.03	0.41
1:G:549:LYS:HA	1:G:550:PRO:HD2	1.84	0.41
1:C:106:GLU:HG3	1:C:172:SER:HB2	2.01	0.41
1:C:148:GLY:HA3	1:C:153:PHE:CD1	2.55	0.41
1:C:491:ASN:OD1	1:C:513:PRO:HD2	2.21	0.41
1:G:407:LEU:HD23	1:G:407:LEU:H	1.85	0.41
1:G:551:LEU:HD11	1:G:553:VAL:HG13	2.02	0.41
1:G:676:ASP:HB3	1:G:731:TRP:CZ2	2.56	0.41
1:G:853:CYS:SG	1:G:918:VAL:HG11	2.60	0.41
1:A:48:LEU:HD12	1:A:52:TYR:HB2	2.02	0.41
1:C:39:LEU:HD23	1:C:39:LEU:HA	1.87	0.41
1:C:106:GLU:OE2	1:C:179:ARG:NH2	2.50	0.41
1:C:424:ASP:O	1:C:428:MET:HG3	2.20	0.41
1:C:937:ASP:OD2	1:C:940:LYS:N	2.54	0.41
1:E:370:LEU:HD21	1:E:413:GLY:C	2.45	0.41
1:G:249:ARG:C	1:G:251:ILE:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:410:ARG:NH1	2:H:9:DA:P	2.94	0.41
1:G:502:ARG:HG3	1:G:504:ARG:HG3	2.02	0.41
1:G:504:ARG:HG2	1:G:504:ARG:NH1	2.33	0.41
1:G:737:LEU:HD23	1:G:780:ALA:HB1	2.03	0.41
1:A:375:TRP:CZ3	1:A:381:ALA:HB1	2.56	0.41
1:A:474:LEU:O	1:A:475:ASP:HB2	2.20	0.41
2:B:5:DA:C6	2:B:6:DA:C6	3.09	0.41
1:C:832:GLY:HA2	2:D:5:DA:N6	2.28	0.41
1:E:414:LEU:HA	1:E:414:LEU:HD23	1.80	0.41
2:H:4:DA:H2''	2:H:5:DA:H5'	2.03	0.41
1:A:122:TRP:CE3	1:A:123:LEU:HD13	2.56	0.41
1:A:520:PRO:HG3	1:A:545:THR:HG23	2.03	0.41
1:A:673:MET:HE2	1:A:673:MET:HB3	1.74	0.41
1:C:270:PHE:HE2	1:C:284:GLN:HB3	1.85	0.41
1:G:34:LEU:HD23	1:G:88:LEU:HD22	2.02	0.41
1:G:272:GLU:O	1:G:275:PRO:HD3	2.21	0.41
1:G:756:GLN:C	1:G:757:ILE:HD12	2.46	0.41
1:G:836:VAL:HG23	1:G:881:ILE:HG23	2.02	0.41
1:A:375:TRP:CZ2	1:A:408:MET:HG2	2.56	0.41
1:A:450:VAL:HG22	1:A:480:LEU:HD12	2.03	0.41
1:C:263:ILE:HD12	1:C:365:SER:CB	2.51	0.41
1:C:314:ALA:O	1:C:318:VAL:HG23	2.20	0.41
1:G:20:PHE:HA	1:G:93:GLN:OE1	2.21	0.41
1:G:76:ILE:HA	1:G:79:TRP:CE3	2.55	0.41
1:G:471:LEU:HD22	1:G:476:VAL:CG2	2.51	0.41
1:G:519:TYR:HA	1:G:520:PRO:HA	1.86	0.41
1:G:534:ARG:HG3	1:G:535:SER:H	1.85	0.41
1:G:619:LEU:HA	1:G:619:LEU:HD12	1.83	0.41
4:G:1003:ATP:H5'1	4:G:1003:ATP:C8	2.56	0.41
1:A:65:MET:HE3	1:A:79:TRP:CH2	2.56	0.41
1:C:156:HIS:HA	1:C:157:PRO:HD3	1.90	0.41
1:E:265:VAL:HA	1:E:266:PRO:HD3	1.76	0.41
1:G:16:LEU:HD21	1:G:35:VAL:HG11	2.03	0.41
1:G:78:PHE:CE1	1:G:82:LEU:HD11	2.56	0.41
1:G:632:THR:O	1:G:636:VAL:HG22	2.20	0.41
1:G:680:VAL:O	1:G:684:LEU:HD22	2.21	0.41
1:G:772:ASP:OD1	1:G:772:ASP:N	2.54	0.41
1:A:255:LEU:HD23	1:A:255:LEU:HA	1.83	0.40
1:A:291:LEU:HD12	1:A:291:LEU:HA	1.91	0.40
1:A:334:ALA:HB1	1:A:423:ILE:HA	2.04	0.40
1:E:187:PHE:CE1	1:E:193:PRO:HD2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:578:LEU:CD1	1:E:583:GLY:CA	2.99	0.40
1:G:39:LEU:HD23	1:G:39:LEU:HA	1.78	0.40
1:G:345:HIS:CD2	1:G:367:LEU:HD12	2.57	0.40
1:A:28:ARG:HD3	1:A:28:ARG:C	2.37	0.40
1:A:454:HIS:HB3	1:A:482:SER:OG	2.22	0.40
1:C:838:CYS:HA	1:C:914:ILE:O	2.21	0.40
1:E:459:TYR:CG	1:E:829:PHE:HB2	2.55	0.40
1:E:742:ARG:HH11	1:E:742:ARG:HD2	1.71	0.40
1:G:407:LEU:CD1	1:G:416:ALA:HB2	2.50	0.40
1:A:67:THR:OG1	1:A:71:HIS:ND1	2.41	0.40
1:A:150:HIS:ND1	2:B:11:DA:H5'	2.37	0.40
1:A:439:ARG:HG3	1:A:439:ARG:NH1	2.35	0.40
1:C:49:TRP:CH2	1:C:58:ARG:HG2	2.57	0.40
1:C:454:HIS:HB3	1:C:482:SER:OG	2.21	0.40
1:E:172:SER:HA	1:E:173:PRO:HD3	1.84	0.40
1:E:443:LEU:HD12	1:E:443:LEU:HA	1.90	0.40
1:E:583:GLY:O	1:E:653:GLY:HA2	2.21	0.40
1:G:351:TYR:O	1:G:355:ARG:HB3	2.20	0.40
1:G:660:GLN:HB3	1:G:663:GLU:OE1	2.21	0.40
1:G:699:ILE:O	1:G:699:ILE:HG13	2.21	0.40
1:E:687:ALA:C	1:E:689:ARG:N	2.79	0.40
1:E:691:TRP:CE3	1:E:708:PRO:HD3	2.56	0.40
1:G:217:LEU:HA	1:G:217:LEU:HD12	1.83	0.40
1:G:580:LYS:N	1:G:580:LYS:CD	2.73	0.40
1:G:937:ASP:HA	1:G:938:PRO:HD2	1.91	0.40
1:A:156:HIS:O	1:A:157:PRO:C	2.65	0.40
1:A:439:ARG:HG3	1:A:439:ARG:HH11	1.87	0.40
1:C:37:HIS:CE1	1:C:215:ASP:OD1	2.74	0.40
1:C:259:GLY:HA3	1:C:366:THR:CG2	2.51	0.40
1:C:265:VAL:HA	1:C:266:PRO:HD3	1.86	0.40
1:C:275:PRO:CD	1:C:354:TYR:CZ	3.04	0.40
1:C:451:ASP:HA	1:C:481:LEU:HB2	2.03	0.40
1:C:842:ASP:O	1:C:845:GLY:CA	2.70	0.40
1:E:24:GLU:OE1	1:E:25:ARG:HG2	2.21	0.40
1:E:405:ASP:O	1:E:408:MET:HB2	2.21	0.40
1:E:742:ARG:NH1	1:E:784:ARG:HH11	2.19	0.40
1:G:306:PRO:HD2	1:G:309:GLU:HG3	2.02	0.40
1:G:377:ASN:HA	1:G:378:PRO:HD3	1.84	0.40
1:G:676:ASP:OD1	1:G:676:ASP:N	2.54	0.40
1:G:841:VAL:O	1:G:918:VAL:HG12	2.21	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	889/964 (92%)	825 (93%)	60 (7%)	4 (0%)	30	59
1	C	887/964 (92%)	803 (90%)	79 (9%)	5 (1%)	21	51
1	E	891/964 (92%)	844 (95%)	46 (5%)	1 (0%)	48	76
1	G	869/964 (90%)	792 (91%)	75 (9%)	2 (0%)	43	71
All	All	3536/3856 (92%)	3264 (92%)	260 (7%)	12 (0%)	36	65

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	703	GLN
1	A	749	ARG
1	C	374	ALA
1	C	660	GLN
1	G	752	GLY
1	C	540	PRO
1	G	250	ARG
1	A	903	ARG
1	A	687	ALA
1	E	660	GLN
1	C	543	ILE
1	C	550	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	746/796 (94%)	643 (86%)	103 (14%)	3	15
1	C	740/796 (93%)	632 (85%)	108 (15%)	3	14
1	E	741/796 (93%)	647 (87%)	94 (13%)	4	18
1	G	734/796 (92%)	621 (85%)	113 (15%)	2	12
All	All	2961/3184 (93%)	2543 (86%)	418 (14%)	3	15

All (418) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
1	A	28	ARG
1	A	30	LYS
1	A	35	VAL
1	A	48	LEU
1	A	53	LEU
1	A	58	ARG
1	A	85	ILE
1	A	88	LEU
1	A	98	ILE
1	A	101	SER
1	A	121	LYS
1	A	123	LEU
1	A	127	LEU
1	A	130	LEU
1	A	146	LEU
1	A	165	LEU
1	A	186	VAL
1	A	198	MET
1	A	217	LEU
1	A	228	LEU
1	A	238	SER
1	A	251	ILE
1	A	254	LEU
1	A	264	THR
1	A	265	VAL
1	A	271	THR
1	A	279	LYS
1	A	283	LEU
1	A	293	CYS
1	A	333	LEU
1	A	358	ASN
1	A	359	THR

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Mol	Chain	Res	Type
1	A	361	LEU
1	A	366	THR
1	A	367	LEU
1	A	370	LEU
1	A	375	TRP
1	A	420	VAL
1	A	431	LEU
1	A	432	ARG
1	A	438	LEU
1	A	440	LEU
1	A	443	LEU
1	A	446	LYS
1	A	448	VAL
1	A	450	VAL
1	A	456	VAL
1	A	458	PRO
1	A	464	LEU
1	A	473	THR
1	A	474	LEU
1	A	476	VAL
1	A	480	LEU
1	A	481	LEU
1	A	488	SER
1	A	504	ARG
1	A	518	SER
1	A	523	LEU
1	A	528	ARG
1	A	541	LEU
1	A	545	THR
1	A	548	ARG
1	A	551	LEU
1	A	553	VAL
1	A	560	VAL
1	A	565	LEU
1	A	570	VAL
1	A	576	THR
1	A	579	VAL
1	A	581	GLN
1	A	601	LEU
1	A	602	LEU
1	A	634	THR
1	A	635	ILE

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Mol	Chain	Res	Type
1	A	673	MET
1	A	680	VAL
1	A	681	SER
1	A	683	LEU
1	A	690	CYS
1	A	696	LEU
1	A	714	THR
1	A	730	SER
1	A	734	VAL
1	A	739	LEU
1	A	765	VAL
1	A	789	LEU
1	A	792	ARG
1	A	804	ASP
1	A	816	PHE
1	A	817	SER
1	A	818	PHE
1	A	833	SER
1	A	836	VAL
1	A	842	ASP
1	A	843	THR
1	A	849	LEU
1	A	852	GLU
1	A	892	LEU
1	A	894	GLU
1	A	908	LEU
1	A	928	GLU
1	A	939	CYS
1	C	16	LEU
1	C	24	GLU
1	C	25	ARG
1	C	35	VAL
1	C	48	LEU
1	C	54	SER
1	C	70	GLU
1	C	88	LEU
1	C	91	GLU
1	C	113	ARG
1	C	123	LEU
1	C	127	LEU
1	C	130	LEU
1	C	134	ASN

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Mol	Chain	Res	Type
1	C	137	LEU
1	C	139	THR
1	C	142	VAL
1	C	145	MET
1	C	152	THR
1	C	158	SER
1	C	186	VAL
1	C	202	PRO
1	C	217	LEU
1	C	251	ILE
1	C	253	SER
1	C	254	LEU
1	C	265	VAL
1	C	271	THR
1	C	278	SER
1	C	279	LYS
1	C	281	ASN
1	C	283	LEU
1	C	311	LYS
1	C	333	LEU
1	C	355	ARG
1	C	356	VAL
1	C	358	ASN
1	C	366	THR
1	C	367	LEU
1	C	407	LEU
1	C	411	LYS
1	C	414	LEU
1	C	420	VAL
1	C	431	LEU
1	C	438	LEU
1	C	439	ARG
1	C	440	LEU
1	C	443	LEU
1	C	448	VAL
1	C	450	VAL
1	C	452	GLU
1	C	464	LEU
1	C	473	THR
1	C	474	LEU
1	C	476	VAL
1	C	478	VAL

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Mol	Chain	Res	Type
1	C	480	LEU
1	C	481	LEU
1	C	492	SER
1	C	494	VAL
1	C	506	TRP
1	C	518	SER
1	C	538	VAL
1	C	541	LEU
1	C	567	ARG
1	C	570	VAL
1	C	574	GLU
1	C	576	THR
1	C	579	VAL
1	C	581	GLN
1	C	590	THR
1	C	602	LEU
1	C	609	LEU
1	C	629	THR
1	C	630	GLU
1	C	651	THR
1	C	655	VAL
1	C	662	VAL
1	C	680	VAL
1	C	683	LEU
1	C	686	ARG
1	C	692	ARG
1	C	703	GLN
1	C	729	ARG
1	C	734	VAL
1	C	739	LEU
1	C	745	THR
1	C	763	GLN
1	C	768	VAL
1	C	774	LEU
1	C	824	VAL
1	C	827	THR
1	C	833	SER
1	C	838	CYS
1	C	855	VAL
1	C	860	GLN
1	C	876	LEU
1	C	879	ARG

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Mol	Chain	Res	Type
1	C	881	ILE
1	C	893	THR
1	C	910	ASP
1	C	919	THR
1	C	921	GLU
1	C	924	VAL
1	C	925	LEU
1	C	932	ARG
1	C	939	CYS
1	C	944	PHE
1	E	16	LEU
1	E	35	VAL
1	E	48	LEU
1	E	67	THR
1	E	88	LEU
1	E	113	ARG
1	E	121	LYS
1	E	123	LEU
1	E	127	LEU
1	E	129	SER
1	E	137	LEU
1	E	138	VAL
1	E	146	LEU
1	E	165	LEU
1	E	172	SER
1	E	186	VAL
1	E	194	THR
1	E	203	THR
1	E	206	VAL
1	E	217	LEU
1	E	224	LEU
1	E	228	LEU
1	E	230	SER
1	E	246	THR
1	E	248	LEU
1	E	250	ARG
1	E	251	ILE
1	E	254	LEU
1	E	264	THR
1	E	265	VAL
1	E	271	THR
1	E	273	SER

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Mol	Chain	Res	Type
1	E	279	LYS
1	E	283	LEU
1	E	291	LEU
1	E	296	THR
1	E	307	MET
1	E	353	ARG
1	E	355	ARG
1	E	356	VAL
1	E	366	THR
1	E	367	LEU
1	E	375	TRP
1	E	408	MET
1	E	420	VAL
1	E	431	LEU
1	E	438	LEU
1	E	440	LEU
1	E	443	LEU
1	E	448	VAL
1	E	450	VAL
1	E	452	GLU
1	E	464	LEU
1	E	473	THR
1	E	474	LEU
1	E	476	VAL
1	E	481	LEU
1	E	494	VAL
1	E	508	ARG
1	E	510	GLU
1	E	517	VAL
1	E	518	SER
1	E	528	ARG
1	E	553	VAL
1	E	570	VAL
1	E	574	GLU
1	E	581	GLN
1	E	584	CYS
1	E	603	SER
1	E	608	THR
1	E	615	ASP
1	E	616	LEU
1	E	628	ARG
1	E	634	THR

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Mol	Chain	Res	Type
1	E	636	VAL
1	E	652	ARG
1	E	673	MET
1	E	676	ASP
1	E	684	LEU
1	E	686	ARG
1	E	694	GLU
1	E	698	ILE
1	E	729	ARG
1	E	734	VAL
1	E	739	LEU
1	E	815	GLU
1	E	836	VAL
1	E	843	THR
1	E	849	LEU
1	E	865	GLU
1	E	881	ILE
1	E	892	LEU
1	E	924	VAL
1	E	929	THR
1	G	16	LEU
1	G	35	VAL
1	G	48	LEU
1	G	53	LEU
1	G	57	LEU
1	G	58	ARG
1	G	63	SER
1	G	70	GLU
1	G	75	CYS
1	G	88	LEU
1	G	96	ILE
1	G	113	ARG
1	G	119	THR
1	G	121	LYS
1	G	123	LEU
1	G	127	LEU
1	G	137	LEU
1	G	142	VAL
1	G	146	LEU
1	G	152	THR
1	G	158	SER
1	G	161	SER

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Mol	Chain	Res	Type
1	G	165	LEU
1	G	186	VAL
1	G	190	THR
1	G	200	ASP
1	G	206	VAL
1	G	217	LEU
1	G	228	LEU
1	G	246	THR
1	G	249	ARG
1	G	254	LEU
1	G	264	THR
1	G	271	THR
1	G	281	ASN
1	G	283	LEU
1	G	287	LEU
1	G	291	LEU
1	G	296	THR
1	G	300	LEU
1	G	311	LYS
1	G	338	MET
1	G	340	THR
1	G	366	THR
1	G	367	LEU
1	G	370	LEU
1	G	373	MET
1	G	375	TRP
1	G	407	LEU
1	G	408	MET
1	G	410	ARG
1	G	420	VAL
1	G	431	LEU
1	G	438	LEU
1	G	440	LEU
1	G	443	LEU
1	G	448	VAL
1	G	450	VAL
1	G	464	LEU
1	G	473	THR
1	G	474	LEU
1	G	476	VAL
1	G	481	LEU
1	G	494	VAL

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Mol	Chain	Res	Type
1	G	504	ARG
1	G	505	ARG
1	G	506	TRP
1	G	507	ASN
1	G	509	SER
1	G	510	GLU
1	G	518	SER
1	G	528	ARG
1	G	529	ILE
1	G	534	ARG
1	G	541	LEU
1	G	548	ARG
1	G	551	LEU
1	G	553	VAL
1	G	568	SER
1	G	580	LYS
1	G	591	THR
1	G	598	VAL
1	G	635	ILE
1	G	672	LEU
1	G	683	LEU
1	G	684	LEU
1	G	686	ARG
1	G	690	CYS
1	G	694	GLU
1	G	698	ILE
1	G	699	ILE
1	G	709	GLU
1	G	718	ASN
1	G	734	VAL
1	G	739	LEU
1	G	745	THR
1	G	755	VAL
1	G	764	LEU
1	G	779	GLU
1	G	782	MET
1	G	789	LEU
1	G	804	ASP
1	G	849	LEU
1	G	855	VAL
1	G	856	GLU
1	G	869	THR

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Mol	Chain	Res	Type
1	G	881	ILE
1	G	895	ASP
1	G	898	PRO
1	G	924	VAL
1	G	925	LEU
1	G	939	CYS
1	G	943	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	664	GLN
1	A	823	HIS
1	A	891	GLN
1	C	358	ASN
1	C	486	HIS
1	C	645	GLN
1	C	763	GLN
1	C	809	ASN
1	E	94	GLN
1	E	112	GLN
1	E	154	HIS
1	E	160	GLN
1	E	243	HIS
1	E	290	HIS
1	E	751	ASN
1	E	811	ASN
1	E	846	ASN
1	E	896	ASN
1	G	435	HIS
1	G	791	GLN
1	G	860	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 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$
4	ATP	C	1003	-	32,33,33	1.32	5 (15%)	48,52,52	1.79	10 (20%)
4	ATP	A	1003	-	32,33,33	1.34	5 (15%)	48,52,52	1.71	9 (18%)
4	ATP	G	1003	-	32,33,33	1.35	6 (18%)	48,52,52	1.68	9 (18%)
4	ATP	E	1003	-	32,33,33	1.40	4 (12%)	48,52,52	1.73	12 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	C	1003	-	-	4/22/38/38	0/3/3/3
4	ATP	A	1003	-	-	7/22/38/38	0/3/3/3
4	ATP	G	1003	-	-	9/22/38/38	0/3/3/3
4	ATP	E	1003	-	-	7/22/38/38	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1003	ATP	C5-C4	4.15	1.46	1.39
4	G	1003	ATP	C5-C4	4.05	1.46	1.39
4	A	1003	ATP	C5-C4	3.90	1.46	1.39
4	E	1003	ATP	C5-C4	3.68	1.45	1.39
4	E	1003	ATP	C5-N7	-3.27	1.33	1.39
4	E	1003	ATP	C4-N9	-2.98	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1003	ATP	C5-N7	-2.95	1.33	1.39
4	A	1003	ATP	C5-N7	-2.78	1.34	1.39
4	C	1003	ATP	C5-N7	-2.74	1.34	1.39
4	G	1003	ATP	C4-N9	-2.42	1.32	1.37
4	E	1003	ATP	C8-N9	-2.32	1.33	1.37
4	A	1003	ATP	C4-N9	-2.30	1.32	1.37
4	C	1003	ATP	C4-N9	-2.30	1.32	1.37
4	A	1003	ATP	C5-C6	2.23	1.47	1.41
4	G	1003	ATP	C5-C6	2.14	1.46	1.41
4	A	1003	ATP	C8-N7	2.13	1.35	1.31
4	C	1003	ATP	C5-C6	2.12	1.46	1.41
4	G	1003	ATP	C8-N9	-2.08	1.34	1.37
4	C	1003	ATP	C8-N7	2.06	1.35	1.31
4	G	1003	ATP	C8-N7	2.02	1.35	1.31

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1003	ATP	C5-C4-N3	-5.94	118.54	126.72
4	G	1003	ATP	C5-C4-N3	-5.58	119.03	126.72
4	C	1003	ATP	C5-C4-N3	-5.29	119.43	126.72
4	E	1003	ATP	C5-C4-N3	-4.99	119.85	126.72
4	C	1003	ATP	N3-C4-N9	4.56	134.92	127.17
4	A	1003	ATP	N3-C4-N9	4.40	134.65	127.17
4	G	1003	ATP	N3-C4-N9	4.31	134.50	127.17
4	C	1003	ATP	N3-C2-N1	-4.03	122.49	128.58
4	E	1003	ATP	N3-C4-N9	3.93	133.85	127.17
4	C	1003	ATP	C2-N3-C4	3.76	121.01	111.83
4	A	1003	ATP	C2-N3-C4	3.62	120.66	111.83
4	E	1003	ATP	N3-C2-N1	-3.54	123.22	128.58
4	A	1003	ATP	C4-C5-N7	-3.49	106.59	110.58
4	E	1003	ATP	C2-N3-C4	3.42	120.18	111.83
4	G	1003	ATP	C2-N3-C4	3.40	120.13	111.83
4	G	1003	ATP	C4-C5-N7	-3.36	106.73	110.58
4	E	1003	ATP	C4-C5-N7	-3.19	106.93	110.58
4	C	1003	ATP	C4-N9-C8	3.16	109.06	105.74
4	G	1003	ATP	N3-C2-N1	-3.05	123.97	128.58
4	E	1003	ATP	C4-N9-C8	2.97	108.86	105.74
4	A	1003	ATP	N3-C2-N1	-2.93	124.15	128.58
4	C	1003	ATP	C4-C5-N7	-2.79	107.39	110.58
4	G	1003	ATP	C4-N9-C8	2.51	108.37	105.74
4	A	1003	ATP	C5-N7-C8	2.47	107.33	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1003	ATP	C5-N7-C8	2.40	107.22	103.45
4	E	1003	ATP	C5-N7-C8	2.34	107.13	103.45
4	A	1003	ATP	C4-N9-C8	2.30	108.15	105.74
4	C	1003	ATP	C5-N7-C8	2.24	106.97	103.45
4	C	1003	ATP	C2-N1-C6	2.23	122.39	118.73
4	E	1003	ATP	N9-C8-N7	-2.23	110.78	113.94
4	E	1003	ATP	C2-N1-C6	2.16	122.29	118.73
4	C	1003	ATP	O3'-C3'-C2'	-2.15	104.93	111.82
4	A	1003	ATP	C6-C5-N7	2.13	136.20	132.09
4	E	1003	ATP	O3G-PG-O2G	2.13	115.79	107.80
4	C	1003	ATP	N9-C8-N7	-2.12	110.93	113.94
4	G	1003	ATP	O3'-C3'-C2'	-2.10	105.10	111.82
4	E	1003	ATP	C6-C5-N7	2.06	136.06	132.09
4	E	1003	ATP	O3'-C3'-C2'	-2.04	105.28	111.82
4	G	1003	ATP	C2-N1-C6	2.04	122.08	118.73
4	A	1003	ATP	O3G-PG-O2G	2.01	115.33	107.80

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1003	ATP	C5'-O5'-PA-O3A
4	E	1003	ATP	PB-O3B-PG-O2G
4	E	1003	ATP	C5'-O5'-PA-O1A
4	G	1003	ATP	C5'-O5'-PA-O2A
4	G	1003	ATP	C5'-O5'-PA-O3A
4	C	1003	ATP	O4'-C1'-N9-C8
4	C	1003	ATP	O4'-C1'-N9-C4
4	G	1003	ATP	C3'-C4'-C5'-O5'
4	E	1003	ATP	C3'-C4'-C5'-O5'
4	G	1003	ATP	O4'-C4'-C5'-O5'
4	E	1003	ATP	O4'-C4'-C5'-O5'
4	A	1003	ATP	C2'-C1'-N9-C8
4	G	1003	ATP	PB-O3A-PA-O1A
4	A	1003	ATP	C5'-O5'-PA-O1A
4	A	1003	ATP	C5'-O5'-PA-O2A
4	A	1003	ATP	C5'-O5'-PA-O3A
4	C	1003	ATP	C5'-O5'-PA-O1A
4	E	1003	ATP	C5'-O5'-PA-O2A
4	G	1003	ATP	C5'-O5'-PA-O1A
4	A	1003	ATP	C2'-C1'-N9-C4
4	E	1003	ATP	C2'-C1'-N9-C8

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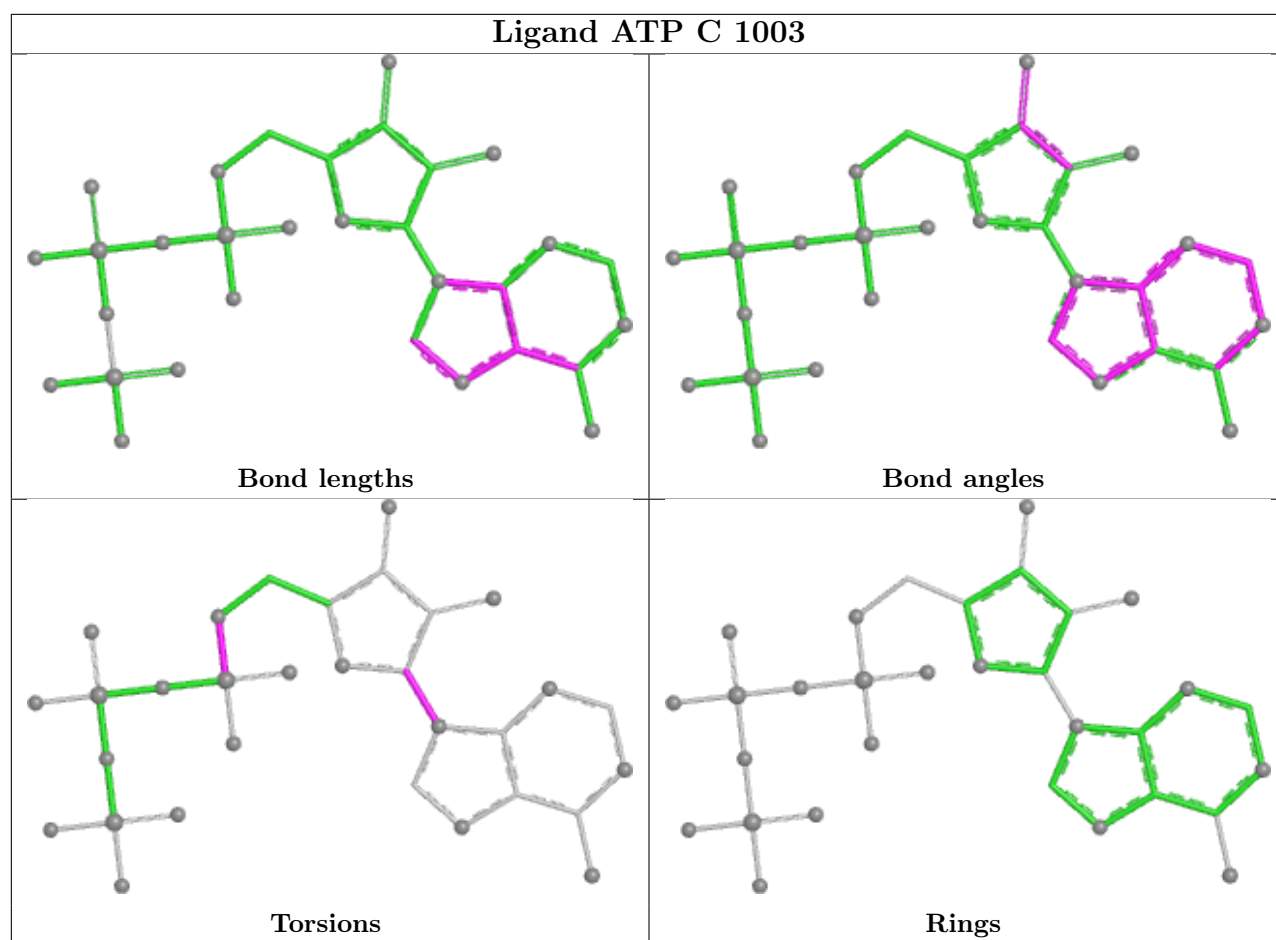
Mol	Chain	Res	Type	Atoms
4	E	1003	ATP	PB-O3B-PG-O3G
4	A	1003	ATP	O4'-C1'-N9-C8
4	A	1003	ATP	PB-O3A-PA-O1A
4	G	1003	ATP	PG-O3B-PB-O1B
4	G	1003	ATP	PB-O3A-PA-O2A
4	G	1003	ATP	C2'-C1'-N9-C8

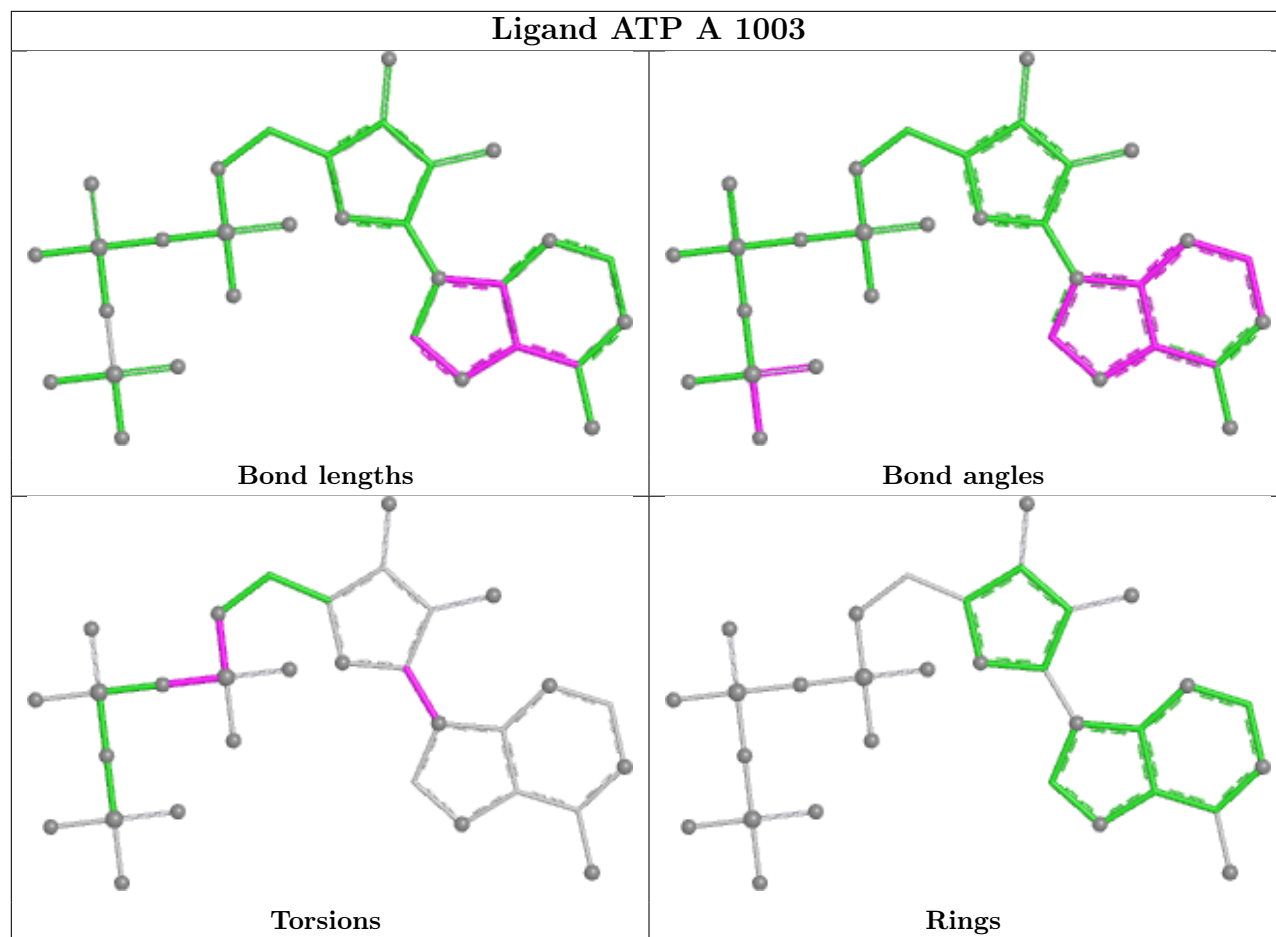
There are no ring outliers.

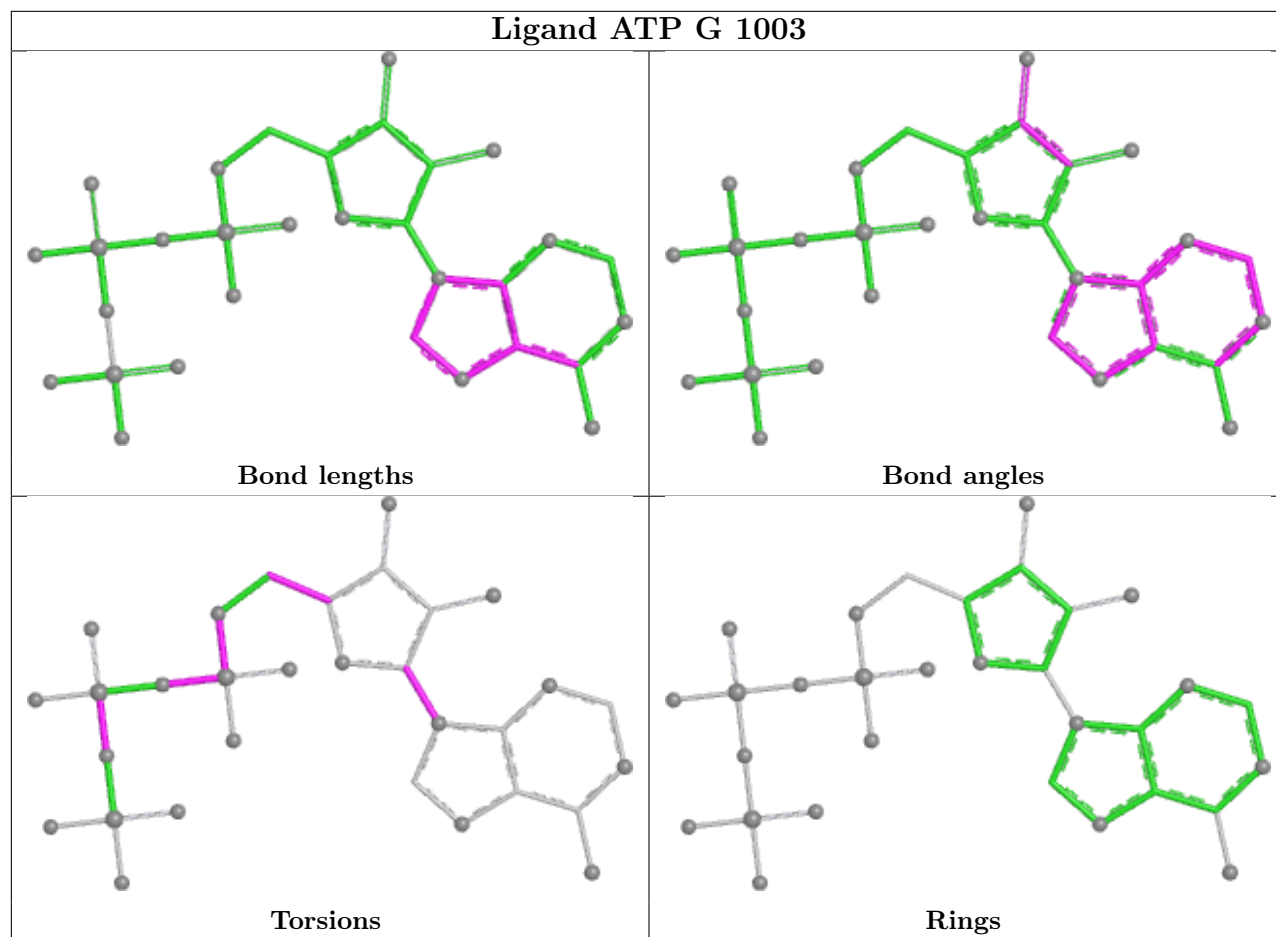
4 monomers are involved in 16 short contacts:

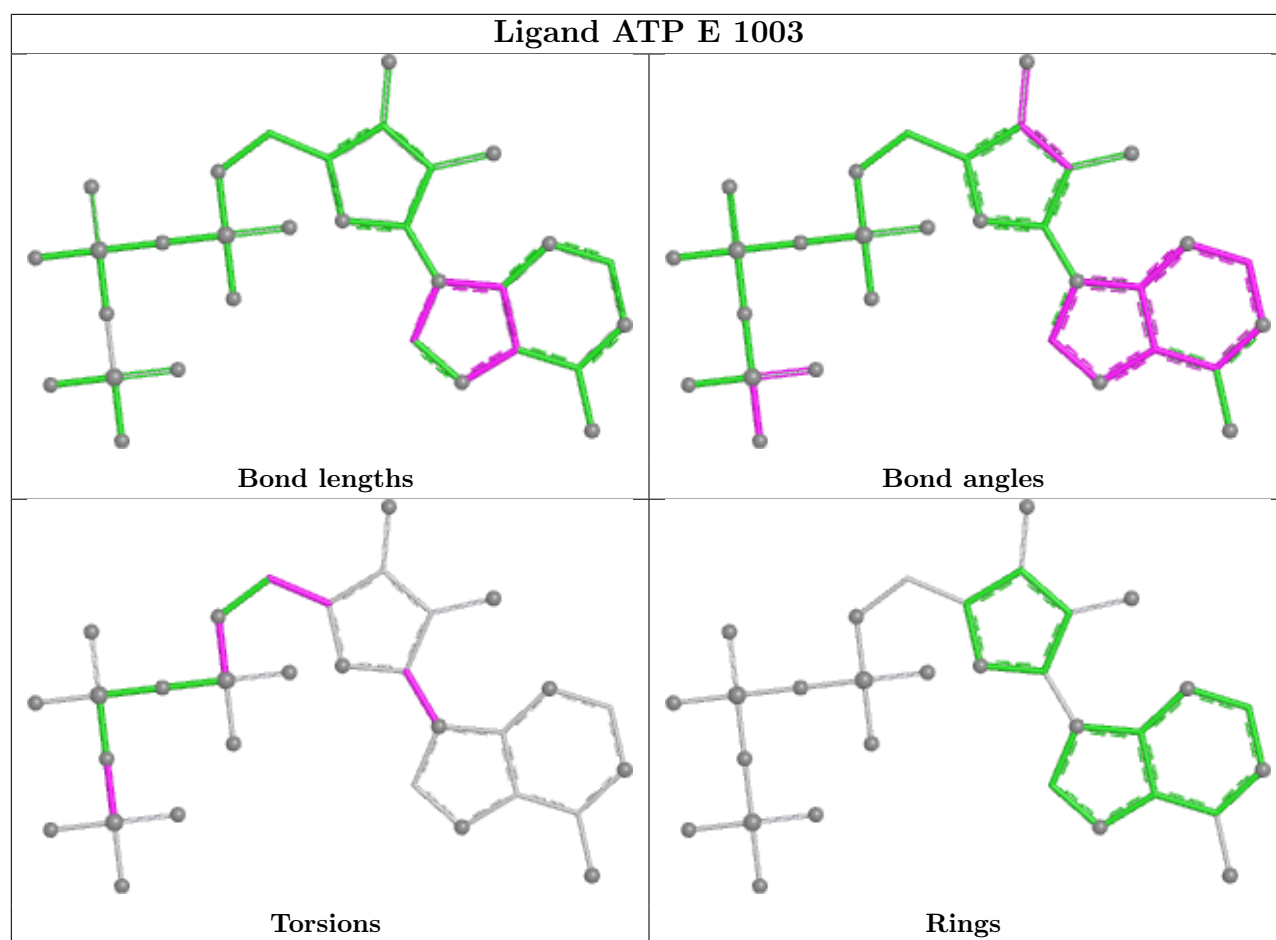
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1003	ATP	6	0
4	A	1003	ATP	1	0
4	G	1003	ATP	7	0
4	E	1003	ATP	2	0

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.









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	903/964 (93%)	-0.57	1 (0%) 92 91	61, 100, 153, 226	0
1	C	899/964 (93%)	-0.45	3 (0%) 90 83	65, 105, 153, 202	0
1	E	901/964 (93%)	-0.58	1 (0%) 92 91	57, 91, 141, 181	0
1	G	887/964 (92%)	-0.46	3 (0%) 90 83	66, 114, 170, 234	0
2	B	11/12 (91%)	-0.38	0 100 100	95, 98, 170, 217	0
2	D	11/12 (91%)	-0.28	0 100 100	91, 106, 184, 194	0
2	F	11/12 (91%)	-0.36	0 100 100	80, 95, 175, 217	0
2	H	11/12 (91%)	-0.42	0 100 100	94, 113, 199, 208	0
All	All	3634/3904 (93%)	-0.51	8 (0%) 91 87	57, 103, 157, 234	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	865	GLU	3.9
1	A	651	THR	2.7
1	E	609	LEU	2.6
1	C	383	ALA	2.4
1	C	364	SER	2.3
1	G	383	ALA	2.2
1	G	668	LEU	2.2
1	G	845	GLY	2.1

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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

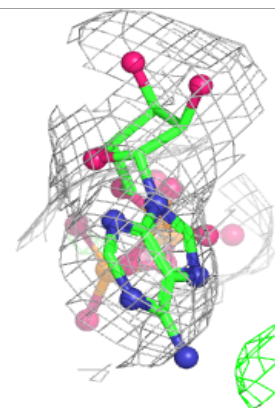
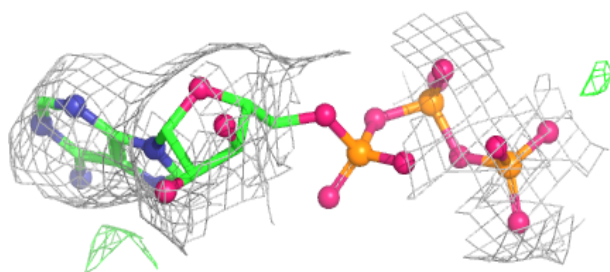
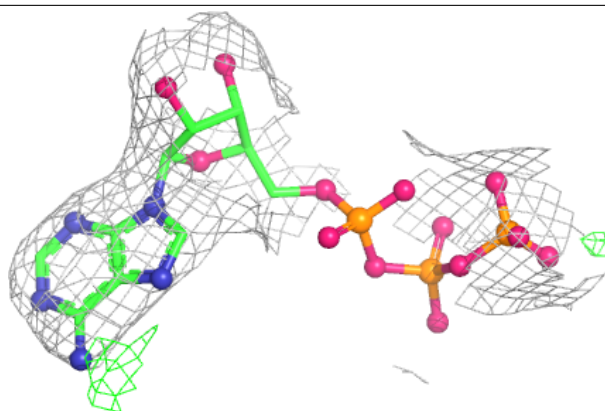
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ATP	G	1003	31/31	0.89	0.08	128,151,159,161	0
4	ATP	C	1003	31/31	0.92	0.07	124,143,160,164	0
4	ATP	A	1003	31/31	0.93	0.08	97,119,131,132	0
4	ATP	E	1003	31/31	0.94	0.07	91,111,120,128	0
3	FE	E	1001	1/1	0.99	0.03	80,80,80,80	0
3	FE	E	1002	1/1	0.99	0.02	70,70,70,70	0
3	FE	A	1001	1/1	0.99	0.06	79,79,79,79	0
3	FE	A	1002	1/1	0.99	0.02	73,73,73,73	0
3	FE	C	1001	1/1	0.99	0.03	77,77,77,77	0
3	FE	C	1002	1/1	0.99	0.03	82,82,82,82	0
3	FE	G	1001	1/1	1.00	0.05	77,77,77,77	0
3	FE	G	1002	1/1	1.00	0.02	79,79,79,79	0

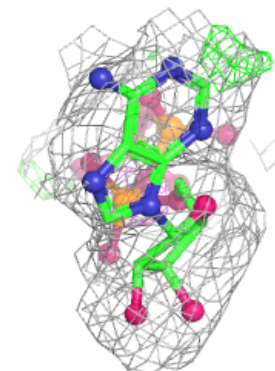
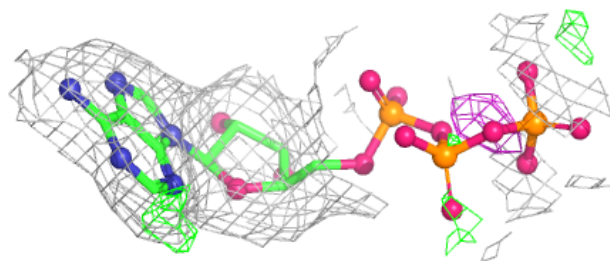
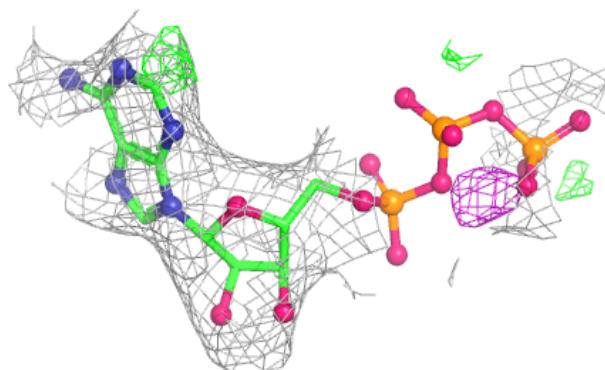
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP G 1003:

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

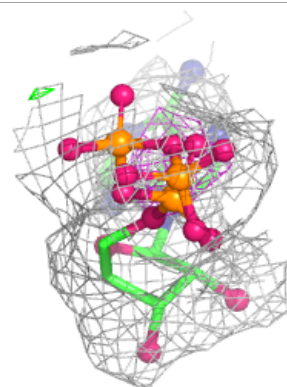
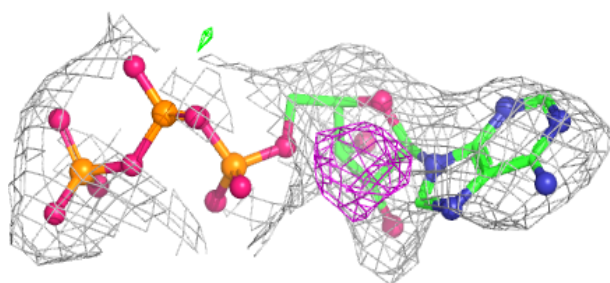
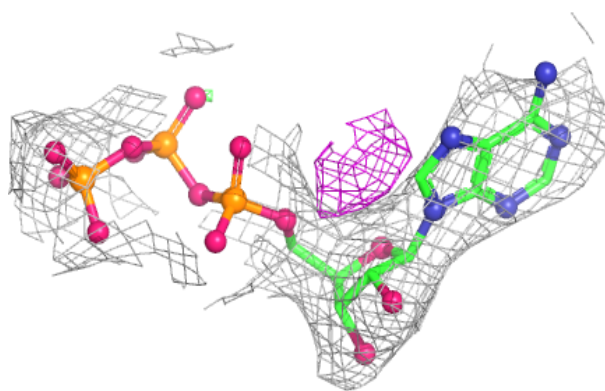
**Electron density around ATP C 1003:**

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

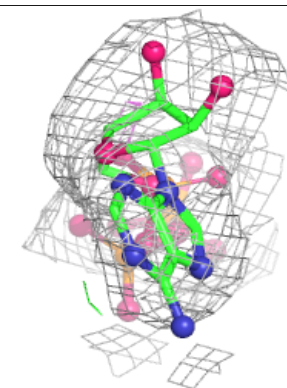
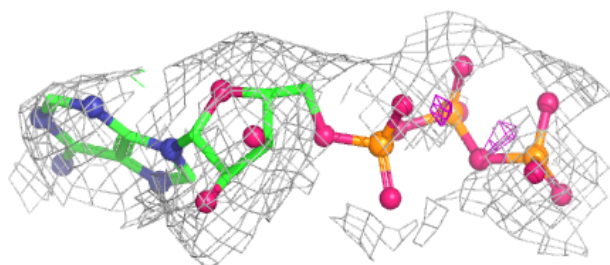


Electron density around ATP A 1003:

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

**Electron density around ATP E 1003:**

$2mF_o-DF_c$ (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.