



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:59 AM UTC

PDB ID : 1Q12 / pdb_00001q12
Title : Crystal Structure of the ATP-bound E. coli MalK
Authors : Chen, J.; Lu, G.; Lin, J.; Davidson, A.L.; Quiocho, F.A.
Deposited on : 2003-07-18
Resolution : 2.60 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

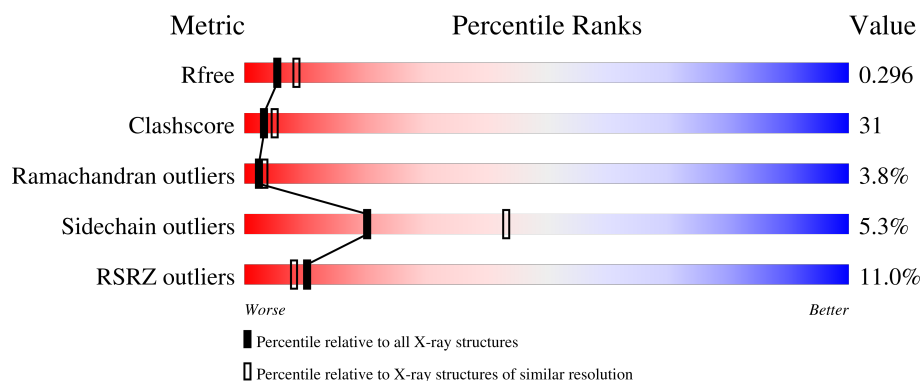
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	381	7% 48% 44% . .
1	B	381	11% 49% 41% 6% . .
1	C	381	8% 49% 43% 5% .
1	D	381	17% 49% 40% 6% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11546 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 Maltose/maltodextrin transport ATP-binding protein malK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	0	0
			2853	1805	511	524	13			
1	B	367	Total	C	N	O	S	0	0	0
			2853	1805	511	524	13			
1	C	367	Total	C	N	O	S	0	0	0
			2853	1805	511	524	13			
1	D	367	Total	C	N	O	S	0	0	0
			2853	1805	511	524	13			

There are 40 discrepancies between the modelled and reference sequences:

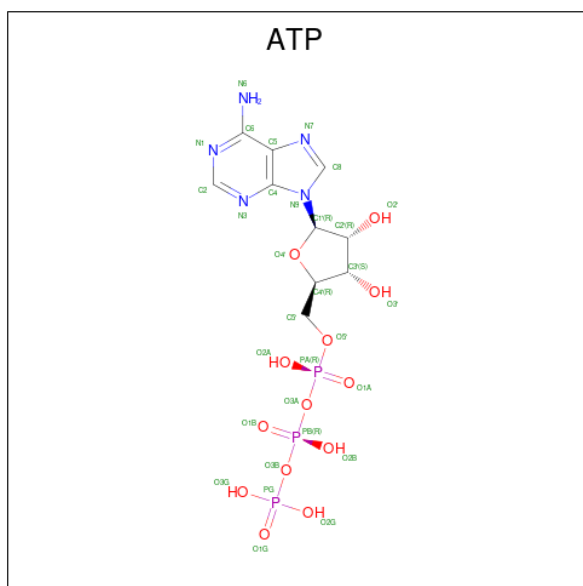
Chain	Residue	Modelled	Actual	Comment	Reference
A	372	ALA	-	expression tag	UNP P68187
A	373	SER	-	expression tag	UNP P68187
A	374	ALA	-	expression tag	UNP P68187
A	375	SER	-	expression tag	UNP P68187
A	376	HIS	-	expression tag	UNP P68187
A	377	HIS	-	expression tag	UNP P68187
A	378	HIS	-	expression tag	UNP P68187
A	379	HIS	-	expression tag	UNP P68187
A	380	HIS	-	expression tag	UNP P68187
A	381	HIS	-	expression tag	UNP P68187
B	372	ALA	-	expression tag	UNP P68187
B	373	SER	-	expression tag	UNP P68187
B	374	ALA	-	expression tag	UNP P68187
B	375	SER	-	expression tag	UNP P68187
B	376	HIS	-	expression tag	UNP P68187
B	377	HIS	-	expression tag	UNP P68187
B	378	HIS	-	expression tag	UNP P68187
B	379	HIS	-	expression tag	UNP P68187
B	380	HIS	-	expression tag	UNP P68187
B	381	HIS	-	expression tag	UNP P68187
C	372	ALA	-	expression tag	UNP P68187

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Chain	Residue	Modelled	Actual	Comment	Reference
C	373	SER	-	expression tag	UNP P68187
C	374	ALA	-	expression tag	UNP P68187
C	375	SER	-	expression tag	UNP P68187
C	376	HIS	-	expression tag	UNP P68187
C	377	HIS	-	expression tag	UNP P68187
C	378	HIS	-	expression tag	UNP P68187
C	379	HIS	-	expression tag	UNP P68187
C	380	HIS	-	expression tag	UNP P68187
C	381	HIS	-	expression tag	UNP P68187
D	372	ALA	-	expression tag	UNP P68187
D	373	SER	-	expression tag	UNP P68187
D	374	ALA	-	expression tag	UNP P68187
D	375	SER	-	expression tag	UNP P68187
D	376	HIS	-	expression tag	UNP P68187
D	377	HIS	-	expression tag	UNP P68187
D	378	HIS	-	expression tag	UNP P68187
D	379	HIS	-	expression tag	UNP P68187
D	380	HIS	-	expression tag	UNP P68187
D	381	HIS	-	expression tag	UNP P68187

- 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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

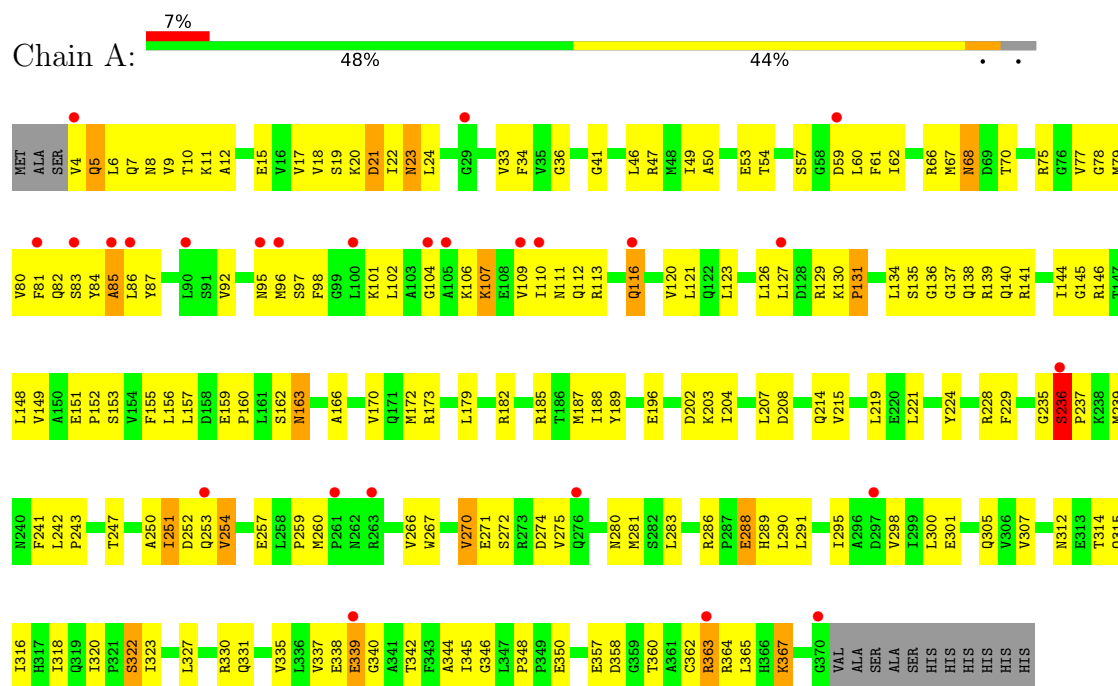
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	9	Total	O	0	0
			9	9		
3	D	1	Total	O	0	0
			1	1		

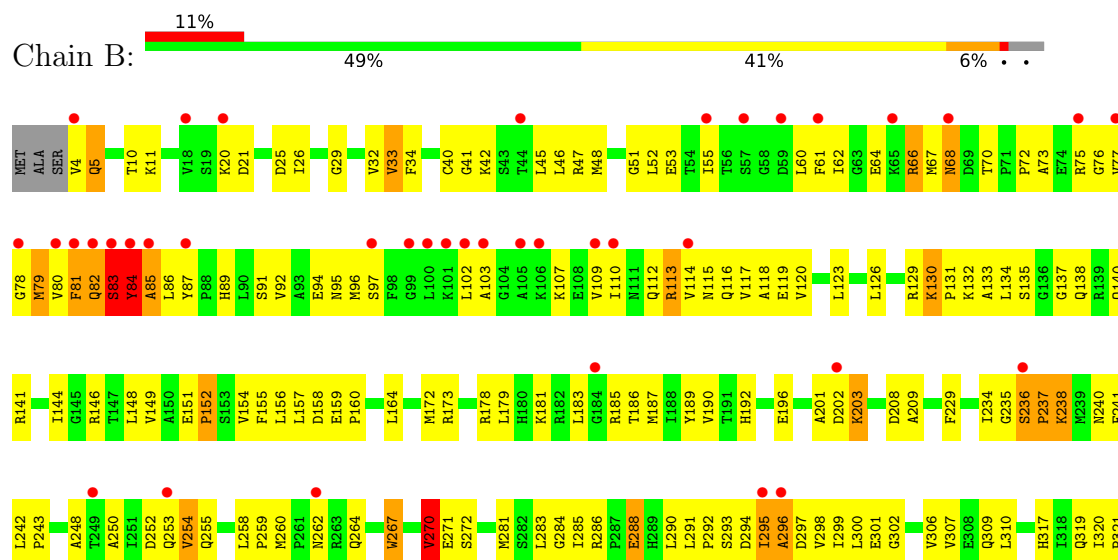
3 Residue-property plots

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: Maltose/maltodextrin transport ATP-binding protein malK

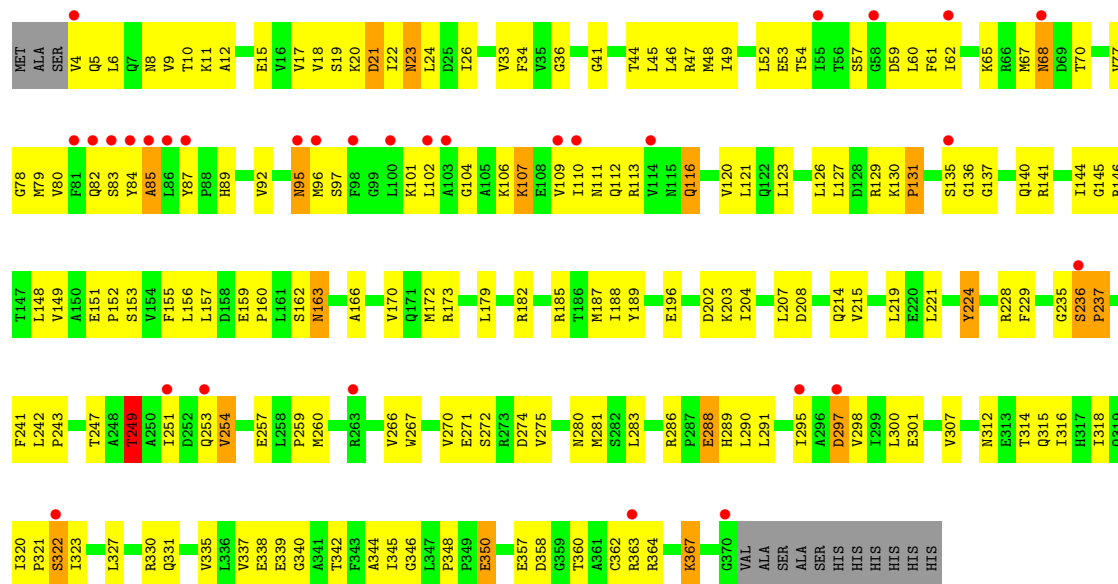


- Molecule 1: Maltose/maltodextrin transport ATP-binding protein malK

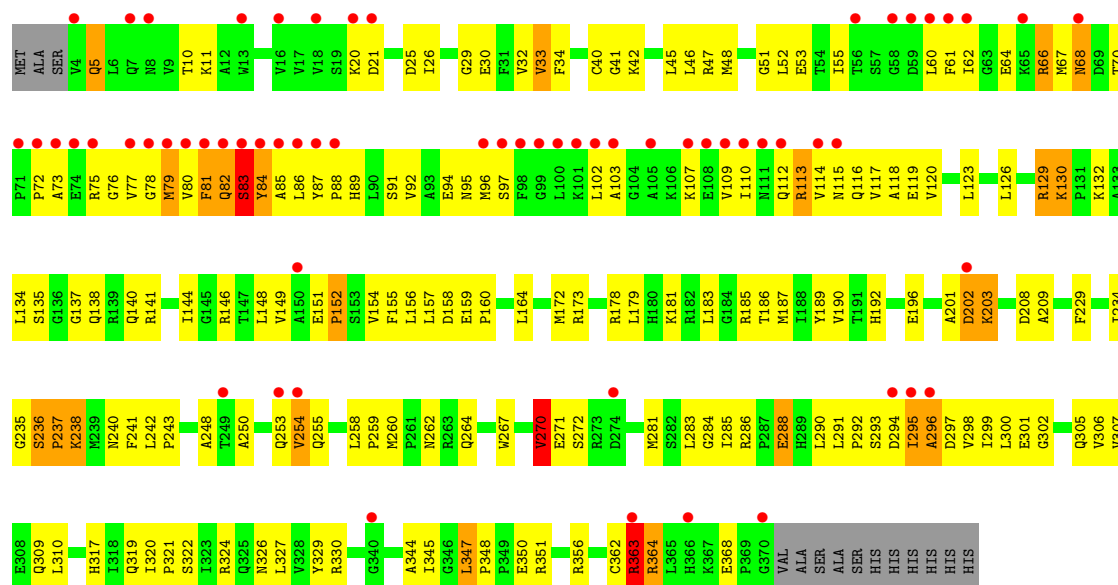




• Molecule 1: Maltose/maltodextrin transport ATP-binding protein malK



• Molecule 1: Maltose/maltodextrin transport ATP-binding protein malK



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	59.88Å 97.28Å 101.86Å 74.59° 82.47° 76.85°	Depositor
Resolution (Å)	14.80 – 2.60 14.80 – 2.60	Depositor EDS
% Data completeness (in resolution range)	86.4 (14.80-2.60) 87.0 (14.80-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.41 (at 2.54Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.258 , 0.286 0.271 , 0.296	Depositor DCC
R_{free} test set	9525 reflections (7.63%)	wwPDB-VP
Wilson B-factor (Å ²)	42.7	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	11546	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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: 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	0/2903	1.05	12/3936 (0.3%)
1	B	0.59	1/2903 (0.0%)	1.06	13/3936 (0.3%)
1	C	0.58	0/2903	1.02	10/3936 (0.3%)
1	D	0.59	0/2903	1.07	16/3936 (0.4%)
All	All	0.59	1/11612 (0.0%)	1.05	51/15744 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	267	TRP	NE1-CE2	-5.29	1.31	1.37

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	79	MET	N-CA-C	8.19	115.50	108.78
1	D	79	MET	N-CA-C	8.17	115.48	108.78
1	B	76	GLY	N-CA-C	-6.03	106.32	115.00
1	C	312	ASN	N-CA-C	-6.00	105.79	113.23
1	A	312	ASN	N-CA-C	-6.00	105.79	113.23
1	D	76	GLY	N-CA-C	-6.00	106.36	115.00
1	A	153	SER	N-CA-C	-5.99	106.13	113.50
1	C	153	SER	N-CA-C	-5.99	106.14	113.50
1	C	36	GLY	CA-C-N	5.97	125.98	119.89
1	C	36	GLY	C-N-CA	5.97	125.98	119.89
1	D	270	VAL	N-CA-C	5.96	118.29	108.99
1	A	36	GLY	CA-C-N	5.94	125.95	119.89
1	A	36	GLY	C-N-CA	5.94	125.95	119.89
1	B	270	VAL	N-CA-C	5.94	118.26	108.99
1	B	84	TYR	O-C-N	5.71	130.18	122.59
1	D	84	TYR	O-C-N	5.68	130.15	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	192	HIS	N-CA-C	-5.61	107.08	114.31
1	D	192	HIS	N-CA-C	-5.59	107.09	114.31
1	D	5	GLN	N-CA-C	5.50	117.35	108.32
1	B	5	GLN	N-CA-C	5.50	117.33	108.32
1	C	202	ASP	N-CA-C	-5.42	106.79	113.41
1	C	364	ARG	NE-CZ-NH2	5.41	124.07	119.20
1	D	85	ALA	O-C-N	5.36	129.72	122.59
1	D	363	ARG	NE-CZ-NH2	5.35	124.02	119.20
1	A	66	ARG	NE-CZ-NH2	5.35	124.02	119.20
1	D	286	ARG	N-CA-C	5.35	116.56	109.93
1	D	364	ARG	NE-CZ-NH2	5.35	124.01	119.20
1	B	364	ARG	NE-CZ-NH2	5.35	124.01	119.20
1	B	286	ARG	N-CA-C	5.34	116.55	109.93
1	A	364	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	A	202	ASP	N-CA-C	-5.29	106.95	113.41
1	A	224	TYR	N-CA-C	5.26	118.21	109.79
1	C	224	TYR	N-CA-C	5.25	118.20	109.79
1	B	79	MET	CB-CA-C	-5.22	109.55	117.07
1	A	239	MET	CA-C-O	-5.20	115.83	121.44
1	D	79	MET	CB-CA-C	-5.19	109.59	117.07
1	C	95	ASN	N-CA-C	-5.19	104.03	110.41
1	D	347	LEU	CA-C-N	5.18	125.72	120.38
1	D	347	LEU	C-N-CA	5.18	125.72	120.38
1	A	363	ARG	NE-CZ-NH2	5.17	123.85	119.20
1	A	47	ARG	NE-CZ-NH2	5.17	123.85	119.20
1	B	347	LEU	CA-C-N	5.15	125.68	120.38
1	B	347	LEU	C-N-CA	5.15	125.68	120.38
1	C	237	PRO	O-C-N	5.15	129.59	122.64
1	C	249	THR	O-C-N	-5.13	117.13	123.33
1	D	202	ASP	N-CA-C	-5.12	105.76	112.41
1	B	85	ALA	O-C-N	5.10	129.37	122.59
1	D	81	PHE	O-C-N	5.06	128.92	123.10
1	A	236	SER	O-C-N	-5.06	115.50	121.32
1	D	129	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	B	81	PHE	O-C-N	5.02	128.87	123.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2853	0	2918	181	0
1	B	2853	0	2918	183	1
1	C	2853	0	2918	179	1
1	D	2853	0	2918	176	0
2	A	31	0	12	3	0
2	B	31	0	12	2	0
2	C	31	0	12	3	0
2	D	31	0	12	2	0
3	C	9	0	0	0	0
3	D	1	0	0	0	0
All	All	11546	0	11720	719	1

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 31.

All (719) 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:253:GLN:O	1:A:254:VAL:HG23	1.32	1.29
1:D:253:GLN:O	1:D:254:VAL:HG23	1.14	1.25
1:B:236:SER:OG	1:B:237:PRO:HD2	1.36	1.25
1:A:236:SER:OG	1:A:237:PRO:HD2	1.36	1.25
1:C:236:SER:OG	1:C:237:PRO:HD2	1.36	1.24
1:D:236:SER:OG	1:D:237:PRO:HD2	1.34	1.24
1:D:253:GLN:O	1:D:254:VAL:CG2	1.89	1.19
1:C:236:SER:HB2	1:C:237:PRO:HD3	1.34	1.08
1:D:236:SER:OG	1:D:237:PRO:CD	2.01	1.08
1:A:236:SER:OG	1:A:237:PRO:CD	2.04	1.06
1:C:236:SER:CB	1:C:237:PRO:CD	2.34	1.05
1:B:236:SER:OG	1:B:237:PRO:CD	2.04	1.05
1:D:83:SER:O	1:D:84:TYR:CD2	2.11	1.04
1:B:83:SER:O	1:B:84:TYR:CD2	2.15	0.99
1:C:253:GLN:O	1:C:254:VAL:HB	1.63	0.99
1:C:68:ASN:HD22	1:C:68:ASN:H	1.12	0.97
1:D:236:SER:CB	1:D:237:PRO:CD	2.42	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:SER:CB	1:B:237:PRO:CD	2.44	0.96
1:C:288:GLU:HG3	1:C:330:ARG:HD3	1.49	0.94
1:A:288:GLU:HG3	1:A:330:ARG:HD3	1.49	0.94
1:C:236:SER:OG	1:C:237:PRO:CD	2.15	0.94
1:A:253:GLN:O	1:A:254:VAL:CG2	2.17	0.93
1:C:236:SER:HB2	1:C:237:PRO:CD	1.97	0.92
1:C:4:VAL:HG13	1:C:26:ILE:O	1.70	0.91
1:D:236:SER:HB2	1:D:237:PRO:HD3	1.53	0.88
1:D:87:TYR:H	1:D:95:ASN:HD21	1.21	0.88
1:B:236:SER:HB2	1:B:237:PRO:HD3	1.54	0.88
1:C:314:THR:CG2	1:C:316:ILE:HD11	2.05	0.87
1:C:110:ILE:HG12	1:C:111:ASN:H	1.38	0.87
1:A:110:ILE:HG12	1:A:111:ASN:H	1.38	0.87
1:B:87:TYR:H	1:B:95:ASN:HD21	1.21	0.87
1:A:101:LYS:HG3	1:A:102:LEU:H	1.39	0.86
1:C:101:LYS:HG3	1:C:102:LEU:H	1.39	0.86
1:D:236:SER:CB	1:D:237:PRO:HD3	2.06	0.85
1:D:253:GLN:C	1:D:254:VAL:HG23	2.01	0.85
1:B:135:SER:H	1:B:138:GLN:HE21	1.22	0.85
1:A:314:THR:CG2	1:A:316:ILE:HD11	2.05	0.85
1:C:314:THR:HG22	1:C:316:ILE:HD11	1.59	0.84
1:D:135:SER:H	1:D:138:GLN:HE21	1.22	0.84
1:A:314:THR:HG22	1:A:316:ILE:HD11	1.59	0.84
1:A:96:MET:HA	1:A:146:ARG:HA	1.61	0.82
1:B:236:SER:CB	1:B:237:PRO:HD3	2.09	0.82
1:D:253:GLN:O	1:D:254:VAL:CB	2.28	0.81
1:D:20:LYS:HG3	1:D:21:ASP:H	1.45	0.81
1:B:253:GLN:O	1:B:254:VAL:HB	1.79	0.81
1:C:96:MET:HA	1:C:146:ARG:HA	1.61	0.81
1:C:260:MET:HE1	1:C:323:ILE:HD11	1.63	0.81
1:B:20:LYS:HG3	1:B:21:ASP:H	1.45	0.80
1:C:253:GLN:O	1:C:254:VAL:CB	2.27	0.80
1:A:236:SER:CB	1:A:237:PRO:CD	2.57	0.80
1:B:250:ALA:HB3	1:B:253:GLN:HB2	1.64	0.79
1:C:271:GLU:O	1:C:272:SER:HB3	1.82	0.78
1:D:130:LYS:HD3	1:D:130:LYS:N	1.98	0.78
1:A:260:MET:HE1	1:A:323:ILE:HD11	1.64	0.78
1:B:82:GLN:HA	1:B:140:GLN:OE1	1.84	0.78
1:C:68:ASN:HD22	1:C:68:ASN:N	1.79	0.78
1:B:130:LYS:HD3	1:B:130:LYS:N	1.98	0.78
1:B:135:SER:H	1:B:138:GLN:NE2	1.82	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:TYR:CG	1:C:363:ARG:NH2	2.52	0.77
1:B:68:ASN:N	1:B:68:ASN:HD22	1.80	0.77
1:D:68:ASN:N	1:D:68:ASN:HD22	1.80	0.77
1:C:291:LEU:HG	1:C:348:PRO:HG3	1.65	0.77
1:D:82:GLN:HA	1:D:140:GLN:OE1	1.84	0.77
1:A:68:ASN:HD22	1:A:68:ASN:H	1.30	0.77
1:B:202:ASP:O	1:B:203:LYS:HB2	1.85	0.77
1:D:86:LEU:HD23	1:D:146:ARG:NH2	2.00	0.77
1:A:60:LEU:H	1:A:68:ASN:HD21	1.33	0.76
1:B:248:ALA:HB3	1:B:267:TRP:CH2	2.20	0.76
1:A:271:GLU:O	1:A:272:SER:HB3	1.83	0.76
1:D:135:SER:H	1:D:138:GLN:NE2	1.82	0.76
1:A:291:LEU:HG	1:A:348:PRO:HG3	1.68	0.76
1:D:86:LEU:HA	1:D:146:ARG:HH22	1.51	0.76
1:A:34:PHE:HD1	1:A:207:LEU:HD11	1.51	0.75
1:C:236:SER:CB	1:C:237:PRO:HD2	2.10	0.75
1:B:86:LEU:HD23	1:B:146:ARG:NH2	2.01	0.75
1:C:236:SER:CB	1:C:237:PRO:HD3	2.05	0.75
1:A:110:ILE:C	1:A:112:GLN:H	1.95	0.74
1:A:4:VAL:HG12	1:A:4:VAL:O	1.88	0.74
1:D:283:LEU:C	1:D:283:LEU:HD23	2.13	0.74
1:C:34:PHE:HD1	1:C:207:LEU:HD11	1.51	0.74
1:B:283:LEU:C	1:B:283:LEU:HD23	2.13	0.73
1:B:86:LEU:HA	1:B:146:ARG:HH22	1.51	0.73
1:C:110:ILE:C	1:C:112:GLN:H	1.95	0.73
1:B:78:GLY:HA3	1:B:152:PRO:HG2	1.70	0.73
1:A:250:ALA:HB3	1:A:253:GLN:HB2	1.70	0.73
1:A:78:GLY:HA3	1:A:152:PRO:HG2	1.70	0.73
1:A:121:LEU:HA	1:A:172:MET:HE1	1.70	0.72
1:D:78:GLY:HA3	1:D:152:PRO:HG2	1.70	0.72
1:D:173:ARG:NE	1:D:196:GLU:HG3	2.04	0.72
1:C:121:LEU:HA	1:C:172:MET:HE1	1.70	0.72
1:A:95:ASN:O	1:A:96:MET:HB2	1.89	0.72
1:B:173:ARG:NE	1:B:196:GLU:HG3	2.04	0.72
1:C:78:GLY:HA3	1:C:152:PRO:HG2	1.70	0.71
1:B:253:GLN:O	1:B:254:VAL:CB	2.38	0.71
1:A:237:PRO:HG2	1:A:330:ARG:HD2	1.73	0.70
1:D:237:PRO:HG2	1:D:330:ARG:HD2	1.74	0.70
1:C:95:ASN:O	1:C:96:MET:HB2	1.92	0.69
1:A:67:MET:HE2	1:A:70:THR:HG21	1.74	0.69
1:C:68:ASN:H	1:C:68:ASN:ND2	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:LYS:HZ3	1:A:102:LEU:HG	1.56	0.68
1:C:235:GLY:O	1:C:236:SER:O	2.11	0.68
1:A:92:VAL:HG12	1:A:96:MET:HE2	1.75	0.68
1:C:300:LEU:HB3	1:C:320:ILE:HD13	1.76	0.68
1:C:60:LEU:H	1:C:68:ASN:HD21	1.41	0.68
1:A:85:ALA:HB1	1:A:146:ARG:NH1	2.07	0.67
1:A:300:LEU:HB3	1:A:320:ILE:HD13	1.76	0.67
1:C:110:ILE:HG12	1:C:111:ASN:N	2.09	0.67
1:C:101:LYS:NZ	1:C:102:LEU:HG	2.10	0.67
1:B:84:TYR:O	1:B:84:TYR:CD1	2.48	0.67
1:A:101:LYS:NZ	1:A:102:LEU:HG	2.09	0.67
1:D:84:TYR:O	1:D:84:TYR:CD1	2.47	0.67
1:A:110:ILE:HG12	1:A:111:ASN:N	2.09	0.67
1:A:33:VAL:CG2	1:A:204:ILE:HG12	2.25	0.67
1:C:208:ASP:HB2	1:C:229:PHE:CE2	2.30	0.67
1:C:155:PHE:HB2	1:C:187:MET:HG2	1.77	0.66
1:A:208:ASP:HB2	1:A:229:PHE:CE2	2.30	0.66
1:B:255:GLN:HB2	1:B:267:TRP:CE3	2.28	0.66
1:A:140:GLN:OE1	1:A:163:ASN:HB2	1.96	0.66
1:A:68:ASN:HD22	1:A:68:ASN:N	1.93	0.66
1:B:270:VAL:HG13	1:B:362:CYS:HB3	1.76	0.66
1:B:157:LEU:HD11	1:B:187:MET:HE2	1.78	0.66
1:D:87:TYR:H	1:D:95:ASN:ND2	1.93	0.66
1:C:6:LEU:HD22	1:C:22:ILE:HD11	1.78	0.66
1:B:60:LEU:H	1:B:68:ASN:HD21	1.44	0.65
1:B:309:GLN:O	1:B:310:LEU:HD23	1.96	0.65
1:D:60:LEU:H	1:D:68:ASN:HD21	1.44	0.65
1:D:157:LEU:HD11	1:D:187:MET:HE2	1.78	0.65
1:A:236:SER:CB	1:A:237:PRO:HD3	2.27	0.65
1:B:148:LEU:HD22	1:B:179:LEU:CD1	2.27	0.65
1:B:237:PRO:HG2	1:B:330:ARG:HD2	1.78	0.65
1:C:45:LEU:HA	1:C:48:MET:HE2	1.78	0.65
1:D:130:LYS:HD3	1:D:130:LYS:H	1.62	0.64
1:D:254:VAL:HG21	1:D:270:VAL:HG12	1.79	0.64
1:C:140:GLN:OE1	1:C:163:ASN:HB2	1.96	0.64
1:B:87:TYR:H	1:B:95:ASN:ND2	1.93	0.64
1:B:144:ILE:HD11	1:B:160:PRO:O	1.98	0.64
1:B:262:ASN:HD21	1:B:264:GLN:HB2	1.63	0.64
1:D:148:LEU:HD22	1:D:179:LEU:CD1	2.27	0.64
1:D:270:VAL:HG13	1:D:362:CYS:HB3	1.79	0.64
1:C:243:PRO:O	1:C:259:PRO:HG3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:VAL:HG13	1:D:201:ALA:HB2	1.77	0.64
1:D:309:GLN:O	1:D:310:LEU:HD23	1.96	0.64
1:B:236:SER:HB2	1:B:237:PRO:CD	2.20	0.64
1:C:4:VAL:HG12	1:C:4:VAL:O	1.97	0.64
1:D:288:GLU:HG3	1:D:330:ARG:HD3	1.80	0.64
1:C:33:VAL:CG2	1:C:204:ILE:HG12	2.27	0.64
1:D:144:ILE:HD11	1:D:160:PRO:O	1.98	0.64
1:A:87:TYR:CE1	1:A:98:PHE:CE2	2.86	0.64
1:A:155:PHE:HB2	1:A:187:MET:HG2	1.78	0.64
1:A:173:ARG:HE	1:A:196:GLU:HG3	1.63	0.64
1:B:248:ALA:CB	1:B:267:TRP:CH2	2.81	0.64
1:A:123:LEU:HD21	1:A:141:ARG:HB3	1.79	0.63
1:A:243:PRO:O	1:A:259:PRO:HG3	1.97	0.63
1:B:130:LYS:HD3	1:B:130:LYS:H	1.62	0.63
1:A:214:GLN:HG2	1:A:221:LEU:CD2	2.29	0.63
1:A:331:GLN:OE1	1:A:335:VAL:HG21	1.99	0.63
1:B:288:GLU:HG3	1:B:330:ARG:HD3	1.80	0.63
1:C:173:ARG:HE	1:C:196:GLU:HG3	1.63	0.63
1:D:262:ASN:HD21	1:D:264:GLN:HB2	1.63	0.63
1:B:34:PHE:HB2	1:B:190:VAL:HG22	1.80	0.62
1:D:270:VAL:HG22	1:D:362:CYS:O	1.99	0.62
1:A:260:MET:HE1	1:A:323:ILE:CD1	2.29	0.62
1:B:271:GLU:O	1:B:272:SER:HB3	1.99	0.62
1:C:123:LEU:HD21	1:C:141:ARG:HB3	1.79	0.62
1:D:34:PHE:HB2	1:D:190:VAL:HG22	1.80	0.62
1:C:314:THR:HG22	1:C:316:ILE:CD1	2.30	0.62
1:D:155:PHE:O	1:D:156:LEU:HD23	2.00	0.62
1:B:155:PHE:O	1:B:156:LEU:HD23	2.00	0.62
1:C:260:MET:HE1	1:C:323:ILE:CD1	2.29	0.62
1:C:214:GLN:HG2	1:C:221:LEU:CD2	2.29	0.62
1:D:271:GLU:O	1:D:272:SER:HB3	1.99	0.62
1:C:331:GLN:OE1	1:C:335:VAL:HG21	1.99	0.62
1:C:67:MET:HE2	1:C:70:THR:HG21	1.80	0.61
1:B:47:ARG:NH2	1:B:52:LEU:HB3	2.15	0.61
1:B:173:ARG:HE	1:B:196:GLU:HG3	1.65	0.61
1:B:141:ARG:HD2	1:B:164:LEU:HD21	1.82	0.61
1:B:309:GLN:C	1:B:310:LEU:HD23	2.25	0.61
1:C:92:VAL:HG12	1:C:96:MET:HE2	1.82	0.61
1:C:33:VAL:HG22	1:C:204:ILE:HG12	1.82	0.61
1:A:367:LYS:HE3	1:A:367:LYS:HA	1.82	0.61
1:D:309:GLN:C	1:D:310:LEU:HD23	2.25	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:ARG:HE	1:D:196:GLU:HG3	1.65	0.61
1:A:79:MET:HE3	1:A:156:LEU:HD12	1.83	0.61
1:B:62:ILE:HB	1:B:67:MET:HE3	1.83	0.61
1:D:141:ARG:HD2	1:D:164:LEU:HD21	1.82	0.61
1:D:208:ASP:HB2	1:D:229:PHE:CE2	2.36	0.61
1:A:87:TYR:HE1	1:A:98:PHE:CE2	2.19	0.60
1:D:62:ILE:HB	1:D:67:MET:HE3	1.83	0.60
1:B:208:ASP:HB2	1:B:229:PHE:CE2	2.36	0.60
1:C:79:MET:HE3	1:C:156:LEU:HD12	1.83	0.60
1:B:255:GLN:HB2	1:B:267:TRP:CZ3	2.36	0.60
1:C:288:GLU:CG	1:C:330:ARG:HD3	2.28	0.60
1:C:367:LYS:HE3	1:C:367:LYS:HA	1.82	0.60
1:C:253:GLN:HB3	1:C:267:TRP:CE3	2.37	0.60
1:D:47:ARG:NH2	1:D:52:LEU:HB3	2.15	0.60
1:B:262:ASN:ND2	1:B:264:GLN:HB2	2.17	0.60
1:D:301:GLU:HG2	1:D:344:ALA:HB2	1.84	0.60
1:A:236:SER:HB2	1:A:237:PRO:HD3	1.83	0.59
1:B:202:ASP:O	1:B:203:LYS:CB	2.50	0.59
1:B:248:ALA:CB	1:B:267:TRP:HH2	2.16	0.59
1:A:33:VAL:HG22	1:A:204:ILE:HG12	1.84	0.59
1:D:262:ASN:ND2	1:D:264:GLN:HB2	2.17	0.59
1:A:126:LEU:O	1:A:129:ARG:HB2	2.03	0.59
1:B:236:SER:O	1:B:238:LYS:N	2.35	0.59
1:C:126:LEU:O	1:C:129:ARG:HB2	2.03	0.59
1:A:314:THR:HG22	1:A:316:ILE:CD1	2.30	0.59
1:D:243:PRO:O	1:D:259:PRO:HD3	2.03	0.59
1:B:33:VAL:HA	1:B:189:TYR:O	2.03	0.58
1:B:81:PHE:CE2	1:B:157:LEU:HA	2.38	0.58
1:D:33:VAL:HA	1:D:189:TYR:O	2.03	0.58
1:D:327:LEU:HD23	1:D:345:ILE:HD11	1.85	0.58
1:B:255:GLN:HB2	1:B:267:TRP:CD2	2.38	0.58
1:A:250:ALA:HB3	1:A:253:GLN:CB	2.34	0.58
1:A:250:ALA:HB3	1:A:253:GLN:CG	2.33	0.58
1:A:110:ILE:O	1:A:112:GLN:N	2.37	0.58
1:C:101:LYS:HZ3	1:C:102:LEU:HG	1.68	0.58
1:C:290:LEU:HD13	1:C:345:ILE:HD12	1.85	0.58
1:A:203:LYS:HD3	1:A:215:VAL:CG1	2.34	0.58
1:D:81:PHE:CE2	1:D:157:LEU:HA	2.39	0.58
1:D:250:ALA:HB3	1:D:253:GLN:HB2	1.86	0.58
1:C:110:ILE:O	1:C:112:GLN:N	2.37	0.58
1:C:228:ARG:HG2	1:C:228:ARG:HH11	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:TYR:O	1:C:85:ALA:HB2	2.04	0.57
1:B:301:GLU:HG2	1:B:344:ALA:HB2	1.84	0.57
1:D:292:PRO:C	1:D:294:ASP:H	2.12	0.57
1:A:236:SER:HG	1:A:237:PRO:HD2	1.62	0.57
1:A:290:LEU:HD13	1:A:345:ILE:HD12	1.85	0.57
1:D:321:PRO:O	1:D:322:SER:OG	2.22	0.57
1:B:243:PRO:O	1:B:259:PRO:HD3	2.03	0.57
1:A:228:ARG:HG2	1:A:228:ARG:HH11	1.68	0.57
1:B:292:PRO:C	1:B:294:ASP:H	2.12	0.57
1:D:236:SER:O	1:D:238:LYS:N	2.37	0.57
1:B:148:LEU:HD22	1:B:179:LEU:HD11	1.86	0.57
1:B:327:LEU:HD23	1:B:345:ILE:HD11	1.85	0.57
1:C:45:LEU:HA	1:C:48:MET:CE	2.34	0.57
1:A:110:ILE:C	1:A:112:GLN:N	2.62	0.56
1:D:148:LEU:HD22	1:D:179:LEU:HD11	1.86	0.56
1:C:10:THR:HB	1:C:57:SER:HB2	1.86	0.56
1:A:6:LEU:HD22	1:A:22:ILE:HD11	1.87	0.56
1:A:141:ARG:HG2	1:A:172:MET:HE3	1.87	0.56
1:C:41:GLY:HA2	2:C:382:ATP:O2A	2.05	0.56
1:A:4:VAL:O	1:A:5:GLN:HB2	2.06	0.56
1:A:49:ILE:O	1:A:62:ILE:HD11	2.06	0.56
1:A:253:GLN:O	1:A:272:SER:HB2	2.06	0.56
1:A:288:GLU:CG	1:A:330:ARG:HD3	2.28	0.56
1:D:60:LEU:HB3	1:D:68:ASN:ND2	2.21	0.56
1:B:60:LEU:HB3	1:B:68:ASN:ND2	2.21	0.56
1:C:44:THR:O	1:C:48:MET:HG3	2.06	0.56
1:C:203:LYS:HD3	1:C:215:VAL:CG1	2.35	0.56
1:A:10:THR:HB	1:A:57:SER:HB2	1.86	0.55
1:B:68:ASN:N	1:B:68:ASN:ND2	2.52	0.55
1:D:290:LEU:HD13	1:D:345:ILE:HD12	1.89	0.55
1:C:95:ASN:C	1:C:97:SER:H	2.14	0.55
1:A:41:GLY:HA2	2:A:382:ATP:O2A	2.05	0.55
1:B:270:VAL:HG22	1:B:362:CYS:O	2.05	0.55
1:C:141:ARG:HG2	1:C:172:MET:HE3	1.87	0.55
1:B:178:ARG:HA	1:B:181:LYS:HG2	1.89	0.55
1:B:290:LEU:HD13	1:B:345:ILE:HD12	1.88	0.55
1:D:281:MET:HE2	1:D:356:ARG:HA	1.89	0.55
1:A:87:TYR:HE1	1:A:98:PHE:CD2	2.25	0.54
1:A:250:ALA:HB3	1:A:253:GLN:HG3	1.89	0.54
1:B:281:MET:HE2	1:B:356:ARG:HA	1.89	0.54
1:D:183:LEU:HB3	1:D:185:ARG:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:GLN:C	1:C:6:LEU:HD12	2.32	0.54
1:A:34:PHE:CE2	1:A:188:ILE:HG23	2.43	0.54
1:A:85:ALA:O	1:A:146:ARG:NH2	2.40	0.54
1:A:126:LEU:HD22	1:A:129:ARG:HG3	1.89	0.54
1:B:183:LEU:HB3	1:B:185:ARG:HG2	1.89	0.54
1:C:8:ASN:HA	1:C:21:ASP:HB2	1.89	0.54
1:D:178:ARG:HA	1:D:181:LYS:HG2	1.89	0.54
1:A:8:ASN:HA	1:A:21:ASP:HB2	1.90	0.54
1:D:236:SER:HB2	1:D:237:PRO:CD	2.20	0.54
1:B:130:LYS:N	1:B:130:LYS:CD	2.70	0.54
1:D:270:VAL:HG13	1:D:271:GLU:N	2.23	0.54
1:A:4:VAL:O	1:A:4:VAL:CG1	2.55	0.54
1:B:126:LEU:HD22	1:B:129:ARG:NH1	2.23	0.54
1:C:126:LEU:HD22	1:C:129:ARG:HG3	1.89	0.54
1:B:350:GLU:H	1:B:350:GLU:CD	2.17	0.53
1:A:83:SER:O	1:A:84:TYR:HB2	2.08	0.53
1:B:81:PHE:CZ	1:B:157:LEU:HD23	2.43	0.53
1:D:81:PHE:CZ	1:D:157:LEU:HD23	2.43	0.53
1:B:130:LYS:H	1:B:130:LYS:CD	2.21	0.53
1:C:275:VAL:HG13	1:C:281:MET:CE	2.39	0.53
2:C:382:ATP:H5'1	1:D:135:SER:HB3	1.90	0.53
1:A:289:HIS:O	1:A:348:PRO:HG2	2.08	0.53
1:B:270:VAL:HG13	1:B:271:GLU:N	2.23	0.53
1:C:34:PHE:CE2	1:C:188:ILE:HG23	2.43	0.53
1:C:47:ARG:HD2	1:C:52:LEU:HD12	1.91	0.53
1:B:248:ALA:HB1	1:B:267:TRP:HH2	1.73	0.53
1:D:242:LEU:HD12	1:D:242:LEU:N	2.23	0.53
1:C:289:HIS:O	1:C:348:PRO:HG2	2.08	0.53
1:C:327:LEU:HD23	1:C:345:ILE:HD11	1.90	0.53
1:D:5:GLN:HB3	1:D:61:PHE:HB2	1.91	0.53
1:B:96:MET:HE1	1:B:118:ALA:HB2	1.91	0.53
1:C:173:ARG:NE	1:C:196:GLU:HG3	2.23	0.53
1:D:110:ILE:O	1:D:113:ARG:HG2	2.09	0.53
1:A:101:LYS:HG3	1:A:102:LEU:N	2.19	0.53
1:D:126:LEU:HD22	1:D:129:ARG:NH1	2.23	0.53
1:D:130:LYS:H	1:D:130:LYS:CD	2.21	0.53
1:D:351:ARG:NE	1:D:368:GLU:OE2	2.42	0.53
2:A:382:ATP:H5'1	1:B:135:SER:HB3	1.90	0.53
1:D:83:SER:O	1:D:84:TYR:CG	2.60	0.53
1:D:96:MET:HE1	1:D:118:ALA:HB2	1.91	0.53
1:A:140:GLN:HE21	1:A:160:PRO:C	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ASP:C	1:A:358:ASP:OD1	2.53	0.52
1:B:117:VAL:HG13	1:B:118:ALA:N	2.24	0.52
1:B:242:LEU:N	1:B:242:LEU:HD12	2.23	0.52
1:D:83:SER:C	1:D:84:TYR:CD2	2.86	0.52
1:A:34:PHE:HE2	1:A:188:ILE:HG23	1.74	0.52
1:D:97:SER:HB3	1:D:114:VAL:HG21	1.91	0.52
1:D:117:VAL:O	1:D:120:VAL:HG22	2.10	0.52
1:A:5:GLN:C	1:A:6:LEU:HD12	2.34	0.52
1:A:286:ARG:HB3	1:A:288:GLU:OE2	2.10	0.52
1:B:295:ILE:O	1:B:296:ALA:HB2	2.09	0.52
1:A:116:GLN:HE22	1:A:182:ARG:HH12	1.58	0.52
1:C:286:ARG:HB3	1:C:288:GLU:OE2	2.10	0.52
1:A:327:LEU:HD23	1:A:345:ILE:HD11	1.90	0.52
1:C:34:PHE:HE2	1:C:188:ILE:HG23	1.73	0.52
1:C:283:LEU:HD23	1:C:283:LEU:C	2.34	0.52
1:B:110:ILE:O	1:B:113:ARG:HG2	2.09	0.52
1:C:140:GLN:HE21	1:C:160:PRO:C	2.18	0.52
1:D:148:LEU:HD22	1:D:179:LEU:HD13	1.91	0.52
1:A:283:LEU:C	1:A:283:LEU:HD23	2.34	0.52
1:B:97:SER:HB3	1:B:114:VAL:HG21	1.91	0.52
1:C:249:THR:HA	1:C:254:VAL:HA	1.92	0.52
1:D:295:ILE:O	1:D:296:ALA:HB2	2.09	0.52
1:B:117:VAL:O	1:B:120:VAL:HG22	2.10	0.52
1:C:101:LYS:HG3	1:C:102:LEU:N	2.19	0.52
1:D:11:LYS:HB2	1:D:48:MET:CE	2.39	0.52
1:A:60:LEU:H	1:A:68:ASN:ND2	2.04	0.51
1:C:92:VAL:O	1:C:96:MET:HE2	2.10	0.51
1:C:335:VAL:HG12	1:C:337:VAL:HG23	1.92	0.51
1:C:80:VAL:O	1:C:80:VAL:HG13	2.10	0.51
1:C:96:MET:HA	1:C:146:ARG:CA	2.38	0.51
1:C:301:GLU:HG3	1:C:344:ALA:HB2	1.91	0.51
1:D:70:THR:HB	1:D:75:ARG:HD3	1.92	0.51
1:A:173:ARG:NE	1:A:196:GLU:HG3	2.23	0.51
1:B:248:ALA:HB3	1:B:255:GLN:HB3	1.93	0.51
1:A:80:VAL:O	1:A:80:VAL:HG13	2.11	0.51
1:A:323:ILE:HD12	1:A:323:ILE:H	1.76	0.51
1:B:11:LYS:HB2	1:B:48:MET:CE	2.39	0.51
1:B:242:LEU:HD11	1:B:327:LEU:HD11	1.93	0.51
1:C:11:LYS:HD3	1:C:54:THR:O	2.11	0.51
1:B:83:SER:O	1:B:84:TYR:CG	2.62	0.51
1:B:141:ARG:HD2	1:B:164:LEU:CD2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242:LEU:HD11	1:D:327:LEU:HD11	1.93	0.51
1:D:141:ARG:HD2	1:D:164:LEU:CD2	2.41	0.51
1:B:70:THR:HB	1:B:75:ARG:HD3	1.92	0.51
1:B:5:GLN:HB3	1:B:61:PHE:HB2	1.91	0.51
1:B:283:LEU:C	1:B:283:LEU:CD2	2.83	0.51
1:C:280:ASN:O	1:C:357:GLU:HG2	2.11	0.51
1:D:117:VAL:HG13	1:D:118:ALA:N	2.24	0.51
1:A:280:ASN:O	1:A:357:GLU:HG2	2.11	0.50
1:B:293:SER:HB3	1:B:345:ILE:HA	1.93	0.50
1:C:358:ASP:C	1:C:358:ASP:OD1	2.53	0.50
1:D:81:PHE:HE2	1:D:156:LEU:O	1.94	0.50
1:D:159:GLU:N	1:D:160:PRO:CD	2.74	0.50
1:A:95:ASN:C	1:A:97:SER:H	2.19	0.50
1:D:82:GLN:HA	1:D:140:GLN:CD	2.36	0.50
1:D:260:MET:HE3	1:D:262:ASN:OD1	2.11	0.50
1:A:251:ILE:N	1:A:251:ILE:HD12	2.26	0.50
1:A:335:VAL:HG12	1:A:337:VAL:HG23	1.92	0.50
1:A:358:ASP:OD1	1:A:360:THR:HG23	2.12	0.50
1:B:148:LEU:HD22	1:B:179:LEU:HD13	1.92	0.50
1:B:297:ASP:O	1:B:299:ILE:HG13	2.12	0.50
1:C:323:ILE:HD12	1:C:323:ILE:H	1.76	0.50
1:C:23:ASN:N	1:C:23:ASN:HD22	2.09	0.50
1:C:144:ILE:HD11	1:C:160:PRO:O	2.12	0.50
1:D:293:SER:HB3	1:D:345:ILE:HA	1.93	0.50
1:A:236:SER:OG	1:A:237:PRO:HD3	2.08	0.50
1:B:81:PHE:HE2	1:B:156:LEU:O	1.94	0.50
1:B:84:TYR:O	1:B:84:TYR:CG	2.65	0.50
1:D:68:ASN:N	1:D:68:ASN:ND2	2.52	0.50
1:D:84:TYR:O	1:D:84:TYR:CG	2.64	0.50
1:B:159:GLU:N	1:B:160:PRO:CD	2.74	0.50
1:B:260:MET:HE3	1:B:262:ASN:OD1	2.11	0.50
1:C:116:GLN:HE22	1:C:182:ARG:HH12	1.58	0.50
1:D:30:GLU:HG2	1:D:202:ASP:OD2	2.12	0.50
1:A:315:GLN:C	1:A:316:ILE:HD13	2.37	0.50
1:B:20:LYS:HG3	1:B:21:ASP:N	2.21	0.50
1:B:29:GLY:HA2	1:B:185:ARG:O	2.12	0.50
1:B:120:VAL:O	1:B:172:MET:HE1	2.12	0.50
1:A:68:ASN:H	1:A:68:ASN:ND2	2.06	0.49
1:A:102:LEU:C	1:A:104:GLY:H	2.20	0.49
1:B:82:GLN:HA	1:B:140:GLN:CD	2.36	0.49
1:C:4:VAL:O	1:C:4:VAL:CG1	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:GLN:C	1:C:316:ILE:HD13	2.37	0.49
1:A:11:LYS:HD3	1:A:54:THR:O	2.11	0.49
1:D:351:ARG:HG3	1:D:351:ARG:HH11	1.77	0.49
1:A:96:MET:HA	1:A:146:ARG:CA	2.39	0.49
1:B:51:GLY:HA3	1:B:72:PRO:HG3	1.94	0.49
1:B:351:ARG:HG3	1:B:351:ARG:HH11	1.77	0.49
1:C:260:MET:SD	1:C:300:LEU:HD22	2.52	0.49
1:A:260:MET:SD	1:A:300:LEU:HD22	2.52	0.49
1:A:23:ASN:N	1:A:23:ASN:HD22	2.09	0.49
1:B:252:ASP:HB3	1:B:365:LEU:CD1	2.43	0.49
1:D:29:GLY:HA2	1:D:185:ARG:O	2.12	0.49
1:D:120:VAL:O	1:D:172:MET:HE1	2.12	0.49
1:D:20:LYS:HG3	1:D:21:ASP:N	2.21	0.49
1:D:51:GLY:HA3	1:D:72:PRO:HG3	1.94	0.49
1:D:92:VAL:CG2	1:D:134:LEU:HD11	2.42	0.49
1:B:11:LYS:HB2	1:B:48:MET:HE1	1.94	0.49
1:B:86:LEU:HA	1:B:146:ARG:NH2	2.25	0.49
1:B:306:VAL:HB	1:B:317:HIS:CG	2.48	0.49
1:A:214:GLN:HG2	1:A:221:LEU:HD21	1.94	0.49
1:C:60:LEU:H	1:C:68:ASN:ND2	2.10	0.49
1:C:68:ASN:N	1:C:68:ASN:ND2	2.50	0.49
1:C:275:VAL:HG13	1:C:281:MET:HE1	1.94	0.49
1:A:144:ILE:HD11	1:A:160:PRO:O	2.12	0.48
1:A:275:VAL:HG13	1:A:281:MET:CE	2.43	0.48
1:B:92:VAL:CG2	1:B:134:LEU:HD11	2.42	0.48
1:D:96:MET:CE	1:D:117:VAL:HG13	2.43	0.48
1:D:132:LYS:O	1:D:132:LYS:HG2	2.13	0.48
1:A:252:ASP:HB3	1:A:365:LEU:CD1	2.43	0.48
1:B:132:LYS:O	1:B:132:LYS:HG2	2.13	0.48
1:C:102:LEU:C	1:C:104:GLY:H	2.20	0.48
1:D:283:LEU:C	1:D:283:LEU:CD2	2.83	0.48
1:A:236:SER:O	1:A:237:PRO:C	2.53	0.48
1:D:40:CYS:SG	1:D:42:LYS:HG3	2.53	0.48
1:D:135:SER:N	1:D:138:GLN:HE21	2.01	0.48
1:D:297:ASP:O	1:D:299:ILE:HG13	2.12	0.48
1:D:306:VAL:HB	1:D:317:HIS:CG	2.48	0.48
1:C:253:GLN:O	1:C:254:VAL:CG2	2.61	0.48
1:A:253:GLN:C	1:A:254:VAL:HG23	2.27	0.48
1:A:301:GLU:HG3	1:A:344:ALA:HB2	1.96	0.48
1:B:96:MET:CE	1:B:117:VAL:HG13	2.43	0.48
1:D:11:LYS:HB2	1:D:48:MET:HE1	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:253:GLN:O	1:D:254:VAL:HB	2.13	0.48
1:C:214:GLN:HG2	1:C:221:LEU:HD21	1.94	0.48
1:C:358:ASP:OD1	1:C:360:THR:HG23	2.13	0.48
1:D:240:ASN:HB2	1:D:285:ILE:O	2.13	0.48
1:A:84:TYR:HE1	1:A:140:GLN:HG3	1.79	0.48
1:B:62:ILE:O	1:B:67:MET:HE3	2.13	0.48
1:B:77:VAL:CG1	1:B:78:GLY:N	2.77	0.48
1:C:109:VAL:HG13	1:C:110:ILE:N	2.29	0.48
1:C:224:TYR:CD1	1:C:363:ARG:NH2	2.81	0.48
1:D:62:ILE:O	1:D:67:MET:HE3	2.13	0.48
1:B:40:CYS:SG	1:B:42:LYS:HG3	2.53	0.48
1:D:77:VAL:CG1	1:D:78:GLY:N	2.77	0.48
1:C:113:ARG:HA	1:C:116:GLN:HG3	1.96	0.48
1:A:145:GLY:O	1:A:149:VAL:HG23	2.14	0.48
1:A:307:VAL:HG13	1:A:316:ILE:CD1	2.44	0.48
1:C:307:VAL:HG13	1:C:316:ILE:CD1	2.44	0.48
1:D:151:GLU:O	1:D:185:ARG:NH1	2.46	0.48
1:D:151:GLU:N	1:D:152:PRO:HD3	2.29	0.47
1:C:145:GLY:O	1:C:149:VAL:HG23	2.14	0.47
1:D:253:GLN:OE1	1:D:267:TRP:CE3	2.68	0.47
1:A:251:ILE:H	1:A:251:ILE:CD1	2.27	0.47
1:A:338:GLU:O	1:A:340:GLY:N	2.47	0.47
1:B:135:SER:N	1:B:138:GLN:HE21	2.01	0.47
1:C:33:VAL:HG12	1:C:189:TYR:HB3	1.96	0.47
1:C:83:SER:O	1:C:84:TYR:HB2	2.14	0.47
1:D:46:LEU:HD11	1:D:156:LEU:HB3	1.97	0.47
1:D:77:VAL:HG12	1:D:78:GLY:N	2.29	0.47
1:B:151:GLU:N	1:B:152:PRO:HD3	2.29	0.47
1:B:152:PRO:O	1:B:185:ARG:NH1	2.48	0.47
1:A:253:GLN:O	1:A:254:VAL:CB	2.62	0.47
1:B:48:MET:HE3	1:B:55:ILE:HA	1.96	0.47
1:B:47:ARG:HG2	1:B:47:ARG:HH11	1.79	0.47
1:C:247:THR:CG2	1:C:257:GLU:HB2	2.45	0.47
1:C:346:GLY:O	1:C:348:PRO:HD3	2.15	0.47
1:A:113:ARG:HA	1:A:116:GLN:HG3	1.96	0.47
1:B:60:LEU:N	1:B:68:ASN:HD21	2.10	0.47
1:B:157:LEU:CD1	1:B:187:MET:HE2	2.43	0.47
1:C:49:ILE:O	1:C:62:ILE:HD11	2.15	0.47
1:C:338:GLU:O	1:C:340:GLY:N	2.47	0.47
1:A:251:ILE:HD12	1:A:251:ILE:H	1.80	0.47
2:A:382:ATP:C5'	1:B:135:SER:HB3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:LEU:HD11	1:B:156:LEU:HB3	1.97	0.47
1:B:178:ARG:HG2	1:B:181:LYS:HE2	1.97	0.47
1:D:47:ARG:HH11	1:D:47:ARG:HG2	1.79	0.47
1:A:109:VAL:HG13	1:A:110:ILE:N	2.29	0.46
1:B:240:ASN:HB2	1:B:285:ILE:O	2.14	0.46
1:B:77:VAL:HG12	1:B:78:GLY:N	2.29	0.46
1:C:6:LEU:CD2	1:C:22:ILE:HD11	2.44	0.46
1:C:6:LEU:HB3	1:C:9:VAL:HG21	1.97	0.46
1:A:50:ALA:O	1:A:75:ARG:HD2	2.15	0.46
1:B:83:SER:C	1:B:84:TYR:CD2	2.89	0.46
1:B:91:SER:H	1:B:94:GLU:HB2	1.81	0.46
1:D:60:LEU:N	1:D:68:ASN:HD21	2.10	0.46
1:D:248:ALA:HB3	1:D:255:GLN:HB3	1.97	0.46
1:A:247:THR:CG2	1:A:257:GLU:HB2	2.45	0.46
1:D:178:ARG:HG2	1:D:181:LYS:HE2	1.97	0.46
1:D:48:MET:HE3	1:D:55:ILE:HA	1.96	0.46
1:B:154:VAL:HG22	1:B:186:THR:HB	1.97	0.46
1:B:351:ARG:NE	1:B:368:GLU:OE2	2.48	0.46
1:D:362:CYS:O	1:D:363:ARG:C	2.58	0.46
1:C:77:VAL:HG13	1:C:156:LEU:HG	1.98	0.46
1:C:137:GLY:O	1:C:141:ARG:HD3	2.16	0.46
1:D:157:LEU:CD1	1:D:187:MET:HE2	2.43	0.46
1:A:33:VAL:HG12	1:A:189:TYR:HB3	1.96	0.46
1:A:235:GLY:O	1:A:236:SER:O	2.34	0.46
1:B:102:LEU:O	1:B:103:ALA:HB3	2.16	0.46
1:B:92:VAL:HG22	1:B:134:LEU:HD11	1.98	0.46
1:B:300:LEU:HB3	1:B:320:ILE:HD13	1.98	0.46
1:A:148:LEU:CD2	1:A:179:LEU:HD22	2.46	0.46
1:A:152:PRO:O	1:A:185:ARG:NH1	2.47	0.46
1:B:51:GLY:C	1:B:53:GLU:H	2.24	0.46
1:B:51:GLY:O	1:B:52:LEU:HB2	2.16	0.46
1:D:236:SER:O	1:D:237:PRO:C	2.59	0.46
1:C:11:LYS:O	1:C:18:VAL:HG12	2.15	0.45
1:D:154:VAL:HG22	1:D:186:THR:HB	1.97	0.45
1:A:11:LYS:O	1:A:18:VAL:HG12	2.15	0.45
1:D:92:VAL:HG22	1:D:134:LEU:HD11	1.98	0.45
1:A:110:ILE:O	1:A:111:ASN:HB3	2.17	0.45
1:A:254:VAL:CG2	1:A:272:SER:HA	2.47	0.45
1:C:148:LEU:CD2	1:C:179:LEU:HD22	2.46	0.45
2:C:382:ATP:C5'	1:D:135:SER:HB3	2.45	0.45
1:D:202:ASP:OD2	1:D:202:ASP:C	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:281:MET:HE1	1:D:356:ARG:HG2	1.98	0.45
1:A:81:PHE:CE1	1:A:83:SER:HB2	2.51	0.45
1:D:41:GLY:O	1:D:45:LEU:HB2	2.17	0.45
1:D:51:GLY:C	1:D:53:GLU:H	2.24	0.45
1:D:51:GLY:O	1:D:52:LEU:HB2	2.16	0.45
1:D:91:SER:H	1:D:94:GLU:HB2	1.81	0.45
1:D:302:GLY:HA3	1:D:319:GLN:O	2.16	0.45
1:B:41:GLY:O	1:B:45:LEU:HB2	2.17	0.45
1:B:110:ILE:C	1:B:110:ILE:HD12	2.41	0.45
1:B:137:GLY:O	1:B:141:ARG:HD3	2.16	0.45
1:B:283:LEU:HD23	1:B:284:GLY:N	2.31	0.45
1:B:302:GLY:HA3	1:B:319:GLN:O	2.16	0.45
1:A:137:GLY:O	1:A:141:ARG:HD3	2.16	0.45
1:A:85:ALA:HB1	1:A:146:ARG:HH12	1.79	0.45
1:A:95:ASN:O	1:A:96:MET:CB	2.59	0.45
1:C:251:ILE:HD12	1:C:251:ILE:N	2.32	0.45
1:D:291:LEU:HD11	1:D:348:PRO:HB3	1.99	0.45
1:A:20:LYS:O	1:A:21:ASP:C	2.60	0.45
1:A:107:LYS:HA	1:A:110:ILE:CG2	2.46	0.45
1:A:130:LYS:O	1:A:131:PRO:C	2.60	0.45
1:A:254:VAL:HG23	1:A:272:SER:HB2	1.99	0.45
1:B:87:TYR:HB3	1:B:89:HIS:CE1	2.52	0.45
1:C:107:LYS:HA	1:C:110:ILE:CG2	2.47	0.45
1:D:283:LEU:HD23	1:D:284:GLY:N	2.31	0.45
1:D:320:ILE:HG23	1:D:321:PRO:HD2	1.99	0.45
1:A:77:VAL:HG13	1:A:156:LEU:HG	1.98	0.45
1:D:110:ILE:HD12	1:D:110:ILE:C	2.41	0.45
1:D:137:GLY:O	1:D:141:ARG:HD3	2.16	0.45
1:D:152:PRO:O	1:D:185:ARG:NH1	2.48	0.45
1:D:300:LEU:HB3	1:D:320:ILE:HD13	1.98	0.45
1:A:102:LEU:C	1:A:104:GLY:N	2.76	0.45
1:B:253:GLN:HB3	1:B:267:TRP:CE3	2.52	0.45
1:D:46:LEU:HD23	1:D:158:ASP:HB2	1.99	0.45
1:A:92:VAL:O	1:A:96:MET:HE2	2.17	0.44
1:B:151:GLU:O	1:B:185:ARG:NH1	2.46	0.44
1:B:236:SER:O	1:B:237:PRO:C	2.54	0.44
1:C:6:LEU:HB3	1:C:9:VAL:CG2	2.47	0.44
1:C:110:ILE:C	1:C:112:GLN:N	2.62	0.44
1:C:152:PRO:O	1:C:185:ARG:NH1	2.47	0.44
1:C:297:ASP:OD1	1:C:297:ASP:N	2.50	0.44
1:C:84:TYR:HE1	1:C:140:GLN:HG3	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:LEU:O	1:D:103:ALA:HB3	2.16	0.44
1:C:130:LYS:O	1:C:131:PRO:C	2.60	0.44
1:D:86:LEU:HA	1:D:146:ARG:NH2	2.25	0.44
1:A:151:GLU:O	1:A:185:ARG:NH1	2.51	0.44
1:A:18:VAL:HG22	1:A:18:VAL:O	2.17	0.44
1:A:49:ILE:HA	1:A:60:LEU:HD21	1.98	0.44
1:A:87:TYR:CE1	1:A:98:PHE:CD2	3.06	0.44
1:B:321:PRO:O	1:B:322:SER:OG	2.22	0.44
1:C:101:LYS:HZ1	1:C:102:LEU:HG	1.80	0.44
1:A:79:MET:HE3	1:A:156:LEU:CD1	2.46	0.44
1:B:281:MET:HE1	1:B:356:ARG:HG2	1.98	0.44
1:C:260:MET:N	1:C:260:MET:HE2	2.33	0.44
1:B:33:VAL:HG13	1:B:201:ALA:HB2	1.98	0.44
1:B:157:LEU:HD11	1:B:187:MET:CE	2.48	0.44
1:B:347:LEU:O	1:B:347:LEU:HD13	2.18	0.44
1:B:362:CYS:O	1:B:363:ARG:C	2.60	0.44
1:A:17:VAL:HG11	1:A:20:LYS:HD2	2.00	0.44
1:B:253:GLN:O	1:B:254:VAL:CG2	2.66	0.44
1:B:291:LEU:HD11	1:B:348:PRO:HB3	1.99	0.44
1:C:135:SER:O	1:C:136:GLY:C	2.61	0.44
1:C:151:GLU:O	1:C:185:ARG:NH1	2.51	0.44
1:C:162:SER:O	1:C:163:ASN:HB2	2.18	0.44
1:A:135:SER:O	1:A:136:GLY:C	2.61	0.44
1:C:20:LYS:O	1:C:21:ASP:C	2.60	0.44
1:A:207:LEU:HD12	1:A:207:LEU:N	2.34	0.43
1:C:102:LEU:C	1:C:104:GLY:N	2.76	0.43
1:C:110:ILE:O	1:C:111:ASN:HB3	2.17	0.43
1:C:159:GLU:N	1:C:160:PRO:CD	2.81	0.43
1:A:121:LEU:O	1:A:123:LEU:HD22	2.19	0.43
1:B:320:ILE:HG23	1:B:321:PRO:HD2	1.99	0.43
1:C:49:ILE:HA	1:C:60:LEU:HD21	1.99	0.43
1:C:135:SER:HB3	2:D:382:ATP:O5'	2.18	0.43
1:D:237:PRO:O	1:D:238:LYS:O	2.35	0.43
1:D:347:LEU:HD13	1:D:347:LEU:O	2.18	0.43
1:A:159:GLU:N	1:A:160:PRO:CD	2.81	0.43
1:B:208:ASP:HB2	1:B:229:PHE:CZ	2.53	0.43
1:C:121:LEU:O	1:C:123:LEU:HD22	2.18	0.43
1:D:26:ILE:HG23	1:D:32:VAL:HG21	2.00	0.43
1:C:259:PRO:HB2	1:C:322:SER:HB3	2.00	0.43
1:C:350:GLU:H	1:C:350:GLU:HG3	1.48	0.43
1:A:162:SER:O	1:A:163:ASN:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:GLY:O	1:A:348:PRO:HD3	2.18	0.43
1:B:235:GLY:O	1:B:236:SER:O	2.37	0.43
1:B:270:VAL:CG1	1:B:362:CYS:HB3	2.46	0.43
1:C:140:GLN:NE2	1:C:160:PRO:C	2.76	0.43
1:D:86:LEU:O	1:D:88:PRO:HD3	2.19	0.43
1:D:87:TYR:HB3	1:D:89:HIS:CE1	2.53	0.43
1:D:253:GLN:HB3	1:D:267:TRP:HE3	1.84	0.43
1:C:18:VAL:HG22	1:C:18:VAL:O	2.17	0.43
1:D:258:LEU:HD12	1:D:260:MET:HE2	2.00	0.43
1:A:260:MET:N	1:A:260:MET:HE2	2.33	0.43
1:C:79:MET:HE3	1:C:156:LEU:CD1	2.46	0.43
1:C:207:LEU:HD12	1:C:207:LEU:N	2.34	0.43
1:B:46:LEU:HD23	1:B:158:ASP:HB2	1.99	0.43
1:C:6:LEU:HD12	1:C:6:LEU:N	2.34	0.43
1:C:120:VAL:HG23	1:C:121:LEU:N	2.34	0.43
1:A:10:THR:HA	1:A:19:SER:O	2.19	0.43
1:A:86:LEU:HD12	1:A:139:ARG:HB3	2.00	0.43
1:B:258:LEU:HD12	1:B:260:MET:HE2	2.00	0.43
1:C:87:TYR:HB3	1:C:89:HIS:CE1	2.54	0.43
1:A:120:VAL:HG23	1:A:121:LEU:N	2.34	0.42
1:A:253:GLN:HB3	1:A:267:TRP:CE3	2.54	0.42
1:D:66:ARG:HG3	1:D:68:ASN:ND2	2.34	0.42
1:A:59:ASP:HB2	1:A:61:PHE:HE1	1.84	0.42
1:A:135:SER:HB3	2:B:382:ATP:O5'	2.18	0.42
1:A:289:HIS:O	1:A:348:PRO:CG	2.67	0.42
1:B:126:LEU:O	1:B:129:ARG:HB2	2.20	0.42
1:C:17:VAL:HG11	1:C:20:LYS:HD2	2.00	0.42
1:D:126:LEU:O	1:D:129:ARG:HB2	2.20	0.42
1:A:92:VAL:HG12	1:A:96:MET:CE	2.46	0.42
1:A:106:LYS:O	1:A:110:ILE:HG22	2.19	0.42
1:A:107:LYS:HA	1:A:110:ILE:HG22	2.02	0.42
1:A:140:GLN:NE2	1:A:160:PRO:C	2.76	0.42
1:B:117:VAL:HG11	1:B:149:VAL:CG2	2.49	0.42
1:B:253:GLN:O	1:B:254:VAL:HG23	2.19	0.42
1:C:107:LYS:HA	1:C:110:ILE:HG22	2.02	0.42
1:D:47:ARG:HG2	1:D:47:ARG:NH1	2.35	0.42
1:A:15:GLU:O	1:A:15:GLU:HG3	2.20	0.42
1:B:253:GLN:C	1:B:254:VAL:HG23	2.44	0.42
1:A:241:PHE:C	1:A:242:LEU:HD12	2.45	0.42
1:B:26:ILE:HG23	1:B:32:VAL:HG21	2.00	0.42
1:B:110:ILE:C	1:B:112:GLN:N	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:PHE:C	1:B:242:LEU:HD12	2.45	0.42
1:C:24:LEU:HD11	1:C:34:PHE:HE1	1.85	0.42
1:C:321:PRO:O	1:C:322:SER:OG	2.30	0.42
1:D:208:ASP:HB2	1:D:229:PHE:CZ	2.54	0.42
1:D:364:ARG:NH2	1:D:368:GLU:HG3	2.35	0.42
1:A:113:ARG:HA	1:A:116:GLN:CG	2.50	0.42
1:A:135:SER:HB3	2:B:382:ATP:C5'	2.50	0.42
1:B:47:ARG:HG2	1:B:47:ARG:NH1	2.35	0.42
1:B:208:ASP:O	1:B:209:ALA:C	2.62	0.42
1:C:10:THR:HA	1:C:19:SER:O	2.19	0.42
1:C:135:SER:HB3	2:D:382:ATP:C5'	2.50	0.42
1:C:235:GLY:O	1:C:236:SER:C	2.63	0.42
1:C:241:PHE:C	1:C:242:LEU:HD12	2.45	0.42
1:D:109:VAL:HG22	1:D:109:VAL:O	2.20	0.42
1:A:24:LEU:HD11	1:A:34:PHE:HE1	1.85	0.42
1:A:259:PRO:HB2	1:A:322:SER:HB3	2.00	0.42
1:B:290:LEU:HB2	1:B:329:TYR:HD1	1.85	0.42
1:D:208:ASP:O	1:D:209:ALA:C	2.62	0.42
1:D:290:LEU:HB2	1:D:329:TYR:HD1	1.85	0.42
1:B:306:VAL:HG12	1:B:307:VAL:N	2.35	0.42
1:C:106:LYS:O	1:C:110:ILE:HG22	2.19	0.42
1:C:157:LEU:HD11	1:C:187:MET:HE2	2.02	0.42
1:C:113:ARG:HA	1:C:116:GLN:CG	2.50	0.42
1:D:117:VAL:HG11	1:D:149:VAL:CG2	2.49	0.42
1:B:66:ARG:HG3	1:B:68:ASN:ND2	2.34	0.41
1:D:241:PHE:C	1:D:242:LEU:HD12	2.45	0.41
1:B:81:PHE:CE2	1:B:156:LEU:O	2.73	0.41
1:B:240:ASN:O	1:B:284:GLY:HA2	2.20	0.41
1:C:289:HIS:O	1:C:348:PRO:CG	2.68	0.41
1:A:270:VAL:HG13	1:A:362:CYS:HB3	2.03	0.41
1:B:109:VAL:HG22	1:B:109:VAL:O	2.20	0.41
1:C:59:ASP:HB2	1:C:61:PHE:HE1	1.84	0.41
1:A:157:LEU:HD11	1:A:187:MET:HE2	2.02	0.41
1:B:131:PRO:C	1:B:133:ALA:H	2.28	0.41
1:C:12:ALA:HB2	1:C:17:VAL:HA	2.03	0.41
1:D:309:GLN:NE2	1:D:309:GLN:HA	2.35	0.41
1:A:134:LEU:HD22	1:A:138:GLN:NE2	2.36	0.41
1:B:117:VAL:C	1:B:119:GLU:N	2.77	0.41
1:B:306:VAL:HB	1:B:317:HIS:HB2	2.01	0.41
1:C:46:LEU:HD11	1:C:188:ILE:HG22	2.03	0.41
1:C:84:TYR:O	1:C:85:ALA:CB	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:300:LEU:HD12	1:D:300:LEU:N	2.35	0.41
1:C:11:LYS:HG3	1:C:18:VAL:CG1	2.51	0.41
1:D:70:THR:HB	1:D:75:ARG:CD	2.51	0.41
1:D:306:VAL:HB	1:D:317:HIS:HB2	2.01	0.41
1:B:11:LYS:HB2	1:B:48:MET:SD	2.61	0.41
1:B:300:LEU:HD12	1:B:300:LEU:N	2.35	0.41
1:C:166:ALA:O	1:C:170:VAL:HG23	2.21	0.41
1:C:228:ARG:HG2	1:C:228:ARG:NH1	2.35	0.41
1:D:240:ASN:O	1:D:284:GLY:HA2	2.20	0.41
1:A:12:ALA:HB2	1:A:17:VAL:HA	2.03	0.41
1:A:166:ALA:O	1:A:170:VAL:HG23	2.21	0.41
1:A:318:ILE:HD12	1:A:345:ILE:HD13	2.03	0.41
1:B:296:ALA:O	1:B:297:ASP:HB2	2.21	0.41
1:B:309:GLN:HA	1:B:309:GLN:NE2	2.35	0.41
1:C:12:ALA:CB	1:C:17:VAL:HA	2.51	0.41
1:C:15:GLU:O	1:C:15:GLU:HG3	2.20	0.41
1:C:92:VAL:HG12	1:C:96:MET:CE	2.50	0.41
1:C:253:GLN:HB3	1:C:267:TRP:HE3	1.86	0.41
1:C:362:CYS:O	1:C:363:ARG:C	2.64	0.41
1:D:202:ASP:O	1:D:203:LYS:HB2	2.21	0.41
1:D:237:PRO:O	1:D:238:LYS:C	2.64	0.41
1:D:306:VAL:HG12	1:D:307:VAL:N	2.35	0.41
1:D:321:PRO:O	1:D:322:SER:CB	2.69	0.41
1:C:65:LYS:O	1:C:67:MET:HG3	2.21	0.41
1:D:157:LEU:HD11	1:D:187:MET:CE	2.48	0.41
1:D:235:GLY:O	1:D:236:SER:O	2.39	0.41
1:A:101:LYS:NZ	1:A:102:LEU:CG	2.82	0.40
1:B:46:LEU:CD2	1:B:158:ASP:HB2	2.51	0.40
1:D:33:VAL:CG1	1:D:201:ALA:HB2	2.47	0.40
1:B:4:VAL:O	1:B:26:ILE:O	2.40	0.40
1:C:173:ARG:HE	1:C:196:GLU:CG	2.31	0.40
1:C:318:ILE:HD12	1:C:345:ILE:HD13	2.03	0.40
1:D:110:ILE:C	1:D:112:GLN:N	2.78	0.40
1:A:7:GLN:C	1:A:9:VAL:N	2.79	0.40
1:A:305:GLN:O	1:A:339:GLU:HG3	2.22	0.40
1:D:117:VAL:C	1:D:119:GLU:N	2.77	0.40
1:B:70:THR:HB	1:B:75:ARG:CD	2.51	0.40
1:C:11:LYS:HG3	1:C:18:VAL:HG12	2.03	0.40
1:D:305:GLN:HG3	1:D:326:ASN:OD1	2.21	0.40
1:A:12:ALA:CB	1:A:17:VAL:HA	2.51	0.40
1:A:46:LEU:HD11	1:A:188:ILE:HG22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ARG:HE	1:A:196:GLU:CG	2.31	0.40
1:A:362:CYS:O	1:A:363:ARG:C	2.64	0.40
1:B:255:GLN:HB2	1:B:267:TRP:CE2	2.56	0.40
1:C:95:ASN:O	1:C:96:MET:CB	2.61	0.40
1:D:296:ALA:O	1:D:297:ASP:HB2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:GLN:NE2	1:C:85:ALA:CB[1_554]	2.02	0.18

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	365/381 (96%)	307 (84%)	47 (13%)	11 (3%)	3	6
1	B	365/381 (96%)	305 (84%)	41 (11%)	19 (5%)	1	2
1	C	365/381 (96%)	304 (83%)	52 (14%)	9 (2%)	4	8
1	D	365/381 (96%)	306 (84%)	42 (12%)	17 (5%)	2	2
All	All	1460/1524 (96%)	1222 (84%)	182 (12%)	56 (4%)	2	3

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	SER
1	A	254	VAL
1	A	322	SER
1	B	73	ALA
1	B	83	SER

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Mol	Chain	Res	Type
1	B	203	LYS
1	B	236	SER
1	B	238	LYS
1	B	324	ARG
1	C	85	ALA
1	C	236	SER
1	C	254	VAL
1	C	322	SER
1	D	73	ALA
1	D	83	SER
1	D	236	SER
1	D	238	LYS
1	D	254	VAL
1	D	324	ARG
1	A	21	ASP
1	A	107	LYS
1	A	251	ILE
1	A	339	GLU
1	B	66	ARG
1	B	107	LYS
1	B	254	VAL
1	B	295	ILE
1	C	21	ASP
1	C	107	LYS
1	C	339	GLU
1	D	66	ARG
1	D	107	LYS
1	D	203	LYS
1	D	295	ILE
1	A	5	GLN
1	A	85	ALA
1	B	64	GLU
1	B	82	GLN
1	B	296	ALA
1	D	64	GLU
1	D	82	GLN
1	D	296	ALA
1	B	80	VAL
1	D	80	VAL
1	D	363	ARG
1	B	84	TYR
1	B	152	PRO

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Mol	Chain	Res	Type
1	B	363	ARG
1	C	298	VAL
1	D	152	PRO
1	A	298	VAL
1	B	85	ALA
1	B	237	PRO
1	D	237	PRO
1	A	295	ILE
1	C	295	ILE

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	312/323 (97%)	296 (95%)	16 (5%)	21	45
1	B	312/323 (97%)	296 (95%)	16 (5%)	21	45
1	C	312/323 (97%)	294 (94%)	18 (6%)	18	39
1	D	312/323 (97%)	296 (95%)	16 (5%)	21	45
All	All	1248/1292 (97%)	1182 (95%)	66 (5%)	20	43

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	53	GLU
1	A	68	ASN
1	A	82	GLN
1	A	116	GLN
1	A	127	LEU
1	A	131	PRO
1	A	163	ASN
1	A	219	LEU
1	A	266	VAL
1	A	270	VAL
1	A	274	ASP

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Mol	Chain	Res	Type
1	A	288	GLU
1	A	342	THR
1	A	350	GLU
1	A	367	LYS
1	B	10	THR
1	B	25	ASP
1	B	33	VAL
1	B	68	ASN
1	B	79	MET
1	B	83	SER
1	B	113	ARG
1	B	115	ASN
1	B	116	GLN
1	B	123	LEU
1	B	130	LYS
1	B	234	ILE
1	B	270	VAL
1	B	288	GLU
1	B	298	VAL
1	B	350	GLU
1	C	23	ASN
1	C	53	GLU
1	C	68	ASN
1	C	82	GLN
1	C	116	GLN
1	C	127	LEU
1	C	131	PRO
1	C	163	ASN
1	C	219	LEU
1	C	249	THR
1	C	266	VAL
1	C	270	VAL
1	C	274	ASP
1	C	288	GLU
1	C	297	ASP
1	C	342	THR
1	C	350	GLU
1	C	367	LYS
1	D	10	THR
1	D	25	ASP
1	D	33	VAL
1	D	68	ASN

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Mol	Chain	Res	Type
1	D	79	MET
1	D	83	SER
1	D	113	ARG
1	D	115	ASN
1	D	116	GLN
1	D	123	LEU
1	D	130	LYS
1	D	234	ILE
1	D	270	VAL
1	D	288	GLU
1	D	298	VAL
1	D	350	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	23	ASN
1	A	68	ASN
1	A	82	GLN
1	A	122	GLN
1	A	255	GLN
1	A	309	GLN
1	A	315	GLN
1	A	353	HIS
1	B	68	ASN
1	B	95	ASN
1	B	116	GLN
1	B	122	GLN
1	B	138	GLN
1	B	163	ASN
1	B	171	GLN
1	B	180	HIS
1	B	265	GLN
1	B	280	ASN
1	B	309	GLN
1	B	315	GLN
1	B	325	GLN
1	B	331	GLN
1	B	332	ASN
1	C	23	ASN
1	C	68	ASN

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Mol	Chain	Res	Type
1	C	82	GLN
1	C	122	GLN
1	C	138	GLN
1	C	255	GLN
1	C	309	GLN
1	C	315	GLN
1	C	353	HIS
1	D	68	ASN
1	D	95	ASN
1	D	116	GLN
1	D	122	GLN
1	D	138	GLN
1	D	163	ASN
1	D	171	GLN
1	D	180	HIS
1	D	265	GLN
1	D	280	ASN
1	D	309	GLN
1	D	315	GLN
1	D	325	GLN
1	D	331	GLN
1	D	332	ASN
1	D	366	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ATP	C	382	-	32,33,33	2.40	8 (25%)	48,52,52	3.06	13 (27%)
2	ATP	B	382	-	32,33,33	2.46	9 (28%)	48,52,52	3.11	12 (25%)
2	ATP	D	382	-	32,33,33	2.46	9 (28%)	48,52,52	3.11	12 (25%)
2	ATP	A	382	-	32,33,33	2.40	6 (18%)	48,52,52	3.06	13 (27%)

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	C	382	-	-	2/22/38/38	0/3/3/3
2	ATP	B	382	-	-	2/22/38/38	0/3/3/3
2	ATP	D	382	-	-	2/22/38/38	0/3/3/3
2	ATP	A	382	-	-	2/22/38/38	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	382	ATP	PB-O3A	9.07	1.69	1.59
2	B	382	ATP	PB-O3A	9.06	1.69	1.59
2	A	382	ATP	PB-O3A	8.94	1.69	1.59
2	C	382	ATP	PB-O3A	8.93	1.69	1.59
2	A	382	ATP	C4-N3	5.12	1.44	1.34
2	C	382	ATP	C4-N3	5.12	1.44	1.34
2	B	382	ATP	C4-N3	5.03	1.43	1.34
2	D	382	ATP	C4-N3	5.01	1.43	1.34
2	D	382	ATP	O5'-C5'	-4.78	1.26	1.44
2	B	382	ATP	O5'-C5'	-4.77	1.26	1.44
2	C	382	ATP	O5'-C5'	-4.58	1.27	1.44
2	A	382	ATP	O5'-C5'	-4.57	1.27	1.44
2	B	382	ATP	PA-O5'	-3.37	1.46	1.59
2	D	382	ATP	PA-O5'	-3.36	1.46	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	382	ATP	PA-O5'	-3.08	1.47	1.59
2	A	382	ATP	PA-O5'	-3.08	1.47	1.59
2	B	382	ATP	PB-O1B	-2.40	1.42	1.50
2	D	382	ATP	PB-O1B	-2.40	1.42	1.50
2	C	382	ATP	C3'-C4'	-2.25	1.47	1.53
2	A	382	ATP	C3'-C4'	-2.23	1.47	1.53
2	D	382	ATP	PB-O2B	-2.15	1.45	1.55
2	B	382	ATP	PB-O2B	-2.14	1.45	1.55
2	A	382	ATP	PB-O1B	-2.14	1.43	1.50
2	D	382	ATP	C3'-C4'	-2.13	1.47	1.53
2	B	382	ATP	C3'-C4'	-2.13	1.47	1.53
2	C	382	ATP	PB-O1B	-2.13	1.43	1.50
2	B	382	ATP	C8-N9	2.11	1.41	1.37
2	D	382	ATP	C8-N9	2.11	1.41	1.37
2	D	382	ATP	O4'-C1'	2.04	1.46	1.42
2	B	382	ATP	O4'-C1'	2.04	1.46	1.42
2	C	382	ATP	C8-N9	2.03	1.41	1.37
2	C	382	ATP	PB-O2B	-2.00	1.46	1.55

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	382	ATP	O5'-C5'-C4'	12.42	151.30	108.99
2	A	382	ATP	O5'-C5'-C4'	12.42	151.27	108.99
2	D	382	ATP	O5'-C5'-C4'	12.30	150.89	108.99
2	B	382	ATP	O5'-C5'-C4'	12.30	150.87	108.99
2	D	382	ATP	O3A-PB-O1B	-8.32	85.69	110.70
2	B	382	ATP	O3A-PB-O1B	-8.30	85.72	110.70
2	C	382	ATP	O3A-PB-O1B	-8.03	86.56	110.70
2	A	382	ATP	O3A-PB-O1B	-8.03	86.56	110.70
2	D	382	ATP	O5'-PA-O1A	-7.10	80.80	108.94
2	B	382	ATP	O5'-PA-O1A	-7.09	80.83	108.94
2	A	382	ATP	O5'-PA-O1A	-6.38	83.64	108.94
2	C	382	ATP	O5'-PA-O1A	-6.37	83.68	108.94
2	B	382	ATP	PA-O5'-C5'	6.10	156.31	121.35
2	D	382	ATP	PA-O5'-C5'	6.10	156.29	121.35
2	C	382	ATP	PA-O5'-C5'	5.85	154.85	121.35
2	A	382	ATP	PA-O5'-C5'	5.84	154.83	121.35
2	B	382	ATP	C5'-C4'-C3'	-5.72	94.63	115.21
2	D	382	ATP	C5'-C4'-C3'	-5.72	94.63	115.21
2	A	382	ATP	C5'-C4'-C3'	-5.47	95.53	115.21
2	C	382	ATP	C5'-C4'-C3'	-5.46	95.57	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	382	ATP	O2A-PA-O3A	4.77	120.16	107.27
2	C	382	ATP	O2A-PA-O3A	4.75	120.12	107.27
2	D	382	ATP	O2B-PB-O3B	4.71	119.99	107.27
2	C	382	ATP	O4'-C4'-C3'	4.70	114.49	105.15
2	B	382	ATP	O2B-PB-O3B	4.70	119.97	107.27
2	A	382	ATP	O4'-C4'-C3'	4.69	114.46	105.15
2	D	382	ATP	O2A-PA-O3A	4.44	119.28	107.27
2	B	382	ATP	O2A-PA-O3A	4.44	119.27	107.27
2	A	382	ATP	O2B-PB-O3B	4.41	119.20	107.27
2	C	382	ATP	O2B-PB-O3B	4.41	119.19	107.27
2	D	382	ATP	O4'-C4'-C3'	4.31	113.71	105.15
2	B	382	ATP	O4'-C4'-C3'	4.30	113.68	105.15
2	D	382	ATP	C3'-C2'-C1'	2.87	106.89	101.46
2	B	382	ATP	C3'-C2'-C1'	2.86	106.87	101.46
2	C	382	ATP	C3'-C2'-C1'	2.58	106.35	101.46
2	A	382	ATP	C3'-C2'-C1'	2.57	106.33	101.46
2	D	382	ATP	O3A-PA-O1A	2.40	117.92	110.70
2	B	382	ATP	O3A-PA-O1A	2.40	117.91	110.70
2	C	382	ATP	O2A-PA-O1A	2.30	123.15	112.44
2	A	382	ATP	O2A-PA-O1A	2.29	123.10	112.44
2	B	382	ATP	O3B-PB-O1B	2.23	117.40	110.70
2	D	382	ATP	O3B-PB-O1B	2.22	117.40	110.70
2	B	382	ATP	O2A-PA-O1A	2.19	122.65	112.44
2	D	382	ATP	O2A-PA-O1A	2.19	122.64	112.44
2	C	382	ATP	O2A-PA-O5'	-2.17	97.71	107.57
2	A	382	ATP	O2A-PA-O5'	-2.17	97.73	107.57
2	A	382	ATP	O2B-PB-O1B	2.09	122.17	112.44
2	C	382	ATP	O2B-PB-O1B	2.08	122.14	112.44
2	C	382	ATP	O3B-PB-O1B	2.06	116.90	110.70
2	A	382	ATP	O3B-PB-O1B	2.05	116.87	110.70

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	382	ATP	C4'-C5'-O5'-PA
2	B	382	ATP	C4'-C5'-O5'-PA
2	C	382	ATP	C4'-C5'-O5'-PA
2	D	382	ATP	C4'-C5'-O5'-PA
2	B	382	ATP	PG-O3B-PB-O2B
2	C	382	ATP	PG-O3B-PB-O2B
2	D	382	ATP	PG-O3B-PB-O2B

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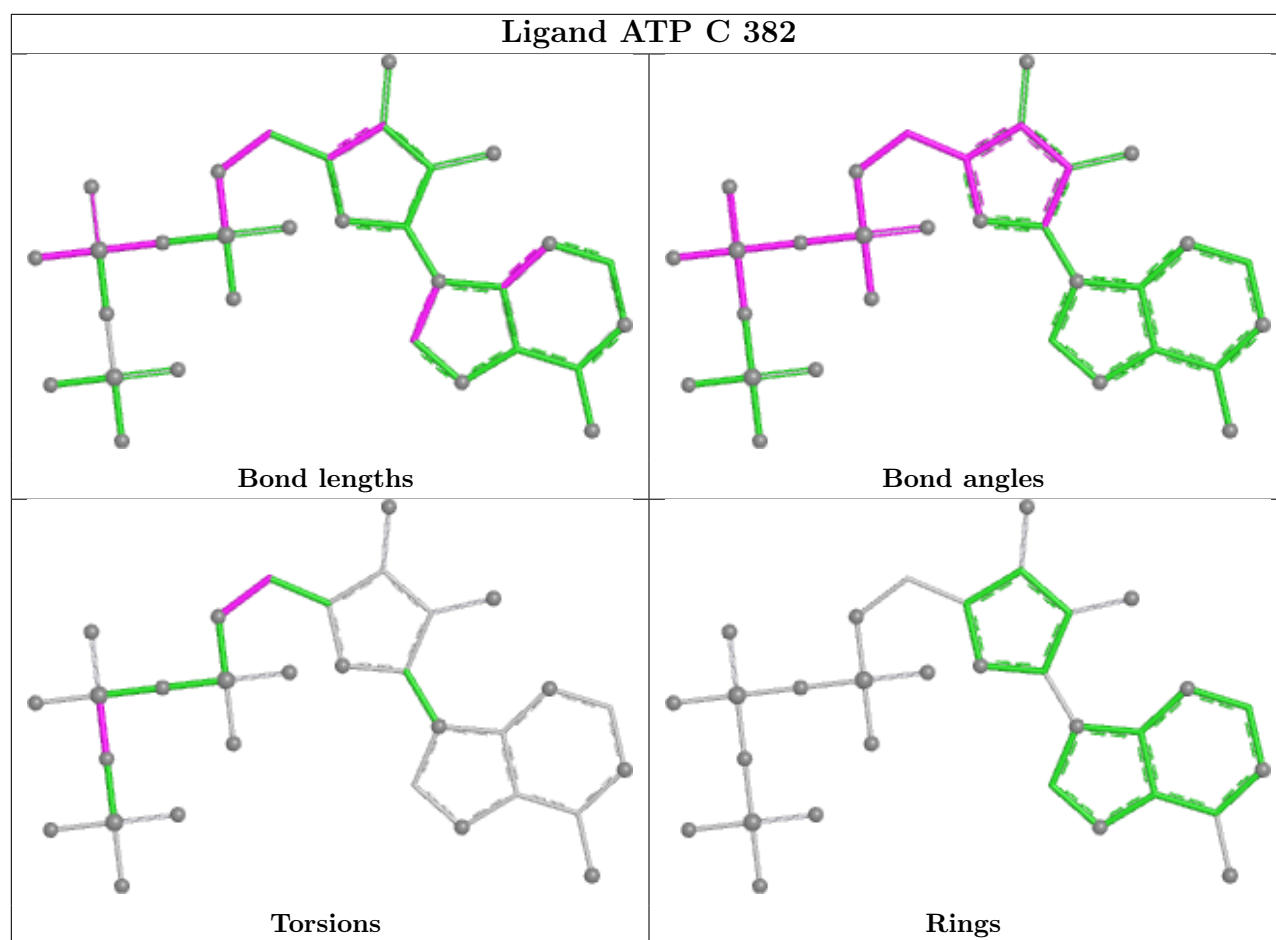
Mol	Chain	Res	Type	Atoms
2	A	382	ATP	PG-O3B-PB-O2B

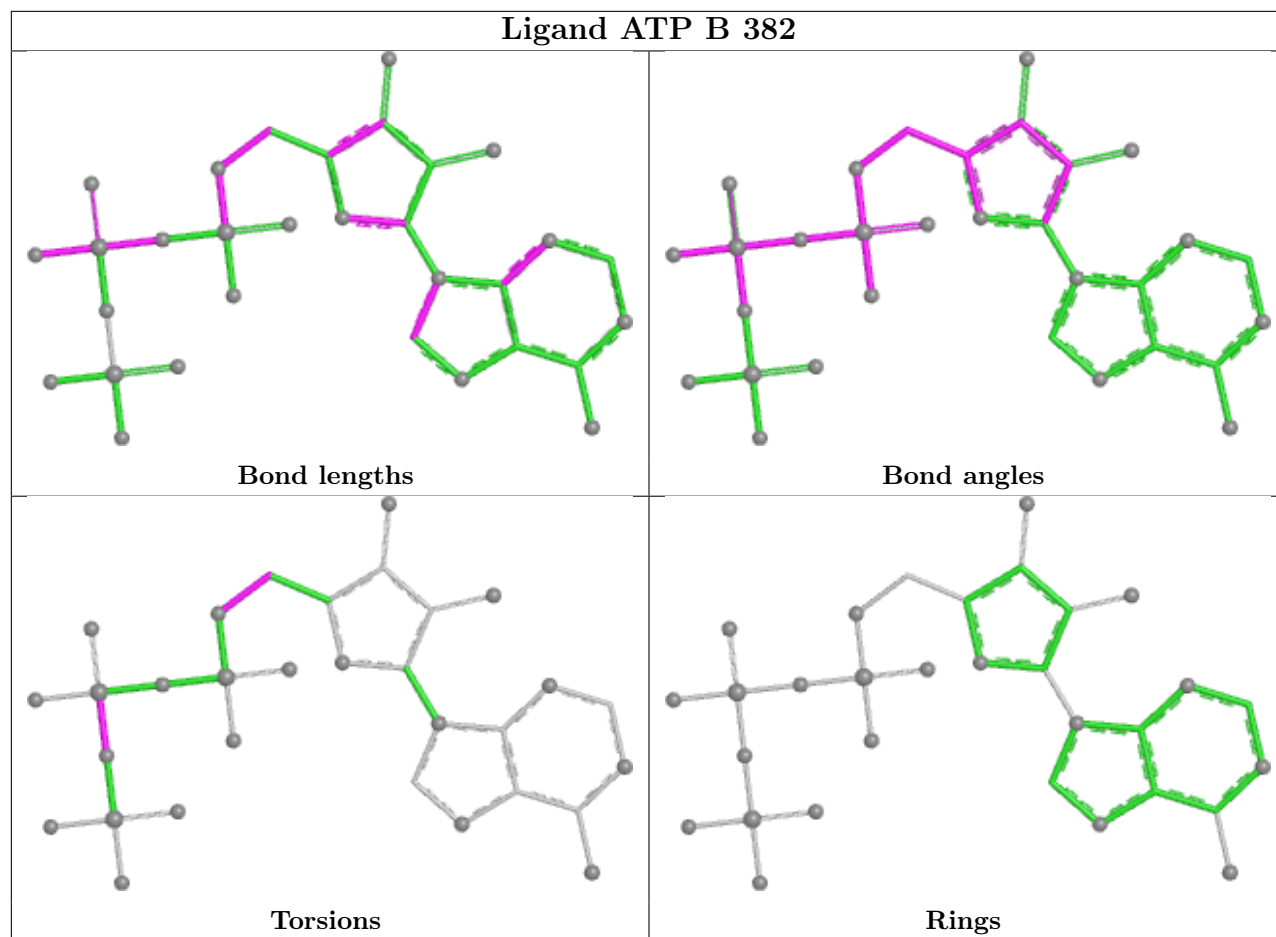
There are no ring outliers.

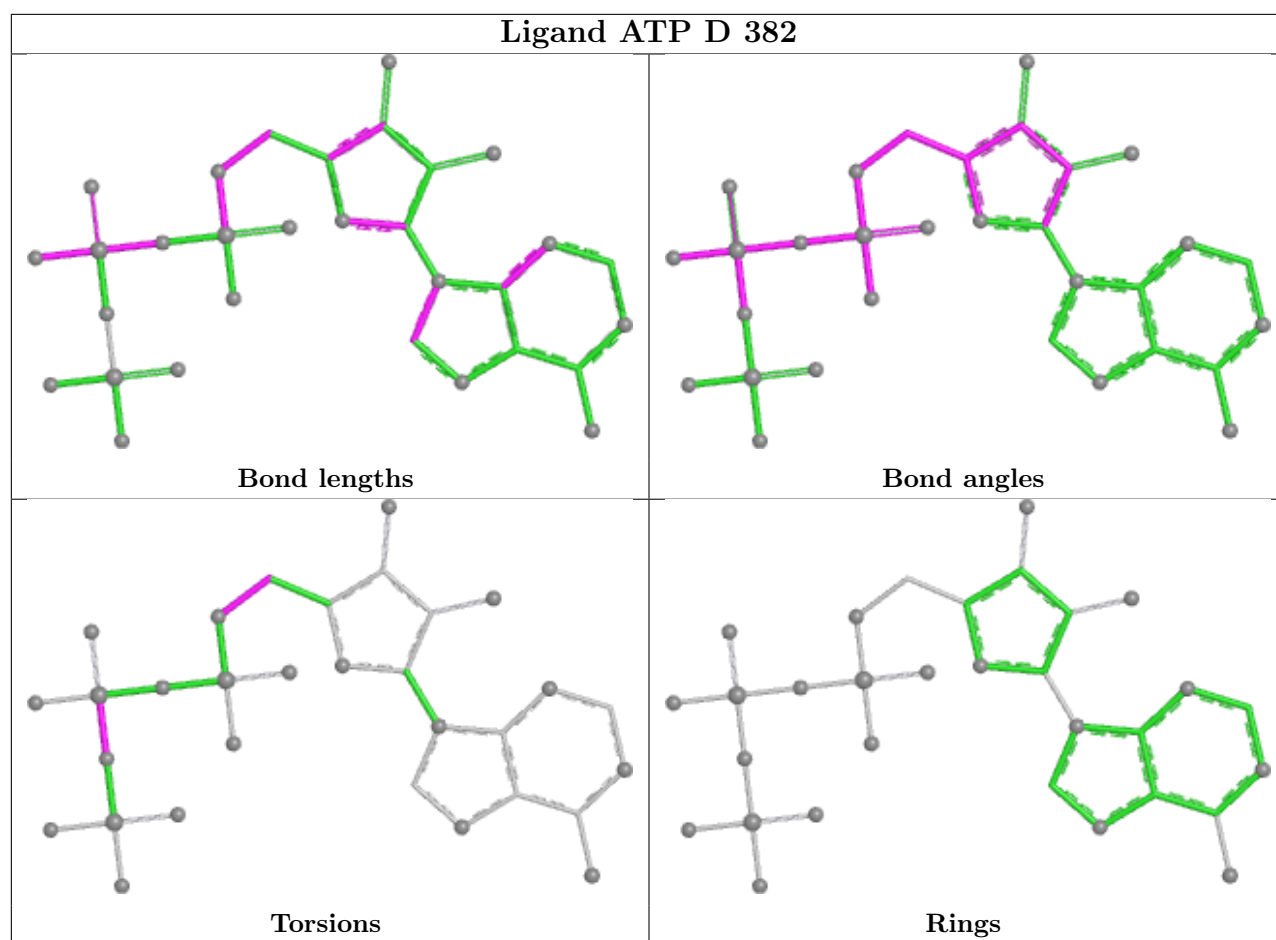
4 monomers are involved in 10 short contacts:

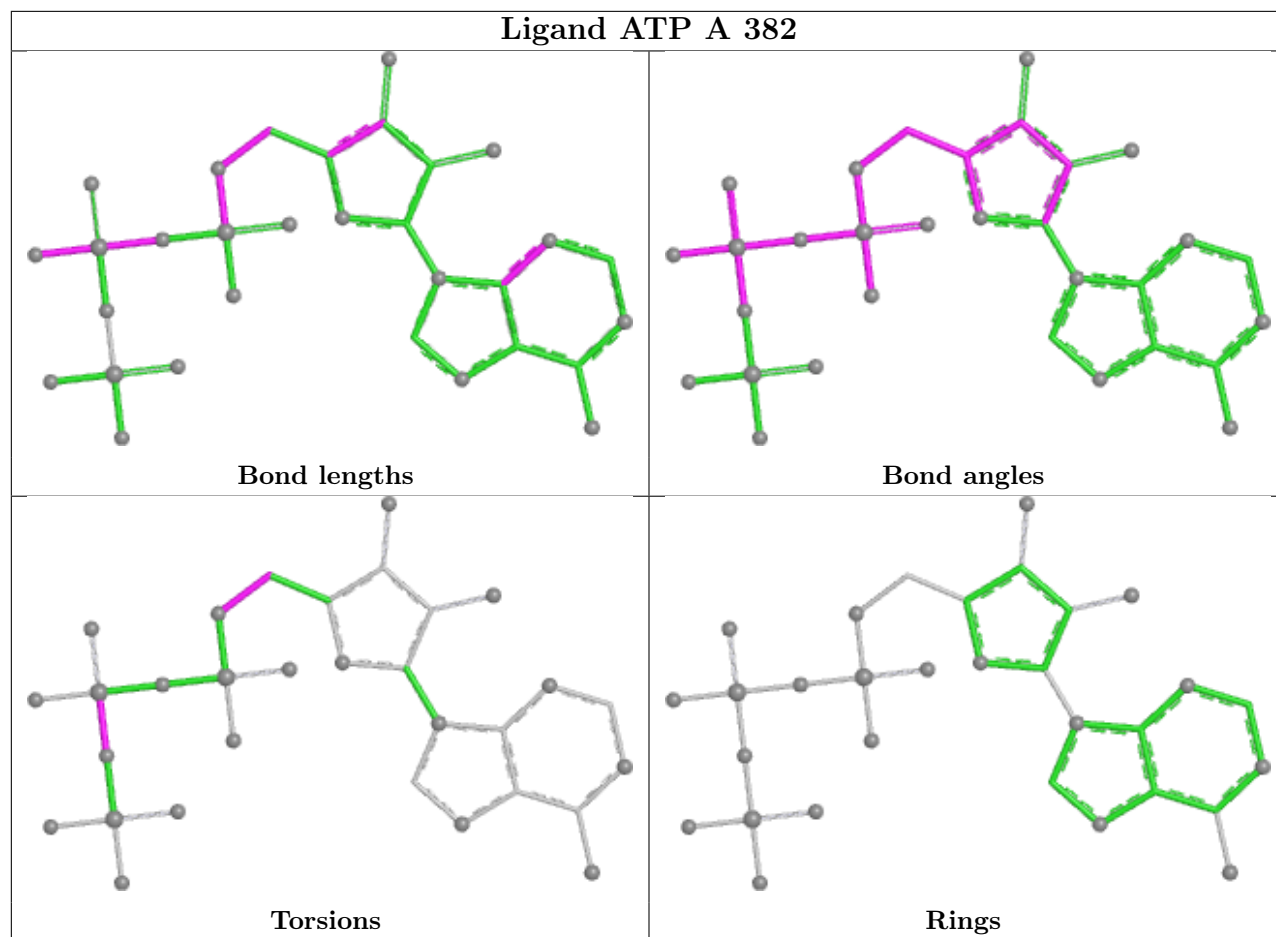
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	382	ATP	3	0
2	B	382	ATP	2	0
2	D	382	ATP	2	0
2	A	382	ATP	3	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	367/381 (96%)	0.46	26 (7%) 22 17	29, 62, 99, 121	0
1	B	367/381 (96%)	0.74	42 (11%) 10 7	36, 71, 130, 149	0
1	C	367/381 (96%)	0.51	31 (8%) 17 13	29, 62, 99, 121	0
1	D	367/381 (96%)	0.92	63 (17%) 4 3	36, 71, 130, 149	0
All	All	1468/1524 (96%)	0.66	162 (11%) 10 8	29, 67, 117, 149	0

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	253	GLN	6.2
1	B	77	VAL	6.0
1	D	102	LEU	5.8
1	B	202	ASP	5.1
1	D	253	GLN	5.0
1	B	84	TYR	5.0
1	A	85	ALA	5.0
1	A	4	VAL	4.7
1	D	105	ALA	4.6
1	B	102	LEU	4.6
1	D	100	LEU	4.6
1	B	109	VAL	4.6
1	B	100	LEU	4.5
1	B	85	ALA	4.4
1	D	85	ALA	4.4
1	D	78	GLY	4.4
1	D	110	ILE	4.4
1	A	86	LEU	4.3
1	B	253	GLN	4.3
1	D	99	GLY	4.2
1	D	103	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	295	ILE	4.0
1	D	61	PHE	4.0
1	D	97	SER	3.9
1	B	363	ARG	3.9
1	B	61	PHE	3.8
1	D	101	LYS	3.7
1	B	80	VAL	3.6
1	C	253	GLN	3.6
1	D	249	THR	3.5
1	D	370	GLY	3.5
1	D	7	GLN	3.5
1	C	85	ALA	3.4
1	B	59	ASP	3.4
1	B	105	ALA	3.3
1	D	18	VAL	3.3
1	B	55	ILE	3.3
1	C	363	ARG	3.3
1	D	108	GLU	3.3
1	D	84	TYR	3.3
1	B	78	GLY	3.2
1	A	110	ILE	3.2
1	A	297	ASP	3.1
1	C	81	PHE	3.1
1	D	65	LYS	3.1
1	B	87	TYR	3.1
1	C	62	ILE	3.1
1	D	80	VAL	3.0
1	C	83	SER	3.0
1	C	322	SER	3.0
1	C	100	LEU	3.0
1	D	202	ASP	3.0
1	B	295	ILE	3.0
1	D	73	ALA	3.0
1	C	82	GLN	2.9
1	C	86	LEU	2.9
1	D	82	GLN	2.9
1	A	95	ASN	2.9
1	B	110	ILE	2.9
1	D	4	VAL	2.9
1	D	114	VAL	2.9
1	C	84	TYR	2.9
1	B	103	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	20	LYS	2.9
1	B	75	ARG	2.8
1	D	83	SER	2.8
1	D	68	ASN	2.8
1	A	236	SER	2.8
1	D	254	VAL	2.8
1	D	81	PHE	2.8
1	D	86	LEU	2.8
1	B	4	VAL	2.8
1	A	104	GLY	2.7
1	C	4	VAL	2.7
1	B	370	GLY	2.7
1	D	13	TRP	2.7
1	B	20	LYS	2.7
1	D	71	PRO	2.7
1	D	98	PHE	2.7
1	A	276	GLN	2.6
1	B	65	LYS	2.6
1	B	68	ASN	2.6
1	B	262	ASN	2.6
1	A	261	PRO	2.6
1	D	109	VAL	2.6
1	D	77	VAL	2.6
1	A	363	ARG	2.5
1	A	29	GLY	2.5
1	C	58	GLY	2.5
1	C	109	VAL	2.5
1	B	99	GLY	2.5
1	B	82	GLN	2.5
1	C	102	LEU	2.5
1	C	135	SER	2.5
1	D	294	ASP	2.5
1	A	116	GLN	2.5
1	D	88	PRO	2.4
1	D	340	GLY	2.4
1	D	87	TYR	2.4
1	B	18	VAL	2.4
1	D	112	GLN	2.4
1	D	363	ARG	2.4
1	C	236	SER	2.4
1	D	16	VAL	2.4
1	D	8	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	297	ASP	2.4
1	B	114	VAL	2.4
1	A	100	LEU	2.3
1	A	127	LEU	2.3
1	B	236	SER	2.3
1	A	81	PHE	2.3
1	C	251	ILE	2.3
1	C	295	ILE	2.3
1	D	96	MET	2.3
1	C	87	TYR	2.3
1	D	107	LYS	2.3
1	D	115	ASN	2.3
1	A	83	SER	2.3
1	B	83	SER	2.3
1	D	150	ALA	2.3
1	B	249	THR	2.3
1	D	111	ASN	2.3
1	A	105	ALA	2.2
1	B	296	ALA	2.2
1	C	103	ALA	2.2
1	D	74	GLU	2.2
1	C	370	GLY	2.2
1	A	263	ARG	2.2
1	C	68	ASN	2.2
1	C	263	ARG	2.2
1	B	322	SER	2.2
1	A	96	MET	2.2
1	C	110	ILE	2.2
1	D	62	ILE	2.2
1	B	57	SER	2.2
1	B	81	PHE	2.2
1	C	98	PHE	2.2
1	D	56	THR	2.1
1	C	95	ASN	2.1
1	D	60	LEU	2.1
1	B	184	GLY	2.1
1	D	58	GLY	2.1
1	D	274	ASP	2.1
1	D	366	HIS	2.1
1	B	97	SER	2.1
1	B	101	LYS	2.1
1	A	90	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	79	MET	2.1
1	A	59	ASP	2.1
1	D	75	ARG	2.1
1	B	106	LYS	2.1
1	C	55	ILE	2.1
1	D	21	ASP	2.1
1	B	44	THR	2.1
1	D	59	ASP	2.0
1	A	339	GLU	2.0
1	C	114	VAL	2.0
1	D	296	ALA	2.0
1	C	96	MET	2.0
1	D	72	PRO	2.0
1	A	370	GLY	2.0
1	A	109	VAL	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](#)

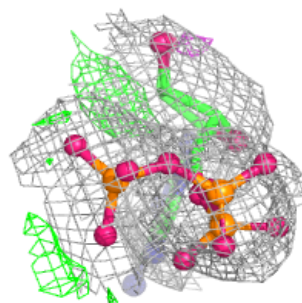
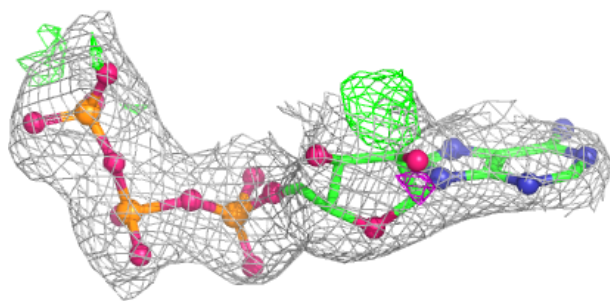
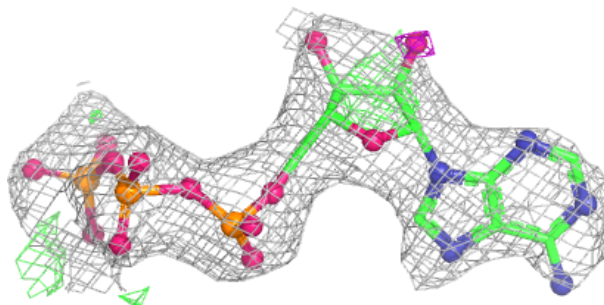
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ATP	D	382	31/31	0.86	0.13	63,87,98,98	0
2	ATP	C	382	31/31	0.91	0.13	38,78,91,92	0
2	ATP	A	382	31/31	0.92	0.12	38,78,91,92	0
2	ATP	B	382	31/31	0.92	0.11	63,87,98,98	0

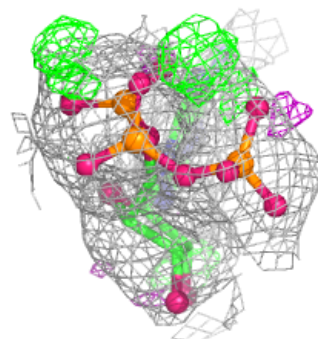
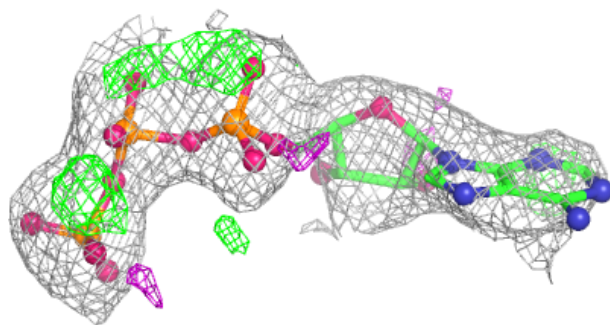
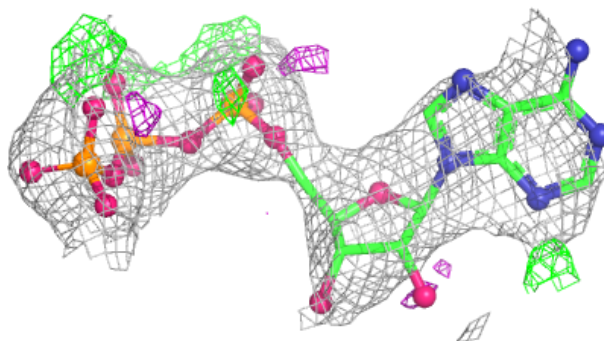
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP D 382:

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

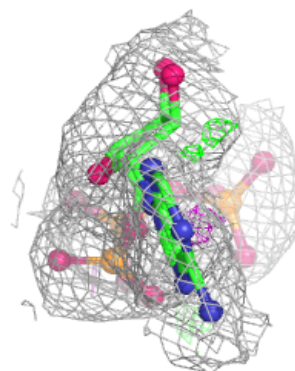
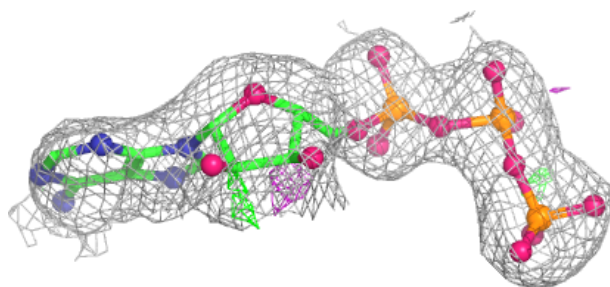
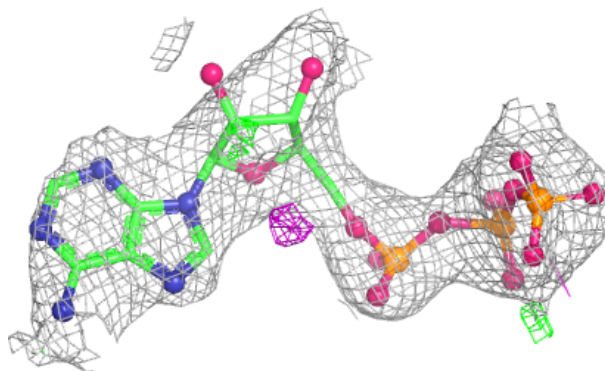
**Electron density around ATP C 382:**

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

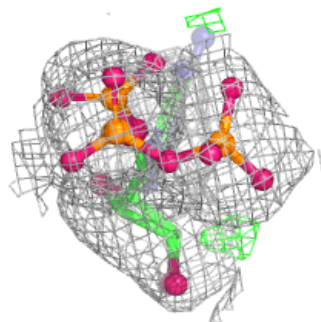
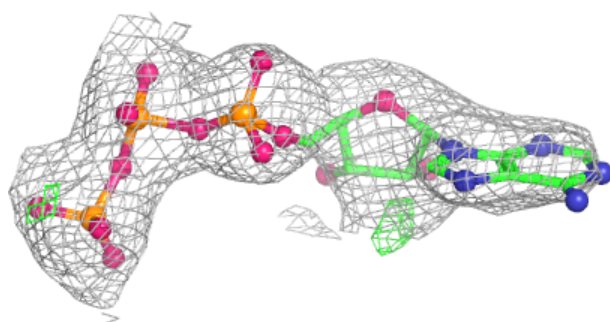
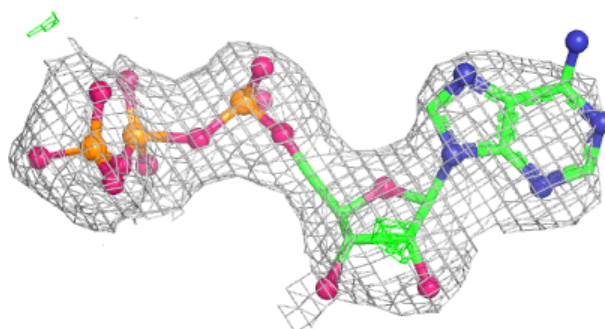


Electron density around ATP A 382:

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

**Electron density around ATP B 382:**

$2mF_o-DF_c$ (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.