



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 10:19 AM BST

PDB ID : 2E89
Title : Crystal structure of Aquifex aeolicus TilS in a complex with ATP, Magnesium ion, and L-lysine
Authors : Kuratani, M.; Yoshikawa, Y.; Takahashi, S.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2007-01-19
Resolution : 2.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.4.dev1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.4.dev1

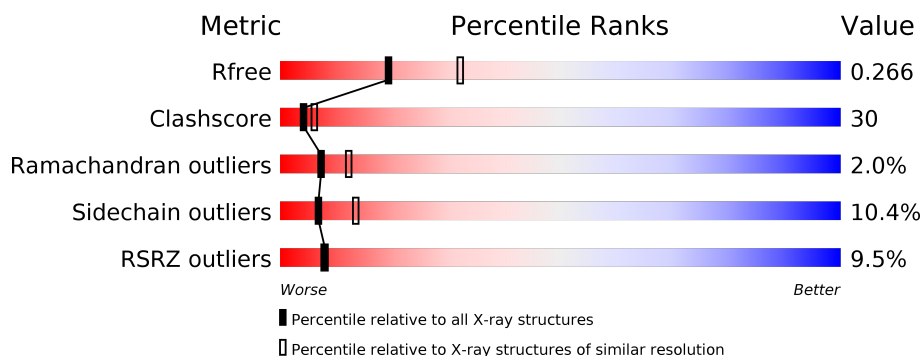
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 on 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	317	<div> <div>7%</div> <div>55%</div> <div>35%</div> <div>8%</div> <div>•</div> </div>
1	B	317	<div> <div>11%</div> <div>51%</div> <div>40%</div> <div>7%</div> <div>••</div> </div>
1	C	317	<div> <div>4%</div> <div>62%</div> <div>32%</div> <div>5%</div> <div>•</div> </div>
1	D	317	<div> <div>16%</div> <div>48%</div> <div>40%</div> <div>10%</div> <div>••</div> </div>

2 Entry composition [i](#)

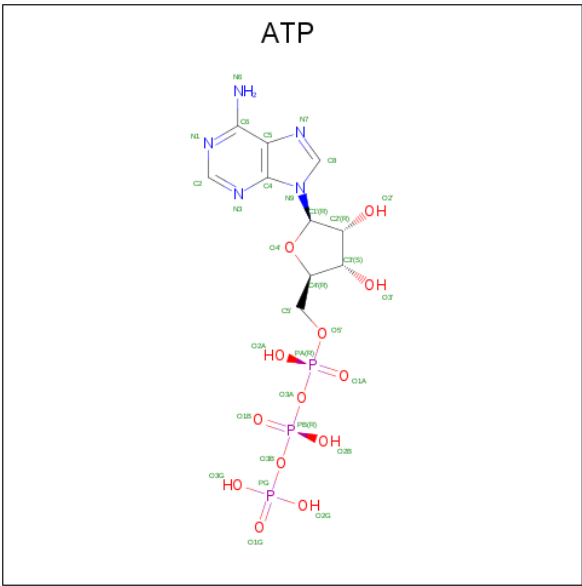
There are 5 unique types of molecules in this entry. The entry contains 10642 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called tRNA(Ile)-lysidine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	0	0
			2630	1682	467	472	9			
1	B	314	Total	C	N	O	S	0	0	0
			2606	1667	464	466	9			
1	C	314	Total	C	N	O	S	0	0	0
			2606	1667	464	466	9			
1	D	313	Total	C	N	O	S	0	0	0
			2600	1664	463	464	9			

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



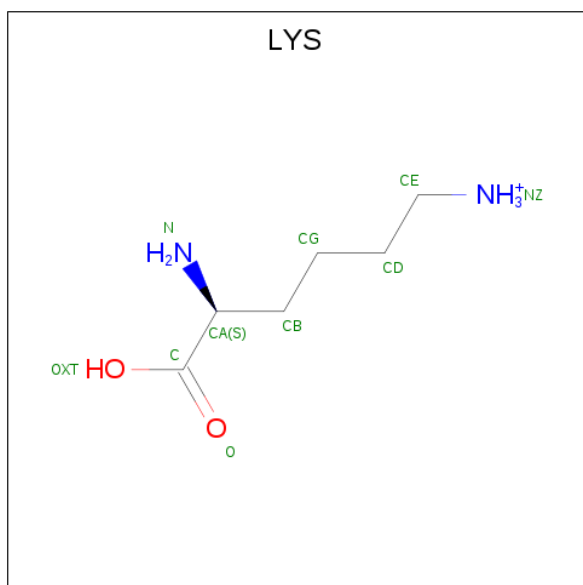
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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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 LYSINE (three-letter code: LYS) (formula: $C_6H_{15}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			10	6	2	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	15	Total	O	0	0
			15	15		
5	B	12	Total	O	0	0
			12	12		
5	C	33	Total	O	0	0
			33	33		

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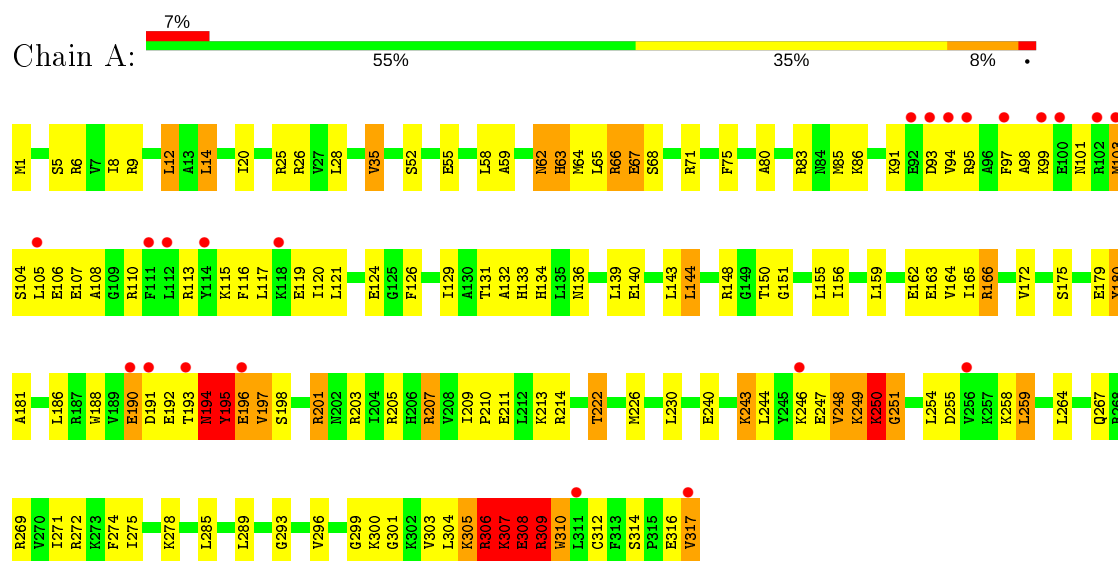
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	5	Total	O	0	0
			5	5		

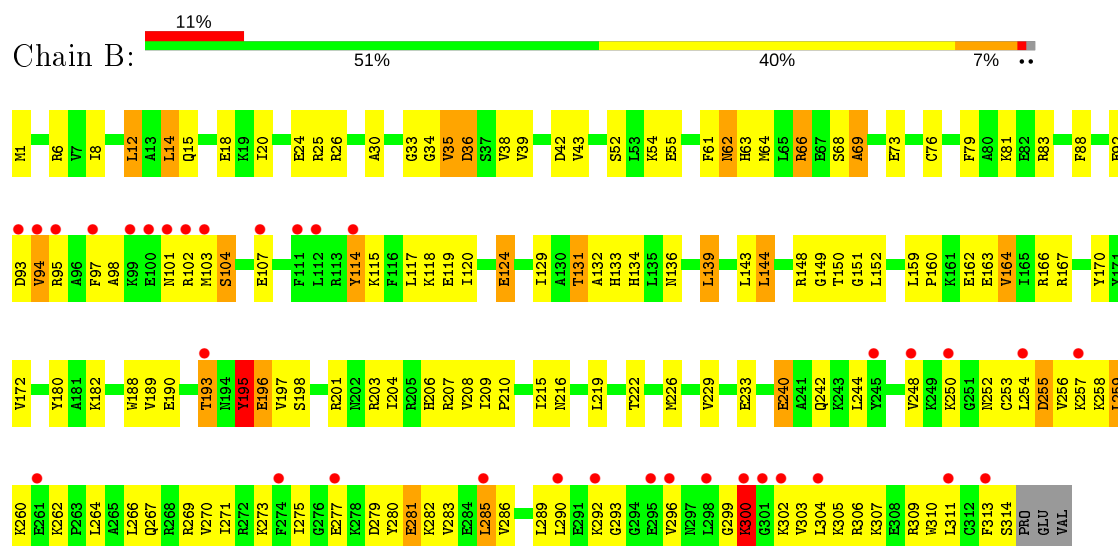
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: tRNA(Ile)-lysine synthase

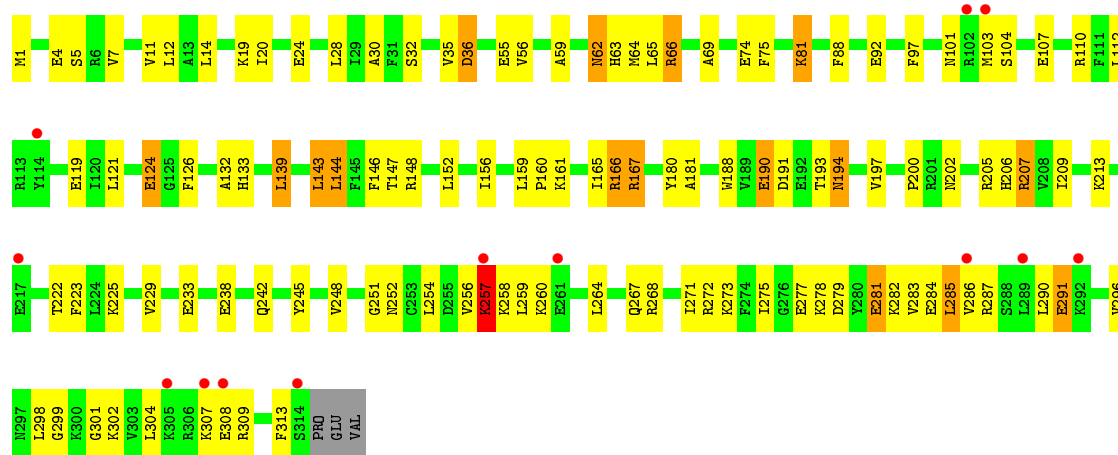


• Molecule 1: tRNA(Ile)-lysine synthase

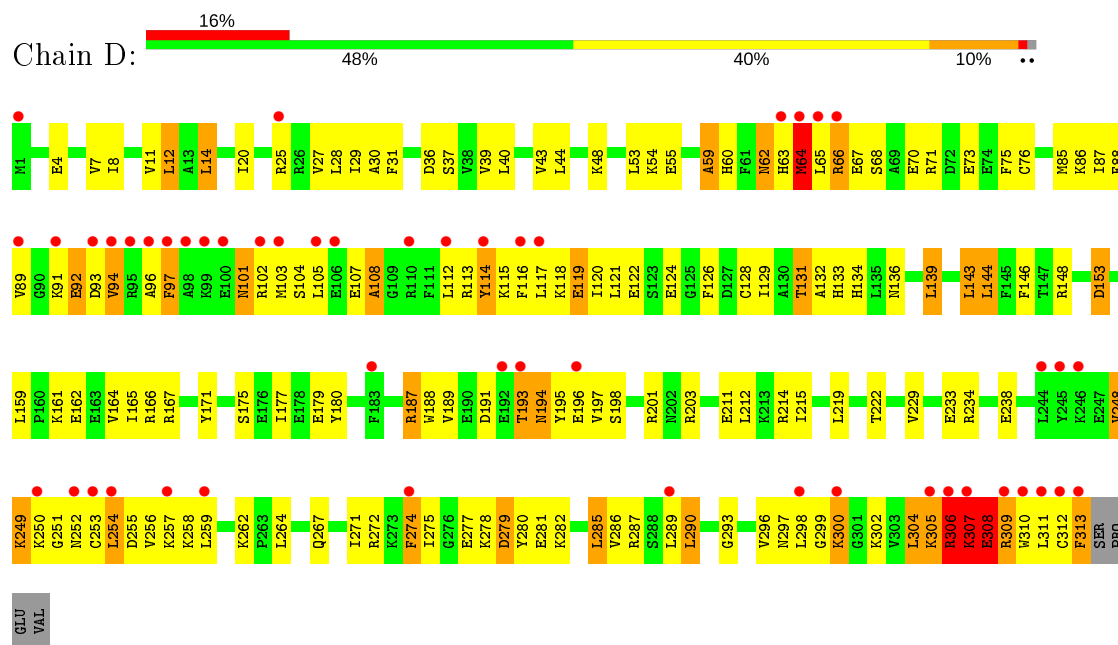


• Molecule 1: tRNA(Ile)-lysine synthase





• Molecule 1: tRNA(Ile)-lysidine synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	97.42Å 81.57Å 109.11Å 90.00° 105.98° 90.00°	Depositor
Resolution (Å)	44.03 – 2.50 44.03 – 2.40	Depositor EDS
% Data completeness (in resolution range)	91.8 (44.03-2.50) 89.4 (44.03-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.229 , 0.274 0.219 , 0.266	Depositor DCC
R_{free} test set	2920 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	41.7	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10642	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	1.03	28/2672 (1.0%)	0.83	11/3569 (0.3%)
1	B	0.53	0/2647	0.69	0/3535
1	C	0.51	0/2647	0.68	0/3535
1	D	0.57	2/2641 (0.1%)	0.82	7/3527 (0.2%)
All	All	0.69	30/10607 (0.3%)	0.76	18/14166 (0.1%)

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	B	0	1
All	All	0	2

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	248	VAL	CB-CG1	-13.83	1.23	1.52
1	A	248	VAL	CB-CG2	-13.79	1.23	1.52
1	A	307	LYS	C-O	-10.62	1.03	1.23
1	A	310	TRP	CG-CD1	-9.67	1.23	1.36
1	A	310	TRP	CD2-CE2	-9.38	1.30	1.41
1	A	248	VAL	C-O	-8.11	1.07	1.23
1	A	310	TRP	C-O	-7.94	1.08	1.23
1	A	308	GLU	C-O	-7.50	1.09	1.23
1	A	250	LYS	CA-C	-7.42	1.33	1.52
1	A	310	TRP	CZ3-CH2	-7.29	1.28	1.40
1	A	308	GLU	N-CA	-7.24	1.31	1.46
1	A	250	LYS	C-O	-7.18	1.09	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	307	LYS	CA-CB	-7.02	1.38	1.53
1	A	306	ARG	C-O	-6.94	1.10	1.23
1	A	249	LYS	CD-CE	-6.93	1.33	1.51
1	A	308	GLU	CA-C	-6.92	1.34	1.52
1	A	249	LYS	CE-NZ	-6.82	1.31	1.49
1	A	250	LYS	CA-CB	-6.80	1.39	1.53
1	D	96	ALA	N-CA	6.34	1.59	1.46
1	A	309	ARG	C-O	-6.33	1.11	1.23
1	A	310	TRP	CD1-NE1	-6.24	1.27	1.38
1	A	306	ARG	CZ-NH2	-6.04	1.25	1.33
1	D	96	ALA	CA-CB	-5.80	1.40	1.52
1	A	310	TRP	CE3-CZ3	-5.75	1.28	1.38
1	A	307	LYS	CA-C	-5.74	1.38	1.52
1	A	306	ARG	CB-CG	-5.69	1.37	1.52
1	A	307	LYS	C-N	-5.63	1.21	1.34
1	A	308	GLU	CD-OE2	-5.61	1.19	1.25
1	A	250	LYS	C-N	-5.51	1.23	1.33
1	A	306	ARG	CZ-NH1	-5.05	1.26	1.33

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	306	ARG	N-CA-C	10.59	139.58	111.00
1	A	248	VAL	CG1-CB-CG2	-9.16	96.25	110.90
1	A	193	THR	N-CA-C	-8.84	87.12	111.00
1	A	307	LYS	CB-CA-C	-8.14	94.13	110.40
1	A	307	LYS	N-CA-C	7.29	130.69	111.00
1	D	108	ALA	N-CA-C	-6.38	93.78	111.00
1	A	309	ARG	CG-CD-NE	6.32	125.07	111.80
1	A	309	ARG	N-CA-C	-6.03	94.73	111.00
1	A	309	ARG	NE-CZ-NH2	5.99	123.30	120.30
1	A	309	ARG	NE-CZ-NH1	-5.97	117.31	120.30
1	D	94	VAL	N-CA-C	5.88	126.87	111.00
1	A	307	LYS	C-N-CA	-5.80	107.20	121.70
1	D	92	GLU	N-CA-C	-5.67	95.70	111.00
1	D	254	LEU	CA-CB-CG	5.56	128.08	115.30
1	D	194	ASN	N-CA-C	-5.38	96.48	111.00
1	D	97	PHE	N-CA-CB	5.30	120.14	110.60
1	A	307	LYS	O-C-N	-5.12	114.51	122.70
1	A	306	ARG	NE-CZ-NH1	5.09	122.84	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	307	LYS	Peptide
1	B	195	TYR	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	2630	0	2722	166	0
1	B	2606	0	2700	152	0
1	C	2606	0	2700	112	0
1	D	2600	0	2695	214	0
2	A	31	0	12	3	0
2	B	31	0	12	1	0
2	C	31	0	12	5	0
2	D	31	0	12	3	0
3	B	10	0	12	4	0
4	C	1	0	0	0	0
5	A	15	0	0	1	0
5	B	12	0	0	0	0
5	C	33	0	0	3	0
5	D	5	0	0	0	0
All	All	10642	0	10877	635	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 30.

All (635) 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:306:ARG:CG	1:A:306:ARG:HH21	1.52	1.14
1:A:249:LYS:O	1:A:250:LYS:HD2	1.44	1.14
1:A:307:LYS:O	1:A:308:GLU:HB2	1.51	1.10
1:A:306:ARG:NH2	1:A:306:ARG:HG2	1.46	1.06
1:D:66:ARG:HG2	1:D:66:ARG:HH11	1.22	1.01
1:A:66:ARG:HH11	1:A:66:ARG:HG3	1.26	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:279:ASP:OD1	1:D:282:LYS:HB2	1.67	0.95
1:A:131:THR:HG21	1:A:133:HIS:ND1	1.81	0.94
1:D:248:VAL:HG21	1:D:259:LEU:CD2	1.99	0.93
1:A:121:LEU:HD12	1:A:126:PHE:HB2	1.51	0.92
1:A:98:ALA:HA	1:A:103:MET:HB2	1.54	0.90
1:A:307:LYS:HG2	1:A:307:LYS:O	1.72	0.90
1:D:131:THR:HG23	1:D:133:HIS:H	1.38	0.89
1:A:307:LYS:O	1:A:308:GLU:CB	2.08	0.89
1:D:197:VAL:HG12	1:D:203:ARG:CZ	2.03	0.88
1:D:131:THR:HG21	1:D:133:HIS:ND1	1.89	0.86
1:B:289:LEU:HB3	1:B:311:LEU:HD21	1.57	0.85
1:D:104:SER:HB3	1:D:107:GLU:HG2	1.59	0.85
1:A:249:LYS:O	1:A:250:LYS:CD	2.25	0.84
1:B:290:LEU:HD23	1:B:311:LEU:HD12	1.58	0.84
1:C:200:PRO:HB3	1:D:215:ILE:HD12	1.60	0.84
1:D:153:ASP:HA	1:D:234:ARG:HH21	1.43	0.84
1:B:282:LYS:O	1:B:286:VAL:HG23	1.79	0.83
1:A:207:ARG:HG2	1:A:207:ARG:HH11	1.43	0.83
1:D:25:ARG:HD2	1:D:54:LYS:HE3	1.58	0.83
1:C:194:ASN:H	1:C:194:ASN:HD22	1.21	0.82
1:C:161:LYS:HG3	1:C:166:ARG:HD2	1.59	0.82
1:C:252:ASN:HD21	1:C:313:PHE:HB2	1.44	0.82
1:A:97:PHE:O	1:A:101:ASN:HB2	1.80	0.81
1:B:289:LEU:O	1:B:306:ARG:HD2	1.81	0.81
1:B:197:VAL:HG11	1:B:207:ARG:HH11	1.42	0.81
1:C:20:ILE:HG23	1:C:166:ARG:HG3	1.63	0.80
1:D:308:GLU:HG2	1:D:308:GLU:O	1.81	0.80
1:A:65:LEU:HA	1:A:95:ARG:NH2	1.97	0.79
1:D:187:ARG:HH11	1:D:187:ARG:HG3	1.47	0.79
1:A:289:LEU:O	1:A:306:ARG:HD2	1.82	0.78
1:C:36:ASP:HB2	1:C:132:ALA:HB1	1.63	0.78
1:C:252:ASN:ND2	1:C:313:PHE:HB2	2.00	0.77
1:D:306:ARG:HG2	1:D:308:GLU:OE2	1.82	0.77
1:D:29:ILE:HD11	1:D:44:LEU:HD12	1.65	0.77
1:D:104:SER:O	1:D:108:ALA:HB2	1.84	0.77
1:A:240:GLU:O	1:A:243:LYS:HG3	1.85	0.77
1:D:64:MET:HB3	1:D:93:ASP:OD1	1.85	0.77
1:A:65:LEU:HA	1:A:95:ARG:HH21	1.50	0.76
1:A:28:LEU:HD11	1:A:59:ALA:HB2	1.65	0.76
1:A:249:LYS:C	1:A:250:LYS:HD2	2.06	0.76
1:A:150:THR:O	1:B:226:MET:HG3	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234:ARG:HD3	1:D:238:GLU:OE1	1.86	0.76
1:A:190:GLU:CD	1:A:190:GLU:H	1.88	0.76
1:A:305:LYS:HB2	1:A:305:LYS:NZ	2.01	0.76
1:B:98:ALA:HB1	1:B:103:MET:O	1.86	0.76
1:D:62:ASN:HD22	1:D:64:MET:H	1.35	0.75
1:D:97:PHE:CE1	1:D:101:ASN:ND2	2.55	0.75
1:D:66:ARG:CG	1:D:66:ARG:HH11	1.99	0.75
1:B:296:VAL:O	1:B:303:VAL:HA	1.87	0.75
1:D:161:LYS:HE3	1:D:166:ARG:CZ	2.16	0.75
1:D:118:LYS:O	1:D:122:GLU:HG3	1.87	0.74
1:B:131:THR:HG23	1:B:133:HIS:H	1.53	0.74
1:C:275:ILE:HG22	1:C:304:LEU:HD21	1.70	0.74
1:C:205:ARG:NH1	5:C:935:HOH:O	2.17	0.73
1:D:248:VAL:HG21	1:D:259:LEU:HD22	1.70	0.73
1:C:190:GLU:CD	1:C:190:GLU:H	1.89	0.73
1:D:197:VAL:HG12	1:D:203:ARG:NH2	2.04	0.73
1:B:139:LEU:HD22	1:B:143:LEU:HD23	1.70	0.73
1:C:133:HIS:HB2	1:C:167:ARG:HD2	1.70	0.73
1:D:121:LEU:HD12	1:D:126:PHE:HB2	1.71	0.73
1:A:66:ARG:NH1	1:A:66:ARG:HG3	1.96	0.72
1:B:131:THR:HG21	1:B:133:HIS:ND1	2.05	0.72
1:C:298:LEU:HB2	1:C:302:LYS:HB2	1.71	0.72
1:D:187:ARG:CG	1:D:187:ARG:HH11	2.01	0.72
1:D:304:LEU:HD23	1:D:312:CYS:O	1.90	0.72
1:C:291:GLU:HA	1:C:291:GLU:OE2	1.89	0.72
2:C:902:ATP:H5'1	2:C:902:ATP:O1G	1.88	0.72
1:D:306:ARG:HG3	1:D:308:GLU:HB3	1.72	0.72
1:A:207:ARG:HG2	1:A:207:ARG:NH1	1.99	0.72
1:B:62:ASN:ND2	1:B:64:MET:H	1.88	0.72
1:D:161:LYS:HE3	1:D:166:ARG:NE	2.05	0.72
1:D:30:ALA:HA	1:D:117:LEU:HD21	1.72	0.71
1:D:65:LEU:HD21	1:D:94:VAL:HB	1.70	0.71
1:A:65:LEU:HD21	1:A:94:VAL:HB	1.72	0.71
1:B:34:GLY:O	1:B:38:VAL:HG23	1.91	0.71
1:A:249:LYS:C	1:A:250:LYS:CD	2.57	0.70
1:A:317:VAL:HG21	1:C:251:GLY:H	1.55	0.70
1:B:131:THR:HG22	1:B:167:ARG:HG2	1.73	0.70
1:B:193:THR:HA	1:B:196:GLU:OE1	1.89	0.70
1:B:103:MET:HG2	1:B:107:GLU:OE1	1.91	0.70
1:D:29:ILE:CD1	1:D:44:LEU:HD12	2.21	0.70
1:A:285:LEU:HB3	1:A:296:VAL:HG11	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:LEU:CD2	1:C:267:GLN:HG2	2.21	0.70
1:D:305:LYS:CG	1:D:306:ARG:H	2.05	0.70
1:B:14:LEU:HD13	1:B:20:ILE:HG13	1.74	0.70
1:B:267:GLN:O	1:B:271:ILE:HG12	1.91	0.70
1:A:20:ILE:HG23	1:A:166:ARG:HG3	1.74	0.70
1:D:119:GLU:HA	1:D:122:GLU:OE1	1.92	0.70
1:D:281:GLU:H	1:D:281:GLU:CD	1.93	0.69
1:B:103:MET:HB3	1:B:107:GLU:HG3	1.74	0.69
1:D:134:HIS:HD2	1:D:136:ASN:H	1.38	0.69
1:D:114:TYR:O	1:D:118:LYS:HG3	1.93	0.69
1:A:104:SER:OG	1:A:107:GLU:HG2	1.93	0.69
1:A:305:LYS:HB2	1:A:305:LYS:HZ2	1.59	0.68
1:B:39:VAL:O	1:B:43:VAL:HG23	1.92	0.68
1:D:248:VAL:O	1:D:249:LYS:C	2.30	0.68
1:C:35:VAL:HG23	1:C:36:ASP:H	1.58	0.68
1:B:197:VAL:HG11	1:B:207:ARG:NH1	2.07	0.68
1:D:131:THR:CG2	1:D:133:HIS:ND1	2.57	0.68
1:C:197:VAL:HG11	1:C:207:ARG:HH11	1.59	0.68
1:C:285:LEU:HD12	1:C:296:VAL:HG13	1.76	0.68
1:C:194:ASN:HD22	1:C:194:ASN:N	1.92	0.68
1:A:131:THR:HG21	1:A:133:HIS:CE1	2.28	0.67
1:D:308:GLU:O	1:D:308:GLU:CG	2.42	0.67
1:C:245:TYR:CZ	1:C:273:LYS:HD2	2.29	0.67
1:A:131:THR:CG2	1:A:133:HIS:ND1	2.56	0.67
1:D:104:SER:O	1:D:108:ALA:CB	2.43	0.67
1:D:306:ARG:CG	1:D:308:GLU:HB3	2.24	0.67
1:D:304:LEU:HG	1:D:313:PHE:CD1	2.30	0.67
1:A:307:LYS:O	1:A:307:LYS:CG	2.32	0.67
1:A:285:LEU:HD13	1:A:296:VAL:HG13	1.77	0.66
1:B:197:VAL:HG21	1:B:207:ARG:NH1	2.10	0.66
1:D:25:ARG:CD	1:D:54:LYS:HE3	2.25	0.66
1:D:304:LEU:HG	1:D:313:PHE:HD1	1.61	0.66
1:B:289:LEU:HD21	1:B:296:VAL:HG23	1.77	0.66
1:A:191:ASP:O	1:A:194:ASN:HB3	1.96	0.66
1:B:62:ASN:HD22	1:B:64:MET:H	1.43	0.66
1:C:81:LYS:HD3	1:C:81:LYS:O	1.95	0.66
1:C:62:ASN:ND2	1:C:64:MET:H	1.94	0.66
1:A:293:GLY:HA2	1:A:306:ARG:HD3	1.77	0.65
1:D:193:THR:CA	1:D:196:GLU:HG3	2.27	0.65
1:D:248:VAL:O	1:D:250:LYS:HG2	1.95	0.65
1:A:191:ASP:O	1:A:194:ASN:CB	2.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:VAL:HG12	1:D:249:LYS:N	2.11	0.65
1:B:97:PHE:HE2	1:B:103:MET:HE1	1.62	0.65
1:C:267:GLN:O	1:C:271:ILE:HG12	1.97	0.64
1:D:139:LEU:HD22	1:D:143:LEU:HD22	1.78	0.64
1:B:36:ASP:HB2	1:B:132:ALA:HB1	1.78	0.64
1:B:229:VAL:O	1:B:233:GLU:HG3	1.98	0.64
1:B:25:ARG:HD2	1:B:54:LYS:HG3	1.80	0.64
1:D:219:LEU:O	1:D:222:THR:HG22	1.98	0.64
1:D:259:LEU:HD12	1:D:267:GLN:HA	1.80	0.64
1:D:251:GLY:C	1:D:253:CYS:H	2.00	0.63
1:C:200:PRO:CB	1:D:215:ILE:HD12	2.28	0.63
1:D:65:LEU:O	1:D:66:ARG:HD2	1.98	0.63
1:C:209:ILE:O	1:C:213:LYS:HG3	1.98	0.63
1:D:62:ASN:ND2	1:D:64:MET:H	1.96	0.63
1:D:132:ALA:HB3	2:D:903:ATP:O3'	1.98	0.63
1:A:306:ARG:HG2	1:A:306:ARG:HH21	0.61	0.63
1:D:94:VAL:HG22	1:D:112:LEU:CD1	2.28	0.63
1:B:188:TRP:NE1	3:B:950:LYS:HE2	2.13	0.63
1:B:305:LYS:HZ1	1:B:307:LYS:HE3	1.63	0.63
1:D:97:PHE:HE1	1:D:101:ASN:ND2	1.96	0.63
1:B:309:ARG:NH1	1:B:310:TRP:CZ2	2.65	0.63
1:C:1:MET:HG3	1:C:5:SER:OG	1.98	0.63
1:C:62:ASN:C	1:C:62:ASN:HD22	2.01	0.63
1:D:197:VAL:CG1	1:D:203:ARG:CZ	2.77	0.63
1:C:238:GLU:O	1:C:242:GLN:HG2	1.98	0.63
1:B:253:CYS:O	1:B:254:LEU:HD12	1.99	0.62
1:D:188:TRP:HD1	1:D:189:VAL:O	1.82	0.62
1:D:193:THR:C	1:D:196:GLU:HG3	2.19	0.62
1:D:27:VAL:HG13	1:D:128:CYS:SG	2.39	0.62
1:B:289:LEU:HD21	1:B:296:VAL:CG2	2.29	0.62
1:C:62:ASN:HD22	1:C:64:MET:H	1.47	0.62
1:A:121:LEU:HD12	1:A:126:PHE:CB	2.29	0.61
1:D:114:TYR:C	1:D:118:LYS:HE2	2.21	0.61
1:A:113:ARG:HD3	2:A:900:ATP:C4	2.35	0.61
1:A:192:GLU:HA	1:A:194:ASN:CG	2.21	0.61
1:B:62:ASN:C	1:B:62:ASN:HD22	2.04	0.61
1:C:4:GLU:HA	1:C:180:TYR:CD1	2.36	0.61
1:A:163:GLU:O	1:A:166:ARG:NH1	2.31	0.61
1:B:306:ARG:HB2	1:B:311:LEU:HD21	1.81	0.61
1:B:256:VAL:HG22	1:B:290:LEU:HD23	1.81	0.60
1:B:299:GLY:H	1:B:302:LYS:HB2	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:191:ASP:OD1	1:D:193:THR:HG23	2.00	0.60
1:D:108:ALA:O	1:D:112:LEU:HG	2.00	0.60
1:D:94:VAL:HG22	1:D:112:LEU:HD13	1.82	0.60
1:B:206:HIS:O	1:B:210:PRO:HG2	2.01	0.60
1:C:167:ARG:CG	1:C:167:ARG:HH11	2.14	0.60
1:D:102:ARG:HH11	1:D:102:ARG:HG3	1.67	0.60
1:D:120:ILE:O	1:D:124:GLU:HB2	2.01	0.60
1:A:131:THR:HG23	2:A:900:ATP:O2'	2.02	0.60
1:B:252:ASN:HD21	1:B:313:PHE:HB2	1.67	0.60
1:C:272:ARG:HD3	1:C:278:LYS:HG2	1.84	0.60
1:D:254:LEU:O	1:D:310:TRP:CE3	2.55	0.60
1:A:98:ALA:HB2	1:A:108:ALA:CB	2.32	0.60
1:D:67:GLU:O	1:D:70:GLU:HG2	2.02	0.60
1:D:63:HIS:C	1:D:65:LEU:H	2.05	0.60
1:B:14:LEU:CD2	1:B:18:GLU:HG3	2.32	0.60
1:C:88:PHE:CZ	1:C:124:GLU:HG2	2.37	0.59
1:C:190:GLU:CD	1:C:190:GLU:N	2.56	0.59
1:C:205:ARG:HD2	5:C:935:HOH:O	2.01	0.59
1:B:115:LYS:HG2	1:B:119:GLU:OE1	2.02	0.59
1:A:207:ARG:CG	1:A:207:ARG:HH11	2.14	0.59
1:A:131:THR:HG22	1:A:133:HIS:H	1.66	0.59
1:B:102:ARG:HH11	1:B:102:ARG:HG3	1.68	0.59
1:B:131:THR:CG2	1:B:133:HIS:ND1	2.65	0.59
1:B:303:VAL:HG13	1:B:314:SER:HB2	1.85	0.59
1:D:64:MET:CB	1:D:93:ASP:OD1	2.51	0.59
1:B:300:LYS:O	1:B:300:LYS:HD2	2.02	0.59
1:D:281:GLU:N	1:D:281:GLU:OE2	2.35	0.59
1:A:308:GLU:H	1:A:310:TRP:H	1.50	0.59
1:A:55:GLU:OE2	1:A:86:LYS:HE2	2.02	0.59
1:D:86:LYS:HD2	1:D:87:ILE:H	1.67	0.59
1:D:287:ARG:O	1:D:290:LEU:HD12	2.03	0.58
1:A:194:ASN:O	1:A:195:TYR:HB2	2.02	0.58
1:B:260:LYS:HE2	1:B:290:LEU:O	2.04	0.58
1:B:66:ARG:N	1:B:66:ARG:HD2	2.18	0.58
1:A:203:ARG:HD2	1:B:215:ILE:HD11	1.85	0.58
1:D:134:HIS:CD2	1:D:136:ASN:HB2	2.38	0.58
1:B:1:MET:HE3	1:B:6:ARG:HE	1.69	0.58
1:D:305:LYS:O	1:D:311:LEU:HD12	2.04	0.58
1:D:97:PHE:HE2	1:D:103:MET:HE2	1.68	0.58
1:A:248:VAL:O	1:A:248:VAL:HG12	2.02	0.58
1:B:305:LYS:HG2	1:B:306:ARG:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:PHE:O	1:D:120:ILE:HG12	2.04	0.58
1:C:248:VAL:HG22	1:C:258:LYS:HD2	1.86	0.57
1:D:299:GLY:O	1:D:302:LYS:N	2.36	0.57
1:A:98:ALA:CA	1:A:103:MET:HB2	2.29	0.57
1:D:256:VAL:HG13	1:D:290:LEU:HD23	1.85	0.57
1:A:194:ASN:H	1:A:194:ASN:ND2	2.01	0.57
1:A:243:LYS:HG3	1:A:244:LEU:N	2.20	0.57
1:B:95:ARG:HH11	1:B:95:ARG:HG3	1.70	0.57
1:C:225:LYS:HG2	1:D:280:TYR:CD2	2.40	0.57
1:D:305:LYS:O	1:D:311:LEU:CD1	2.52	0.57
1:A:35:VAL:HG22	1:A:188:TRP:CD1	2.39	0.57
1:B:14:LEU:HD22	1:B:18:GLU:HG3	1.86	0.57
1:D:128:CYS:HA	1:D:164:VAL:HG22	1.85	0.57
1:D:60:HIS:CD2	1:D:73:GLU:HA	2.39	0.57
1:A:14:LEU:HD13	1:A:20:ILE:HD11	1.87	0.57
1:D:272:ARG:NH2	1:D:278:LYS:NZ	2.52	0.57
1:C:144:LEU:HD22	1:C:148:ARG:HD2	1.86	0.57
1:C:66:ARG:HH11	1:C:66:ARG:HG3	1.70	0.57
1:C:7:VAL:O	1:C:11:VAL:HG23	2.05	0.57
1:A:222:THR:HG23	1:B:149:GLY:HA2	1.87	0.56
1:B:159:LEU:HB2	1:B:162:GLU:HG3	1.86	0.56
1:B:259:LEU:HD22	1:B:267:GLN:HG2	1.87	0.56
1:B:115:LYS:O	1:B:119:GLU:HG3	2.05	0.56
1:D:159:LEU:HB2	1:D:162:GLU:HG3	1.85	0.56
1:D:66:ARG:HG2	1:D:66:ARG:NH1	2.03	0.56
1:C:147:THR:OG1	1:D:212:LEU:HD22	2.05	0.56
1:A:299:GLY:O	1:A:301:GLY:N	2.32	0.56
1:B:30:ALA:HB1	2:B:901:ATP:H1'	1.86	0.56
1:C:242:GLN:HA	1:C:242:GLN:OE1	2.06	0.56
1:C:272:ARG:HD3	1:C:278:LYS:NZ	2.20	0.56
1:C:35:VAL:HG23	1:C:36:ASP:N	2.18	0.56
1:B:242:GLN:OE1	1:B:242:GLN:HA	2.05	0.56
1:B:252:ASN:ND2	1:B:313:PHE:HB2	2.19	0.56
1:D:275:ILE:HG22	1:D:304:LEU:HD11	1.88	0.56
1:B:120:ILE:O	1:B:124:GLU:HB2	2.06	0.56
1:C:275:ILE:HG13	1:C:277:GLU:H	1.71	0.56
1:A:249:LYS:HE2	1:A:251:GLY:O	2.06	0.56
1:C:193:THR:HB	1:C:202:ASN:ND2	2.21	0.56
1:C:268:ARG:HD2	5:C:911:HOH:O	2.06	0.55
1:D:297:ASN:ND2	1:D:299:GLY:H	2.04	0.55
1:A:254:LEU:HD22	1:A:274:PHE:CD1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:305:LYS:HG3	1:D:306:ARG:H	1.70	0.55
1:A:197:VAL:HG12	1:A:197:VAL:O	2.04	0.55
1:D:258:LYS:O	1:D:262:LYS:HG2	2.06	0.55
1:A:124:GLU:HB3	1:A:126:PHE:HE1	1.71	0.55
1:C:281:GLU:HA	1:C:281:GLU:OE1	2.06	0.55
1:D:287:ARG:HA	1:D:290:LEU:HD12	1.87	0.55
1:D:36:ASP:OD2	1:D:37:SER:N	2.38	0.55
1:C:194:ASN:ND2	1:C:194:ASN:H	1.99	0.55
1:A:285:LEU:HD21	1:C:307:LYS:HE2	1.87	0.55
1:B:131:THR:CG2	1:B:167:ARG:HG2	2.36	0.55
1:D:248:VAL:HG12	1:D:249:LYS:H	1.71	0.55
1:A:209:ILE:HB	1:A:210:PRO:HD3	1.89	0.55
1:A:26:ARG:NH1	1:A:55:GLU:OE1	2.40	0.55
1:C:124:GLU:HB3	1:C:126:PHE:CE1	2.42	0.55
1:C:229:VAL:O	1:C:233:GLU:HG3	2.07	0.55
1:A:303:VAL:HG13	1:A:314:SER:HB2	1.89	0.55
1:D:308:GLU:O	1:D:310:TRP:N	2.40	0.55
1:A:269:ARG:HH21	1:B:233:GLU:CD	2.11	0.55
1:A:94:VAL:HG11	1:A:105:LEU:O	2.07	0.55
1:A:64:MET:CE	1:A:91:LYS:HE2	2.36	0.54
1:B:216:ASN:ND2	1:B:219:LEU:HA	2.22	0.54
1:A:196:GLU:O	1:A:198:SER:N	2.40	0.54
1:B:240:GLU:OE1	1:B:240:GLU:HA	2.08	0.54
1:B:279:ASP:O	1:B:283:VAL:HG23	2.06	0.54
1:A:249:LYS:C	1:A:250:LYS:HD3	2.27	0.54
1:C:197:VAL:HG11	1:C:207:ARG:NH1	2.22	0.54
1:C:298:LEU:HD12	1:C:302:LYS:HB3	1.89	0.54
1:D:104:SER:HB3	1:D:107:GLU:CG	2.36	0.54
1:A:316:GLU:O	1:A:317:VAL:HB	2.06	0.54
1:B:33:GLY:C	1:B:189:VAL:HG12	2.28	0.54
1:A:246:LYS:C	1:A:248:VAL:H	2.11	0.54
1:B:305:LYS:HZ2	1:B:307:LYS:HD3	1.72	0.54
1:D:30:ALA:CB	1:D:117:LEU:HD11	2.38	0.54
1:A:196:GLU:C	1:A:198:SER:H	2.11	0.54
1:A:124:GLU:HB3	1:A:126:PHE:CE1	2.42	0.54
1:D:31:PHE:CD1	1:D:37:SER:HB3	2.43	0.54
1:A:243:LYS:HG3	1:A:244:LEU:H	1.72	0.54
1:B:134:HIS:HB2	1:B:172:VAL:O	2.08	0.53
1:B:306:ARG:HA	1:B:311:LEU:HD23	1.90	0.53
1:D:255:ASP:HA	1:D:309:ARG:O	2.08	0.53
1:B:300:LYS:O	1:B:300:LYS:CD	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:ILE:HD12	1:C:165:ILE:N	2.23	0.53
1:B:162:GLU:O	1:B:163:GLU:HB2	2.08	0.53
1:D:4:GLU:HA	1:D:180:TYR:CD1	2.44	0.53
1:B:266:LEU:O	1:B:269:ARG:HB2	2.09	0.53
1:D:274:PHE:C	1:D:274:PHE:CD2	2.81	0.53
1:B:188:TRP:HE1	3:B:950:LYS:HE2	1.73	0.53
1:B:26:ARG:NH2	1:B:55:GLU:OE2	2.41	0.53
1:C:66:ARG:NH1	1:C:66:ARG:HG3	2.24	0.53
1:D:97:PHE:O	1:D:97:PHE:CG	2.62	0.53
1:A:192:GLU:HG2	1:A:194:ASN:OD1	2.09	0.53
1:A:248:VAL:CG1	1:A:248:VAL:O	2.56	0.53
1:B:290:LEU:CD2	1:B:311:LEU:HD12	2.34	0.53
1:D:248:VAL:HG11	1:D:254:LEU:HG	1.91	0.53
1:A:222:THR:HG23	1:B:149:GLY:CA	2.38	0.52
1:B:14:LEU:HD13	1:B:20:ILE:CG1	2.38	0.52
1:C:139:LEU:HD22	1:C:143:LEU:HD22	1.91	0.52
1:D:289:LEU:HD11	1:D:296:VAL:HG22	1.91	0.52
1:C:194:ASN:HA	1:C:206:HIS:CD2	2.44	0.52
1:C:24:GLU:OE1	1:C:24:GLU:N	2.33	0.52
1:D:201:ARG:HH11	1:D:201:ARG:HG2	1.74	0.52
1:A:240:GLU:O	1:A:243:LYS:CG	2.56	0.52
1:B:163:GLU:O	1:B:166:ARG:NH1	2.43	0.52
1:D:161:LYS:HE3	1:D:166:ARG:NH2	2.25	0.52
1:D:257:LYS:CG	1:D:257:LYS:O	2.58	0.52
1:C:167:ARG:HH11	1:C:167:ARG:HG2	1.74	0.52
1:D:116:PHE:HA	1:D:119:GLU:HB2	1.92	0.52
1:D:121:LEU:HD12	1:D:126:PHE:CB	2.38	0.52
1:D:257:LYS:HG2	1:D:257:LYS:O	2.10	0.52
1:A:194:ASN:O	1:A:195:TYR:CB	2.56	0.51
1:A:134:HIS:HD2	1:A:136:ASN:H	1.58	0.51
1:A:35:VAL:HG23	5:A:912:HOH:O	2.10	0.51
1:D:193:THR:HB	1:D:196:GLU:OE2	2.10	0.51
1:B:35:VAL:HG13	1:B:188:TRP:CD2	2.45	0.51
1:C:63:HIS:CD2	1:C:65:LEU:H	2.28	0.51
1:D:251:GLY:C	1:D:253:CYS:N	2.64	0.51
1:A:175:SER:O	1:A:179:GLU:HG3	2.10	0.51
1:A:194:ASN:N	1:A:194:ASN:ND2	2.57	0.51
1:B:34:GLY:HA2	1:B:189:VAL:HG12	1.91	0.51
1:D:86:LYS:HG3	1:D:88:PHE:CE1	2.46	0.51
1:B:139:LEU:HD22	1:B:143:LEU:CD2	2.38	0.51
1:A:26:ARG:NH2	1:A:55:GLU:OE1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:MET:SD	1:A:91:LYS:HG2	2.50	0.51
1:B:139:LEU:O	1:B:143:LEU:HD23	2.11	0.51
1:C:285:LEU:HD12	1:C:296:VAL:CG1	2.40	0.51
1:D:104:SER:O	1:D:108:ALA:N	2.43	0.50
1:D:66:ARG:CG	1:D:66:ARG:NH1	2.65	0.50
1:A:14:LEU:HD13	1:A:20:ILE:CG1	2.42	0.50
1:B:93:ASP:O	1:B:94:VAL:C	2.50	0.50
1:D:187:ARG:CG	1:D:187:ARG:NH1	2.66	0.50
1:D:267:GLN:O	1:D:271:ILE:HG12	2.11	0.50
1:D:306:ARG:CG	1:D:308:GLU:OE2	2.58	0.50
1:D:63:HIS:O	1:D:65:LEU:N	2.43	0.50
1:C:62:ASN:ND2	1:C:69:ALA:HB1	2.26	0.50
1:A:191:ASP:O	1:A:194:ASN:CG	2.49	0.50
1:D:193:THR:O	1:D:196:GLU:HG3	2.12	0.50
1:D:88:PHE:CE2	1:D:124:GLU:HG3	2.47	0.50
1:D:67:GLU:HG2	1:D:68:SER:N	2.27	0.50
1:A:62:ASN:HD22	1:A:64:MET:H	1.58	0.49
1:B:97:PHE:HE2	1:B:103:MET:CE	2.23	0.49
1:D:272:ARG:HG2	1:D:277:GLU:O	2.12	0.49
1:B:309:ARG:HD2	1:B:310:TRP:NE1	2.26	0.49
1:C:75:PHE:CZ	1:C:188:TRP:HA	2.48	0.49
1:D:113:ARG:NH1	2:D:903:ATP:O4'	2.45	0.49
1:A:131:THR:HG22	1:A:132:ALA:N	2.26	0.49
1:A:65:LEU:CA	1:A:95:ARG:NH2	2.73	0.49
1:D:308:GLU:C	1:D:310:TRP:H	2.16	0.49
1:B:25:ARG:CD	1:B:54:LYS:HG3	2.43	0.49
1:C:273:LYS:HD3	1:C:273:LYS:O	2.12	0.49
1:A:63:HIS:CG	1:A:65:LEU:HG	2.47	0.49
1:A:66:ARG:N	1:A:66:ARG:HD2	2.27	0.49
1:B:306:ARG:HG2	1:B:307:LYS:O	2.12	0.49
1:C:36:ASP:OD2	1:C:36:ASP:N	2.43	0.49
1:B:35:VAL:HG13	1:B:188:TRP:CE2	2.48	0.49
1:D:197:VAL:CG1	1:D:203:ARG:NH1	2.76	0.49
1:A:151:GLY:O	1:A:155:LEU:HG	2.13	0.49
1:B:131:THR:HG21	1:B:167:ARG:HH11	1.76	0.49
1:B:248:VAL:HG13	1:B:255:ASP:HB3	1.94	0.49
1:B:281:GLU:N	1:B:281:GLU:OE1	2.46	0.49
3:B:950:LYS:HG3	3:B:950:LYS:OXT	2.13	0.49
1:D:177:ILE:O	1:D:180:TYR:HB3	2.13	0.49
1:A:117:LEU:HB3	1:A:129:ILE:HD13	1.94	0.48
1:A:304:LEU:HA	1:A:312:CYS:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:LEU:HD21	1:C:267:GLN:HA	1.95	0.48
1:B:24:GLU:OE2	1:B:166:ARG:NH2	2.42	0.48
1:B:66:ARG:NE	1:B:66:ARG:HA	2.28	0.48
1:C:97:PHE:CG	1:C:112:LEU:HD11	2.47	0.48
1:D:25:ARG:HB3	1:D:54:LYS:HD2	1.95	0.48
1:A:304:LEU:N	1:A:304:LEU:HD12	2.28	0.48
1:D:254:LEU:O	1:D:310:TRP:HA	2.13	0.48
1:D:305:LYS:CG	1:D:306:ARG:N	2.75	0.48
1:A:180:TYR:C	1:A:180:TYR:CD2	2.86	0.48
1:B:271:ILE:HB	1:B:283:VAL:HG13	1.95	0.48
1:D:59:ALA:HA	1:D:88:PHE:O	2.13	0.48
1:A:116:PHE:O	1:A:119:GLU:HB2	2.14	0.48
1:A:75:PHE:CZ	1:A:188:TRP:HA	2.49	0.48
1:A:14:LEU:HD13	1:A:20:ILE:HG13	1.96	0.48
1:B:305:LYS:NZ	1:B:307:LYS:HE3	2.28	0.48
1:C:260:LYS:HE2	1:C:290:LEU:O	2.12	0.48
1:A:159:LEU:HB2	1:A:162:GLU:HG3	1.95	0.48
1:C:252:ASN:HD21	1:C:313:PHE:CB	2.23	0.48
1:D:73:GLU:O	1:D:76:CYS:HB2	2.13	0.48
1:C:279:ASP:OD1	1:C:282:LYS:HD2	2.13	0.48
1:C:275:ILE:HA	1:C:313:PHE:HZ	1.78	0.48
1:C:81:LYS:HD3	1:C:81:LYS:C	2.34	0.48
1:D:248:VAL:HG13	1:D:255:ASP:H	1.79	0.48
1:A:115:LYS:O	1:A:119:GLU:HG3	2.13	0.48
1:A:62:ASN:HD22	1:A:62:ASN:C	2.17	0.47
1:B:290:LEU:HD23	1:B:311:LEU:CD1	2.36	0.47
1:C:275:ILE:HG21	1:C:286:VAL:HG21	1.96	0.47
1:D:134:HIS:HD2	1:D:136:ASN:N	2.09	0.47
1:B:103:MET:C	1:B:104:SER:O	2.52	0.47
1:B:25:ARG:HD2	1:B:54:LYS:NZ	2.28	0.47
1:A:113:ARG:O	1:A:117:LEU:HG	2.13	0.47
1:A:255:ASP:OD1	1:A:258:LYS:HG3	2.14	0.47
1:D:296:VAL:O	1:D:296:VAL:HG23	2.14	0.47
1:C:139:LEU:HD23	1:C:223:PHE:CD1	2.50	0.47
1:D:293:GLY:HA2	1:D:306:ARG:HB2	1.96	0.47
1:A:93:ASP:O	1:A:94:VAL:C	2.53	0.47
1:B:280:TYR:HD2	1:B:281:GLU:OE1	1.98	0.47
1:C:20:ILE:HD11	1:C:160:PRO:HB2	1.97	0.47
1:A:14:LEU:HD13	1:A:20:ILE:CD1	2.44	0.47
1:A:211:GLU:OE2	1:A:214:ARG:NH1	2.48	0.47
1:A:209:ILE:O	1:A:213:LYS:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:ARG:NH1	1:D:102:ARG:HG3	2.29	0.47
1:A:243:LYS:O	1:A:247:GLU:HB2	2.15	0.47
1:A:303:VAL:CG1	1:A:314:SER:HB2	2.45	0.47
1:B:197:VAL:HG12	1:B:197:VAL:O	2.14	0.47
1:A:205:ARG:HA	1:A:209:ILE:HD12	1.96	0.47
1:A:64:MET:HE3	1:A:91:LYS:HE2	1.96	0.46
1:D:193:THR:HA	1:D:196:GLU:HG3	1.96	0.46
1:D:248:VAL:CG1	1:D:254:LEU:HG	2.46	0.46
1:A:131:THR:HG23	2:A:900:ATP:H4'	1.96	0.46
1:B:197:VAL:HG13	1:B:203:ARG:HA	1.97	0.46
1:B:73:GLU:O	1:B:76:CYS:HB2	2.15	0.46
1:C:279:ASP:O	1:C:283:VAL:HG23	2.15	0.46
1:B:38:VAL:HG13	1:B:79:PHE:CZ	2.50	0.46
1:D:114:TYR:O	1:D:118:LYS:HE2	2.15	0.46
1:D:249:LYS:HG2	1:D:249:LYS:O	2.13	0.46
1:A:250:LYS:N	1:A:250:LYS:CD	2.75	0.46
1:B:197:VAL:CG1	1:B:207:ARG:HH11	2.23	0.46
1:D:39:VAL:O	1:D:43:VAL:HG23	2.14	0.46
1:C:309:ARG:HG2	1:C:309:ARG:O	2.15	0.46
1:C:97:PHE:HE2	1:C:103:MET:HE1	1.81	0.46
1:C:139:LEU:HD13	1:C:209:ILE:CD1	2.46	0.46
1:A:285:LEU:HD13	1:A:296:VAL:CG1	2.46	0.46
1:B:258:LYS:O	1:B:262:LYS:HD3	2.15	0.46
1:B:242:GLN:OE1	1:B:273:LYS:HE3	2.16	0.46
1:D:201:ARG:NH1	1:D:201:ARG:HG2	2.30	0.46
1:D:281:GLU:O	1:D:285:LEU:HB2	2.16	0.46
1:B:281:GLU:H	1:B:281:GLU:CD	2.18	0.46
1:C:194:ASN:ND2	1:C:194:ASN:N	2.60	0.46
1:C:62:ASN:HD21	1:C:69:ALA:HB1	1.81	0.46
1:A:226:MET:O	1:A:230:LEU:HG	2.16	0.45
1:B:305:LYS:HE3	1:B:307:LYS:HG2	1.98	0.45
1:D:27:VAL:CG2	1:D:53:LEU:HD22	2.46	0.45
1:B:163:GLU:HB3	1:B:164:VAL:H	1.30	0.45
1:B:289:LEU:HB3	1:B:311:LEU:CD2	2.38	0.45
1:C:248:VAL:HG12	1:C:248:VAL:O	2.15	0.45
1:D:300:LYS:HE3	1:D:300:LYS:HB2	1.58	0.45
1:D:307:LYS:O	1:D:308:GLU:C	2.54	0.45
1:D:30:ALA:HB2	1:D:117:LEU:HD11	1.98	0.45
1:D:62:ASN:C	1:D:62:ASN:HD22	2.20	0.45
1:A:150:THR:OG1	1:A:151:GLY:N	2.47	0.45
1:A:194:ASN:HD22	1:A:194:ASN:N	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:LEU:O	1:C:167:ARG:NH1	2.49	0.45
1:D:254:LEU:HD22	1:D:274:PHE:CE1	2.51	0.45
1:D:272:ARG:CZ	1:D:278:LYS:HD3	2.45	0.45
1:A:140:GLU:HG3	1:A:209:ILE:HD11	1.98	0.45
1:B:102:ARG:HG3	1:B:102:ARG:NH1	2.29	0.45
1:D:267:GLN:HG2	1:D:287:ARG:HD2	1.99	0.45
1:D:306:ARG:HD3	1:D:308:GLU:OE2	2.16	0.45
1:A:5:SER:O	1:A:9:ARG:HB2	2.17	0.45
1:B:281:GLU:N	1:B:281:GLU:CD	2.70	0.45
1:B:97:PHE:CE2	1:B:103:MET:CE	2.99	0.45
1:D:275:ILE:HD11	1:D:277:GLU:HB2	1.99	0.45
1:A:131:THR:CG2	1:A:132:ALA:N	2.80	0.45
1:A:20:ILE:CG2	1:A:166:ARG:HG3	2.45	0.45
1:A:83:ARG:CB	1:A:85:MET:HG3	2.47	0.45
1:D:75:PHE:CZ	1:D:188:TRP:HA	2.51	0.45
1:A:243:LYS:CG	1:A:244:LEU:N	2.80	0.45
1:B:152:LEU:HA	1:B:152:LEU:HD23	1.84	0.45
1:D:164:VAL:HG22	1:D:164:VAL:O	2.17	0.45
1:D:254:LEU:CD2	1:D:311:LEU:HD23	2.46	0.45
1:A:95:ARG:O	1:A:99:LYS:HB2	2.17	0.45
1:B:88:PHE:CZ	1:B:124:GLU:HG2	2.52	0.45
1:B:134:HIS:HD2	1:B:136:ASN:H	1.65	0.45
1:B:61:PHE:CD2	1:B:63:HIS:CD2	3.05	0.45
1:D:104:SER:OG	1:D:105:LEU:N	2.50	0.45
1:D:274:PHE:C	1:D:274:PHE:HD2	2.21	0.45
1:B:26:ARG:CZ	1:B:55:GLU:OE2	2.65	0.45
1:B:8:ILE:HG22	1:B:12:LEU:HD22	1.99	0.45
1:B:209:ILE:N	1:B:210:PRO:CD	2.80	0.44
1:D:229:VAL:O	1:D:233:GLU:HG3	2.17	0.44
1:D:293:GLY:HA3	1:D:306:ARG:NH2	2.33	0.44
1:B:134:HIS:CD2	1:B:136:ASN:HB2	2.52	0.44
1:A:110:ARG:HH21	1:A:201:ARG:HH22	1.64	0.44
1:A:110:ARG:HH21	1:A:201:ARG:NH2	2.15	0.44
1:B:66:ARG:N	1:B:66:ARG:CD	2.81	0.44
1:D:30:ALA:HB1	1:D:117:LEU:HD11	1.98	0.44
1:D:67:GLU:CG	1:D:68:SER:N	2.80	0.44
1:D:62:ASN:HB3	1:D:91:LYS:HG3	1.99	0.44
1:C:257:LYS:HD2	1:C:257:LYS:HA	1.82	0.44
1:C:272:ARG:HD3	1:C:278:LYS:HZ2	1.82	0.44
1:C:279:ASP:OD2	1:C:282:LYS:HG3	2.18	0.44
1:C:32:SER:HB3	2:C:902:ATP:N7	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ASN:O	1:A:195:TYR:CD1	2.70	0.44
1:B:160:PRO:HD3	1:B:170:TYR:CE1	2.52	0.44
1:B:195:TYR:HB3	1:B:196:GLU:H	1.20	0.44
1:B:259:LEU:HD11	1:B:270:VAL:HG11	2.00	0.44
1:B:68:SER:O	1:B:69:ALA:C	2.56	0.44
1:D:272:ARG:NH2	1:D:278:LYS:HZ1	2.15	0.44
1:D:29:ILE:HG23	1:D:40:LEU:HD23	1.98	0.44
1:D:8:ILE:HG22	1:D:12:LEU:HD22	1.99	0.44
1:A:26:ARG:CZ	1:A:55:GLU:OE1	2.66	0.44
1:B:277:GLU:HG2	1:B:302:LYS:HE2	1.98	0.44
1:C:97:PHE:HE2	1:C:103:MET:CE	2.31	0.44
1:D:64:MET:O	1:D:64:MET:HG3	2.16	0.44
1:B:134:HIS:HD2	1:B:136:ASN:N	2.16	0.44
1:C:30:ALA:HB1	2:C:902:ATP:H1'	2.00	0.44
1:D:63:HIS:C	1:D:65:LEU:N	2.71	0.44
1:B:250:LYS:HB2	1:B:310:TRP:CZ3	2.53	0.44
1:D:211:GLU:O	1:D:214:ARG:HB2	2.17	0.44
1:A:104:SER:O	1:A:105:LEU:C	2.55	0.43
1:B:38:VAL:HG13	1:B:79:PHE:CE1	2.53	0.43
1:C:165:ILE:O	1:C:166:ARG:HD3	2.18	0.43
1:C:284:GLU:CD	1:C:287:ARG:HE	2.22	0.43
1:A:267:GLN:O	1:A:271:ILE:HG12	2.18	0.43
1:A:83:ARG:HB2	1:A:85:MET:HG3	1.99	0.43
1:B:144:LEU:HD22	1:B:148:ARG:NE	2.33	0.43
1:D:304:LEU:CD2	1:D:312:CYS:O	2.62	0.43
1:A:259:LEU:HD21	1:A:267:GLN:HA	2.00	0.43
1:B:292:LYS:HG2	1:B:293:GLY:O	2.18	0.43
1:D:85:MET:CG	1:D:86:LYS:N	2.80	0.43
1:D:94:VAL:HG22	1:D:112:LEU:HD12	1.99	0.43
1:B:15:GLN:OE1	1:B:20:ILE:N	2.52	0.43
1:B:285:LEU:HD12	1:B:296:VAL:CG2	2.49	0.43
1:A:144:LEU:HD22	1:A:148:ARG:HD2	2.01	0.43
1:A:275:ILE:HG22	1:A:304:LEU:HD21	2.01	0.43
1:A:309:ARG:HD2	1:A:309:ARG:HH11	1.60	0.43
1:D:293:GLY:CA	1:D:306:ARG:HB2	2.48	0.43
1:D:248:VAL:O	1:D:250:LYS:N	2.52	0.43
1:A:159:LEU:HD12	1:A:162:GLU:HG2	2.00	0.43
1:A:192:GLU:HA	1:A:194:ASN:ND2	2.33	0.43
1:A:1:MET:HE2	1:A:6:ARG:NH2	2.34	0.43
1:A:64:MET:HE2	1:A:91:LYS:HE2	2.01	0.43
1:C:296:VAL:N	1:C:304:LEU:O	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:THR:HG23	1:D:133:HIS:N	2.20	0.43
1:D:139:LEU:HD22	1:D:143:LEU:CD2	2.47	0.43
1:D:48:LYS:HE2	1:D:53:LEU:O	2.19	0.43
1:A:58:LEU:HD12	1:A:80:ALA:HB2	2.01	0.43
1:B:95:ARG:HG3	1:B:95:ARG:NH1	2.34	0.43
1:D:175:SER:O	1:D:179:GLU:HG3	2.19	0.43
1:A:196:GLU:C	1:A:198:SER:N	2.72	0.42
1:A:25:ARG:NH1	1:A:52:SER:O	2.52	0.42
1:B:15:GLN:HA	1:B:15:GLN:OE1	2.18	0.42
1:B:188:TRP:CD1	3:B:950:LYS:HE2	2.54	0.42
1:C:104:SER:N	1:C:107:GLU:OE2	2.44	0.42
1:C:28:LEU:HD11	1:C:59:ALA:HB2	2.00	0.42
1:D:272:ARG:HH21	1:D:278:LYS:HZ1	1.66	0.42
1:A:156:ILE:HD11	1:A:230:LEU:CB	2.50	0.42
1:C:299:GLY:C	1:C:301:GLY:H	2.22	0.42
1:A:243:LYS:HD2	1:A:247:GLU:OE1	2.19	0.42
1:B:34:GLY:CA	1:B:189:VAL:HG12	2.50	0.42
1:A:12:LEU:HA	1:A:12:LEU:HD12	1.90	0.42
1:B:275:ILE:HG13	1:B:277:GLU:H	1.85	0.42
1:C:139:LEU:HD13	1:C:209:ILE:HD11	2.02	0.42
1:C:181:ALA:HB1	1:C:188:TRP:CZ3	2.55	0.42
1:C:259:LEU:HD22	1:C:267:GLN:HG2	2.00	0.42
1:C:275:ILE:CG2	1:C:304:LEU:HD21	2.45	0.42
1:D:254:LEU:HD23	1:D:311:LEU:HD23	2.00	0.42
1:D:286:VAL:CG2	1:D:298:LEU:HD11	2.50	0.42
1:A:107:GLU:HA	1:A:110:ARG:HD2	2.02	0.42
1:B:117:LEU:HB3	1:B:129:ILE:HD13	2.02	0.42
1:C:146:PHE:C	1:C:146:PHE:CD2	2.93	0.42
1:C:152:LEU:O	1:C:156:ILE:HG13	2.19	0.42
1:D:254:LEU:HD13	1:D:274:PHE:CD1	2.54	0.42
1:B:248:VAL:HG22	1:B:258:LYS:HB3	2.01	0.42
1:C:103:MET:HB3	1:C:107:GLU:HG3	2.02	0.42
1:D:264:LEU:HD11	1:D:287:ARG:CZ	2.49	0.42
1:D:305:LYS:HG2	1:D:306:ARG:H	1.83	0.42
1:D:62:ASN:HD22	1:D:64:MET:N	2.10	0.42
1:A:201:ARG:HB2	1:A:201:ARG:HH11	1.85	0.42
1:A:68:SER:O	1:A:71:ARG:N	2.53	0.42
1:B:114:TYR:CZ	1:B:118:LYS:NZ	2.74	0.42
1:D:146:PHE:CD2	1:D:146:PHE:C	2.92	0.42
1:A:98:ALA:HB2	1:A:108:ALA:HB3	2.02	0.41
1:C:121:LEU:HD12	1:C:126:PHE:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:282:LYS:O	1:D:286:VAL:HG23	2.20	0.41
1:C:121:LEU:CD1	1:C:126:PHE:O	2.69	0.41
1:D:193:THR:O	1:D:196:GLU:HB2	2.20	0.41
1:D:309:ARG:HG3	1:D:309:ARG:O	2.18	0.41
1:D:63:HIS:HB2	1:D:65:LEU:HG	2.02	0.41
1:A:197:VAL:O	1:A:197:VAL:CG1	2.68	0.41
1:B:197:VAL:HG12	1:B:203:ARG:CZ	2.50	0.41
1:C:307:LYS:HB3	1:C:308:GLU:H	1.68	0.41
1:D:165:ILE:HG21	1:D:167:ARG:NH1	2.35	0.41
1:D:248:VAL:HG21	1:D:259:LEU:HD23	1.93	0.41
1:A:116:PHE:O	1:A:120:ILE:HG12	2.20	0.41
1:A:190:GLU:CD	1:A:190:GLU:N	2.66	0.41
1:C:191:ASP:OD1	1:C:193:THR:HG23	2.20	0.41
1:A:181:ALA:HA	1:A:186:LEU:HD12	2.02	0.41
1:A:285:LEU:HD23	1:A:285:LEU:HA	1.92	0.41
1:B:25:ARG:NH1	1:B:52:SER:O	2.53	0.41
1:C:55:GLU:HG3	1:C:56:VAL:N	2.35	0.41
1:D:134:HIS:NE2	1:D:136:ASN:HB2	2.35	0.41
1:A:307:LYS:C	1:A:307:LYS:CD	2.77	0.41
1:C:144:LEU:HA	1:C:144:LEU:HD23	1.89	0.41
1:D:307:LYS:O	1:D:309:ARG:N	2.53	0.41
1:B:62:ASN:C	1:B:62:ASN:ND2	2.72	0.41
1:D:14:LEU:HD13	1:D:20:ILE:HG13	2.01	0.41
1:D:194:ASN:O	1:D:195:TYR:C	2.54	0.41
1:B:42:ASP:OD1	1:B:180:TYR:OH	2.30	0.41
1:B:258:LYS:HG3	1:B:262:LYS:HZ3	1.85	0.41
1:D:164:VAL:HA	1:D:166:ARG:HH12	1.85	0.41
1:D:153:ASP:CA	1:D:234:ARG:HH21	2.23	0.41
1:D:44:LEU:HA	1:D:44:LEU:HD23	1.87	0.41
1:D:64:MET:O	1:D:66:ARG:N	2.54	0.41
1:D:94:VAL:CG1	1:D:108:ALA:HB3	2.51	0.41
1:A:62:ASN:ND2	1:A:64:MET:H	2.17	0.41
1:B:150:THR:OG1	1:B:151:GLY:N	2.54	0.41
1:B:244:LEU:HD23	1:B:266:LEU:HB3	2.03	0.41
1:B:305:LYS:HE2	1:B:305:LYS:HB3	1.83	0.41
1:D:30:ALA:HB1	2:D:903:ATP:H1'	2.03	0.41
1:D:4:GLU:O	1:D:8:ILE:HG12	2.21	0.41
1:A:272:ARG:CG	1:A:278:LYS:HD2	2.51	0.41
1:A:66:ARG:HB3	1:A:67:GLU:H	1.73	0.41
1:D:144:LEU:HD21	1:D:148:ARG:CZ	2.50	0.41
1:D:279:ASP:OD2	1:D:282:LYS:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:HIS:HB2	1:A:172:VAL:O	2.21	0.40
1:B:204:ILE:HA	1:B:208:VAL:HB	2.03	0.40
1:C:30:ALA:CB	2:C:902:ATP:H1'	2.51	0.40
1:D:7:VAL:O	1:D:11:VAL:HG23	2.21	0.40
1:C:32:SER:HB3	2:C:902:ATP:C5	2.56	0.40
1:D:102:ARG:NH1	1:D:102:ARG:CG	2.84	0.40
1:D:14:LEU:HD23	1:D:171:TYR:CE1	2.56	0.40
1:A:105:LEU:H	1:A:105:LEU:HG	1.68	0.40
1:A:165:ILE:O	1:A:166:ARG:HD3	2.22	0.40
1:C:97:PHE:CE2	1:C:101:ASN:ND2	2.89	0.40
1:D:28:LEU:O	1:D:129:ILE:HA	2.21	0.40
1:B:61:PHE:HD2	1:B:63:HIS:CD2	2.40	0.40
1:D:112:LEU:O	1:D:115:LYS:HB3	2.21	0.40
1:D:39:VAL:HG13	1:D:180:TYR:CD2	2.57	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	315/317 (99%)	284 (90%)	24 (8%)	7 (2%)	6	10
1	B	312/317 (98%)	284 (91%)	20 (6%)	8 (3%)	5	8
1	C	312/317 (98%)	296 (95%)	14 (4%)	2 (1%)	25	43
1	D	311/317 (98%)	272 (88%)	31 (10%)	8 (3%)	5	8
All	All	1250/1268 (99%)	1136 (91%)	89 (7%)	25 (2%)	7	12

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	TYR

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Mol	Chain	Res	Type
1	A	197	VAL
1	A	308	GLU
1	B	195	TYR
1	B	196	GLU
1	D	249	LYS
1	D	307	LYS
1	A	106	GLU
1	A	300	LYS
1	B	255	ASP
1	B	300	LYS
1	D	64	MET
1	D	248	VAL
1	D	300	LYS
1	D	309	ARG
1	A	194	ASN
1	A	251	GLY
1	C	257	LYS
1	B	69	ALA
1	D	59	ALA
1	B	94	VAL
1	B	101	ASN
1	B	104	SER
1	D	308	GLU
1	C	256	VAL

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	285/285 (100%)	254 (89%)	31 (11%)	6	12
1	B	282/285 (99%)	253 (90%)	29 (10%)	7	14
1	C	282/285 (99%)	255 (90%)	27 (10%)	8	16
1	D	281/285 (99%)	250 (89%)	31 (11%)	6	12
All	All	1130/1140 (99%)	1012 (90%)	118 (10%)	7	13

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ILE
1	A	12	LEU
1	A	14	LEU
1	A	35	VAL
1	A	62	ASN
1	A	63	HIS
1	A	66	ARG
1	A	67	GLU
1	A	103	MET
1	A	139	LEU
1	A	143	LEU
1	A	144	LEU
1	A	164	VAL
1	A	166	ARG
1	A	180	TYR
1	A	190	GLU
1	A	194	ASN
1	A	195	TYR
1	A	196	GLU
1	A	201	ARG
1	A	207	ARG
1	A	222	THR
1	A	243	LYS
1	A	250	LYS
1	A	259	LEU
1	A	264	LEU
1	A	305	LYS
1	A	306	ARG
1	A	307	LYS
1	A	309	ARG
1	A	317	VAL
1	B	12	LEU
1	B	14	LEU
1	B	35	VAL
1	B	36	ASP
1	B	62	ASN
1	B	66	ARG
1	B	81	LYS
1	B	83	ARG
1	B	92	GLU
1	B	114	TYR
1	B	124	GLU

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Mol	Chain	Res	Type
1	B	131	THR
1	B	139	LEU
1	B	144	LEU
1	B	164	VAL
1	B	182	LYS
1	B	190	GLU
1	B	193	THR
1	B	198	SER
1	B	201	ARG
1	B	222	THR
1	B	240	GLU
1	B	257	LYS
1	B	259	LEU
1	B	264	LEU
1	B	281	GLU
1	B	285	LEU
1	B	300	LYS
1	B	304	LEU
1	C	12	LEU
1	C	14	LEU
1	C	19	LYS
1	C	36	ASP
1	C	62	ASN
1	C	66	ARG
1	C	74	GLU
1	C	81	LYS
1	C	92	GLU
1	C	110	ARG
1	C	119	GLU
1	C	124	GLU
1	C	139	LEU
1	C	143	LEU
1	C	144	LEU
1	C	166	ARG
1	C	167	ARG
1	C	190	GLU
1	C	194	ASN
1	C	207	ARG
1	C	222	THR
1	C	254	LEU
1	C	257	LYS
1	C	264	LEU

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Mol	Chain	Res	Type
1	C	281	GLU
1	C	285	LEU
1	C	291	GLU
1	D	12	LEU
1	D	14	LEU
1	D	55	GLU
1	D	62	ASN
1	D	64	MET
1	D	66	ARG
1	D	71	ARG
1	D	89	VAL
1	D	92	GLU
1	D	101	ASN
1	D	114	TYR
1	D	119	GLU
1	D	131	THR
1	D	139	LEU
1	D	143	LEU
1	D	144	LEU
1	D	153	ASP
1	D	187	ARG
1	D	193	THR
1	D	198	SER
1	D	252	ASN
1	D	274	PHE
1	D	279	ASP
1	D	285	LEU
1	D	290	LEU
1	D	304	LEU
1	D	305	LYS
1	D	306	ARG
1	D	307	LYS
1	D	308	GLU
1	D	313	PHE

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

Mol	Chain	Res	Type
1	A	62	ASN
1	A	63	HIS
1	A	202	ASN
1	A	267	GLN

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Mol	Chain	Res	Type
1	B	62	ASN
1	B	101	ASN
1	B	134	HIS
1	B	218	ASN
1	B	252	ASN
1	C	62	ASN
1	C	63	HIS
1	C	101	ASN
1	C	194	ASN
1	C	202	ASN
1	C	252	ASN
1	D	60	HIS
1	D	62	ASN
1	D	63	HIS
1	D	101	ASN
1	D	134	HIS
1	D	267	GLN
1	D	297	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ATP	D	903	-	26,33,33	0.99	2 (7%)	31,52,52	2.08	11 (35%)
2	ATP	B	901	-	26,33,33	0.99	1 (3%)	31,52,52	2.01	11 (35%)
2	ATP	A	900	-	26,33,33	1.15	3 (11%)	31,52,52	2.04	11 (35%)
2	ATP	C	902	-	26,33,33	1.01	1 (3%)	31,52,52	2.02	11 (35%)
3	LYS	B	950	-	5,9,9	0.77	0	4,10,10	0.51	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	D	903	-	-	4/18/38/38	0/3/3/3
2	ATP	B	901	-	-	6/18/38/38	0/3/3/3
2	ATP	A	900	-	-	1/18/38/38	0/3/3/3
2	ATP	C	902	-	-	3/18/38/38	0/3/3/3
3	LYS	B	950	-	-	0/5/9/9	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	ATP	O4'-C1'	2.48	1.44	1.41
2	C	902	ATP	O4'-C1'	2.45	1.44	1.41
2	A	900	ATP	C4-N3	-2.42	1.32	1.35
2	D	903	ATP	O4'-C1'	2.40	1.44	1.41
2	A	900	ATP	O4'-C1'	2.39	1.44	1.41
2	A	900	ATP	C5-N7	-2.23	1.31	1.39
2	D	903	ATP	C5-N7	-2.19	1.31	1.39

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	902	ATP	O2G-PG-O3B	-4.64	89.09	104.64
2	A	900	ATP	O2G-PG-O3B	-4.47	89.64	104.64
2	C	902	ATP	N3-C2-N1	-4.45	121.73	128.68
2	D	903	ATP	N3-C2-N1	-4.42	121.76	128.68
2	D	903	ATP	O2G-PG-O3B	-4.38	89.94	104.64
2	A	900	ATP	N3-C2-N1	-4.38	121.83	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	ATP	N3-C2-N1	-4.13	122.22	128.68
2	D	903	ATP	O3G-PG-O3B	-3.94	91.42	104.64
2	C	902	ATP	O3G-PG-O3B	-3.91	91.54	104.64
2	B	901	ATP	O3G-PG-O3B	-3.85	91.71	104.64
2	A	900	ATP	O3G-PG-O3B	-3.78	91.94	104.64
2	B	901	ATP	O2G-PG-O3B	-3.76	92.02	104.64
2	D	903	ATP	PB-O3B-PG	-3.74	119.99	132.83
2	B	901	ATP	PB-O3B-PG	-3.39	121.19	132.83
2	B	901	ATP	PA-O3A-PB	-3.37	121.26	132.83
2	A	900	ATP	PA-O3A-PB	-3.30	121.49	132.83
2	A	900	ATP	PB-O3B-PG	-3.26	121.63	132.83
2	D	903	ATP	PA-O3A-PB	-3.14	122.05	132.83
2	C	902	ATP	PB-O3B-PG	-3.09	122.24	132.83
2	B	901	ATP	O3G-PG-O1G	3.04	122.59	110.68
2	C	902	ATP	O3G-PG-O1G	2.98	122.36	110.68
2	D	903	ATP	O3G-PG-O1G	2.96	122.26	110.68
2	A	900	ATP	O3G-PG-O1G	2.93	122.16	110.68
2	D	903	ATP	C2'-C3'-C4'	-2.90	97.02	102.64
2	B	901	ATP	O3B-PG-O1G	-2.85	95.39	111.19
2	C	902	ATP	PA-O3A-PB	-2.84	123.08	132.83
2	C	902	ATP	O2G-PG-O1G	2.79	121.62	110.68
2	B	901	ATP	C4-C5-N7	-2.72	106.57	109.40
2	C	902	ATP	O3B-PG-O1G	-2.66	96.44	111.19
2	D	903	ATP	O2G-PG-O1G	2.65	121.07	110.68
2	D	903	ATP	O2B-PB-O1B	2.64	125.29	112.24
2	D	903	ATP	O3B-PG-O1G	-2.63	96.59	111.19
2	A	900	ATP	O2G-PG-O1G	2.63	120.97	110.68
2	A	900	ATP	O2B-PB-O1B	2.59	125.05	112.24
2	B	901	ATP	O2B-PB-O1B	2.59	125.04	112.24
2	B	901	ATP	O2G-PG-O1G	2.55	120.68	110.68
2	A	900	ATP	O3B-PG-O1G	-2.52	97.22	111.19
2	C	902	ATP	O2B-PB-O1B	2.52	124.68	112.24
2	C	902	ATP	C4-C5-N7	-2.37	106.93	109.40
2	A	900	ATP	O3G-PG-O2G	2.20	116.05	107.64
2	D	903	ATP	O3G-PG-O2G	2.19	116.00	107.64
2	B	901	ATP	O3G-PG-O2G	2.15	115.87	107.64
2	A	900	ATP	C2'-C3'-C4'	-2.15	98.47	102.64
2	C	902	ATP	O3G-PG-O2G	2.05	115.47	107.64

There are no chirality outliers.

All (14) torsion outliers are listed below:

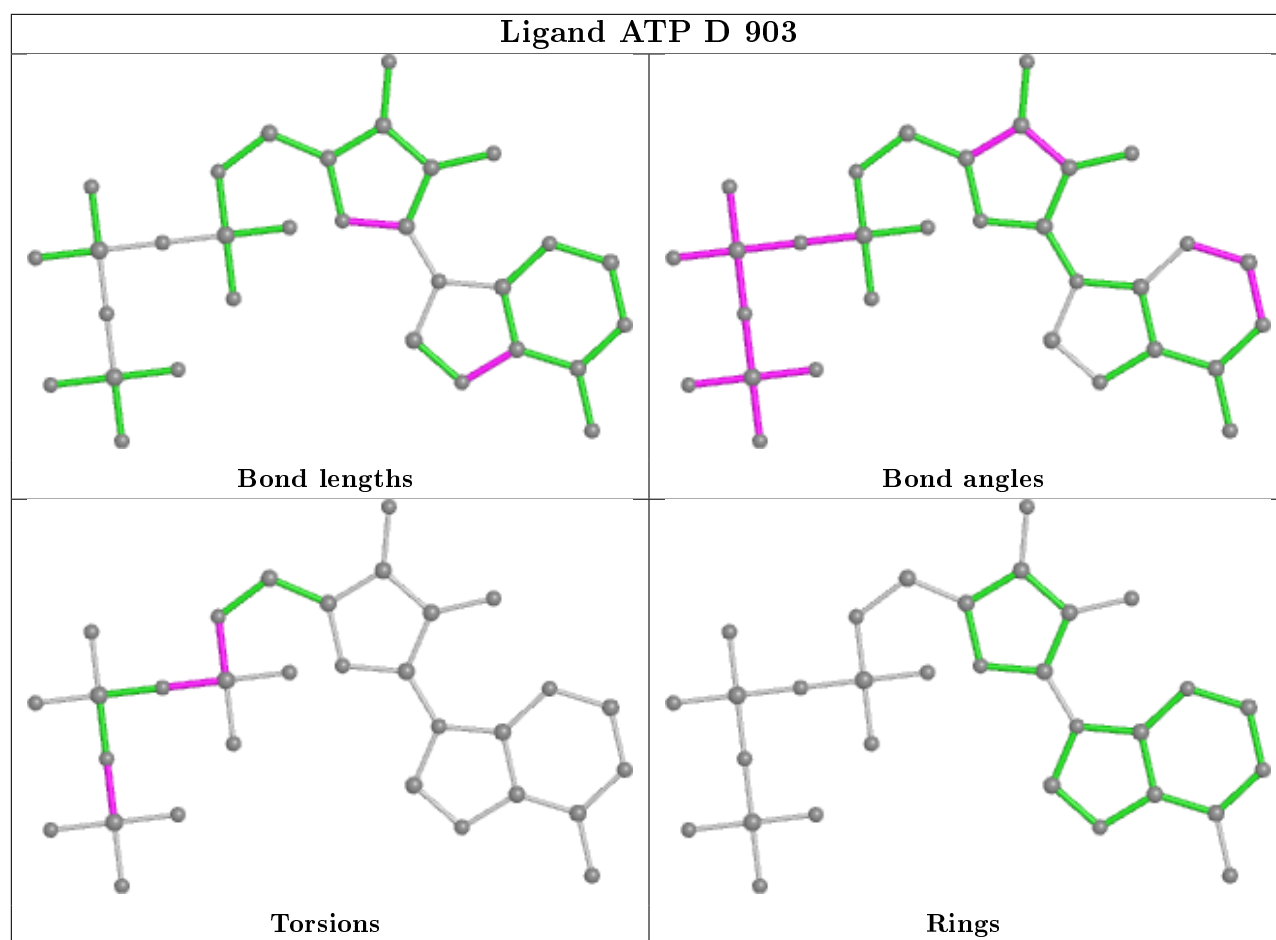
Mol	Chain	Res	Type	Atoms
2	B	901	ATP	C5'-O5'-PA-O2A
2	B	901	ATP	C5'-O5'-PA-O3A
2	A	900	ATP	PG-O3B-PB-O1B
2	B	901	ATP	PB-O3A-PA-O2A
2	B	901	ATP	C5'-O5'-PA-O1A
2	C	902	ATP	PG-O3B-PB-O1B
2	C	902	ATP	PB-O3A-PA-O2A
2	D	903	ATP	PB-O3B-PG-O2G
2	D	903	ATP	C5'-O5'-PA-O3A
2	D	903	ATP	PB-O3A-PA-O1A
2	D	903	ATP	PB-O3A-PA-O2A
2	C	902	ATP	PB-O3A-PA-O1A
2	B	901	ATP	PG-O3B-PB-O1B
2	B	901	ATP	PB-O3A-PA-O1A

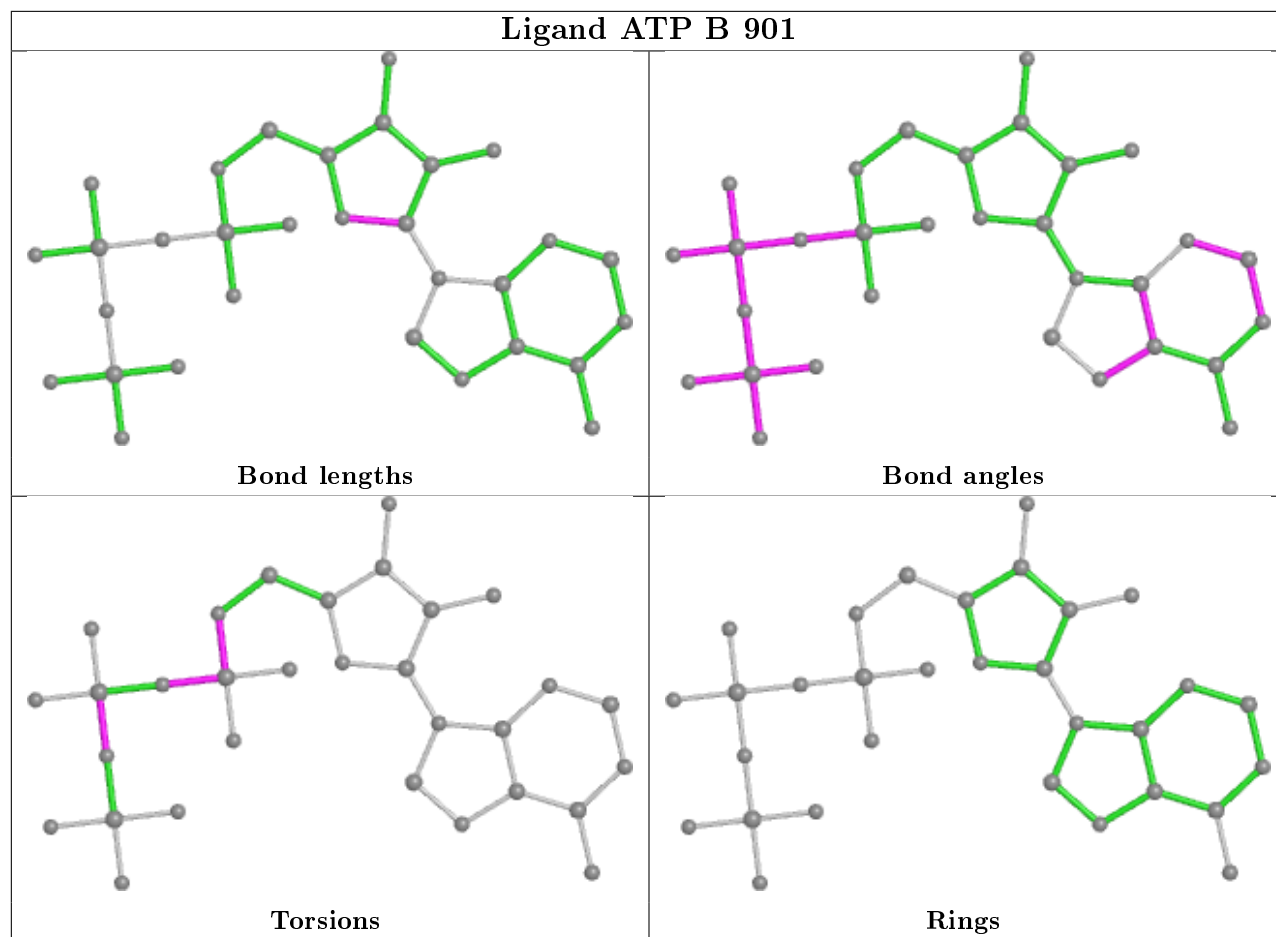
There are no ring outliers.

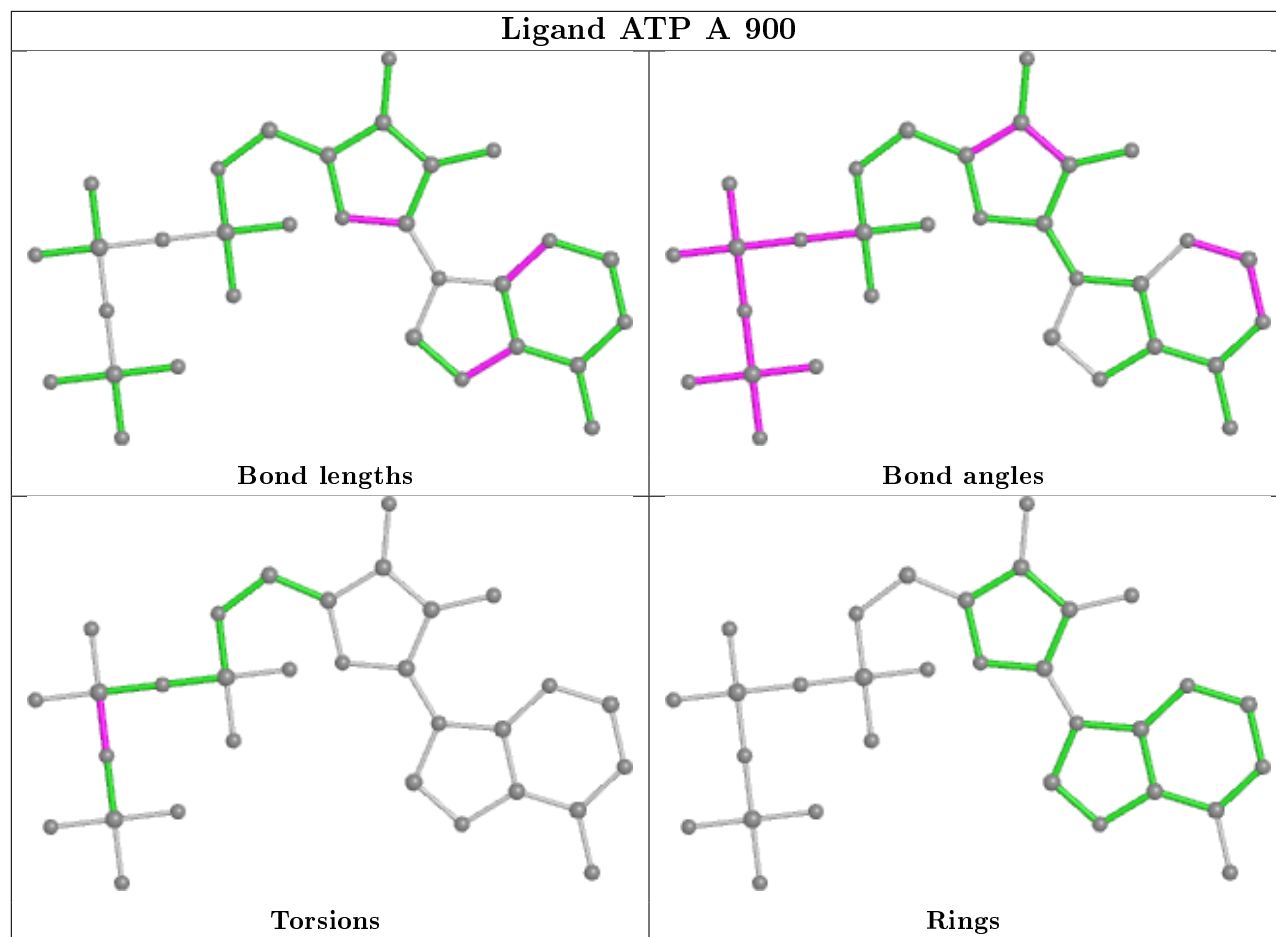
5 monomers are involved in 16 short contacts:

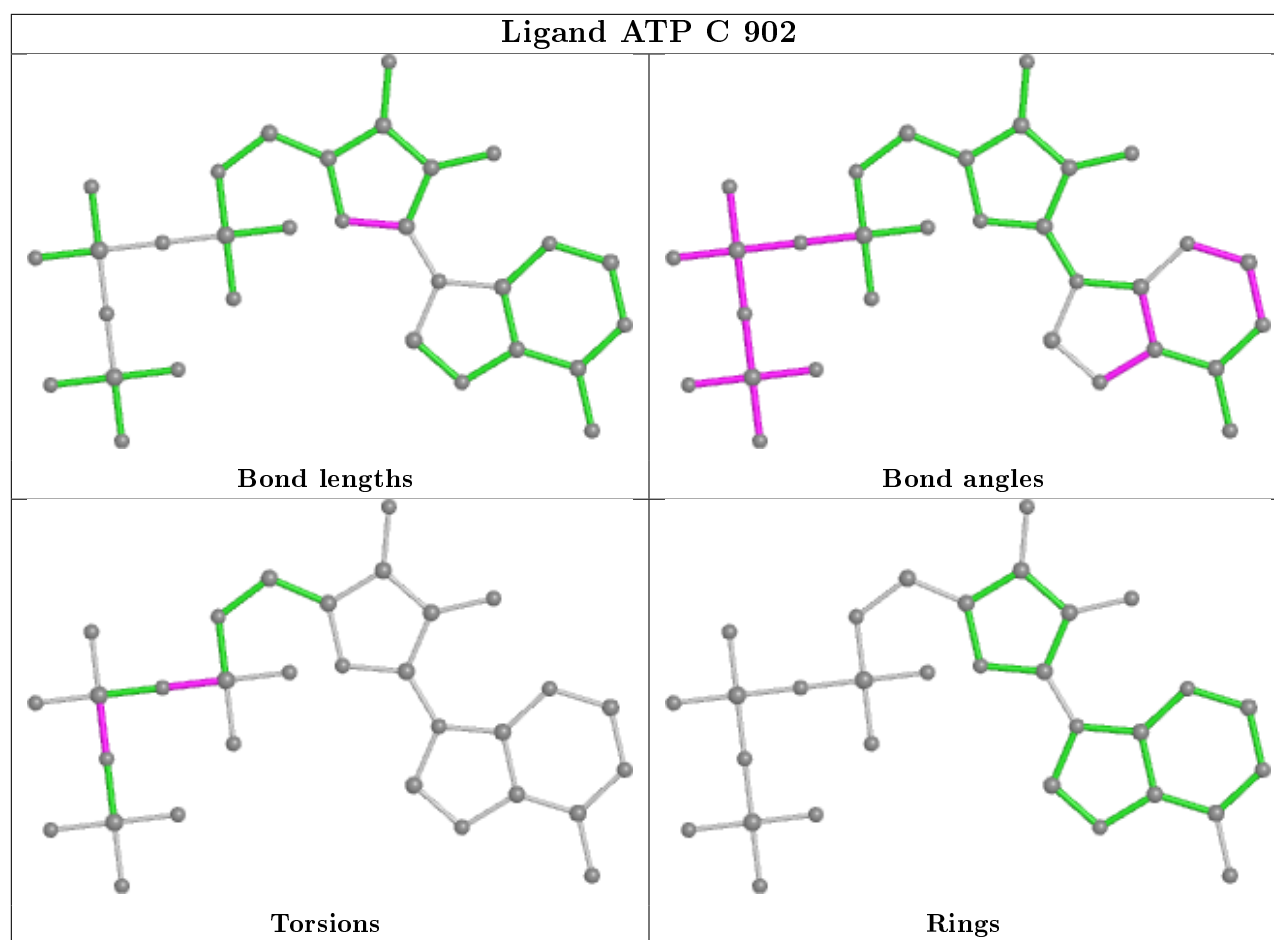
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	903	ATP	3	0
2	B	901	ATP	1	0
2	A	900	ATP	3	0
2	C	902	ATP	5	0
3	B	950	LYS	4	0

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	317/317 (100%)	0.44	22 (6%) 16 17	26, 46, 91, 110	0
1	B	314/317 (99%)	0.61	34 (10%) 5 5	22, 47, 88, 98	0
1	C	314/317 (99%)	0.13	13 (4%) 37 40	21, 42, 79, 85	0
1	D	313/317 (98%)	0.95	50 (15%) 1 1	29, 60, 108, 116	0
All	All	1258/1268 (99%)	0.53	119 (9%) 8 8	21, 49, 94, 116	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	105	LEU	9.5
1	D	305	LYS	8.7
1	A	105	LEU	8.2
1	D	99	LYS	7.0
1	D	98	ALA	7.0
1	D	311	LEU	6.2
1	D	64	MET	6.2
1	D	116	PHE	5.6
1	D	250	LYS	5.6
1	A	102	ARG	5.5
1	D	307	LYS	5.1
1	A	99	LYS	5.1
1	D	94	VAL	5.0
1	D	95	ARG	4.9
1	B	94	VAL	4.9
1	D	110	ARG	4.5
1	A	114	TYR	4.5
1	A	95	ARG	4.4
1	D	112	LEU	4.3
1	D	306	ARG	4.3
1	D	196	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	192	GLU	4.1
1	B	300	LYS	4.0
1	D	65	LEU	3.9
1	D	102	ARG	3.9
1	D	309	ARG	3.8
1	B	97	PHE	3.8
1	D	300	LYS	3.8
1	B	301	GLY	3.8
1	D	106	GLU	3.7
1	D	252	ASN	3.7
1	D	310	TRP	3.7
1	A	112	LEU	3.7
1	D	91	LYS	3.6
1	D	114	TYR	3.6
1	B	102	ARG	3.6
1	B	261	GLU	3.6
1	A	196	GLU	3.5
1	B	311	LEU	3.4
1	D	257	LYS	3.4
1	C	102	ARG	3.4
1	B	95	ARG	3.4
1	D	66	ARG	3.3
1	D	1	MET	3.2
1	A	100	GLU	3.2
1	A	94	VAL	3.2
1	D	96	ALA	3.1
1	D	254	LEU	3.1
1	A	103	MET	3.1
1	D	100	GLU	3.1
1	A	97	PHE	3.1
1	D	274	PHE	3.1
1	C	305	LYS	3.0
1	B	298	LEU	3.0
1	A	317	VAL	3.0
1	B	277	GLU	3.0
1	A	191	ASP	3.0
1	D	259	LEU	3.0
1	D	298	LEU	3.0
1	D	97	PHE	2.9
1	B	99	LYS	2.9
1	B	250	LYS	2.9
1	B	103	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	89	VAL	2.9
1	A	256	VAL	2.8
1	A	92	GLU	2.8
1	C	292	LYS	2.8
1	B	290	LEU	2.8
1	D	103	MET	2.8
1	C	307	LYS	2.7
1	B	302	LYS	2.7
1	C	103	MET	2.7
1	B	274	PHE	2.7
1	B	313	PHE	2.7
1	B	111	PHE	2.6
1	B	248	VAL	2.6
1	D	193	THR	2.6
1	D	117	LEU	2.6
1	B	112	LEU	2.6
1	C	257	LYS	2.6
1	B	257	LYS	2.5
1	A	311	LEU	2.5
1	B	107	GLU	2.5
1	D	246	LYS	2.5
1	A	193	THR	2.5
1	B	193	THR	2.5
1	B	295	GLU	2.5
1	C	217	GLU	2.5
1	B	101	ASN	2.4
1	C	286	VAL	2.4
1	B	292	LYS	2.4
1	C	314	SER	2.4
1	A	93	ASP	2.4
1	B	114	TYR	2.3
1	D	93	ASP	2.3
1	B	296	VAL	2.3
1	D	183	PHE	2.3
1	D	312	CYS	2.3
1	A	246	LYS	2.2
1	B	304	LEU	2.2
1	A	111	PHE	2.2
1	C	289	LEU	2.2
1	D	289	LEU	2.2
1	D	245	TYR	2.2
1	D	253	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	313	PHE	2.2
1	C	114	TYR	2.2
1	C	308	GLU	2.2
1	B	93	ASP	2.2
1	B	245	TYR	2.1
1	A	190	GLU	2.1
1	B	285	LEU	2.1
1	D	244	LEU	2.1
1	B	100	GLU	2.1
1	A	118	LYS	2.1
1	D	25	ARG	2.1
1	D	63	HIS	2.1
1	B	254	LEU	2.1
1	C	261	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

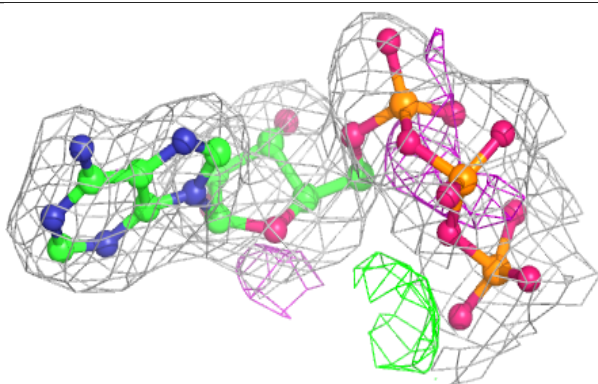
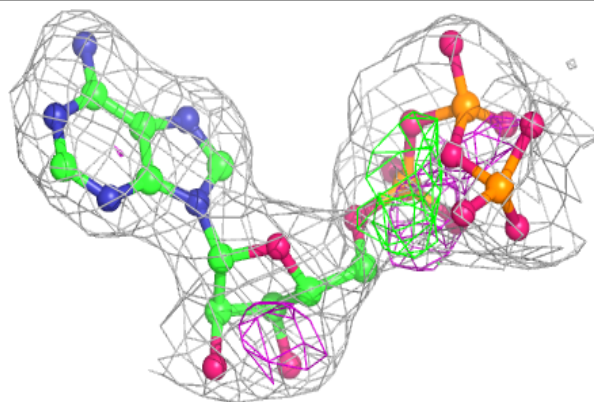
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	LYS	B	950	10/10	0.86	0.26	46,57,59,60	0
2	ATP	B	901	31/31	0.91	0.14	36,46,82,83	0
2	ATP	A	900	31/31	0.92	0.13	36,53,84,86	0
2	ATP	C	902	31/31	0.92	0.17	29,37,69,72	0
4	MG	C	601	1/1	0.94	0.21	59,59,59,59	0
2	ATP	D	903	31/31	0.94	0.14	75,77,81,82	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

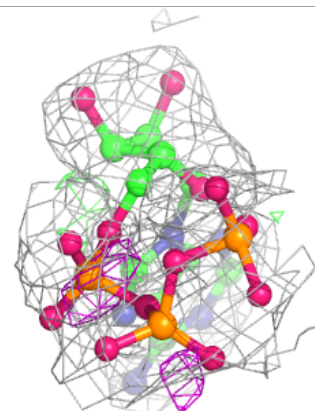
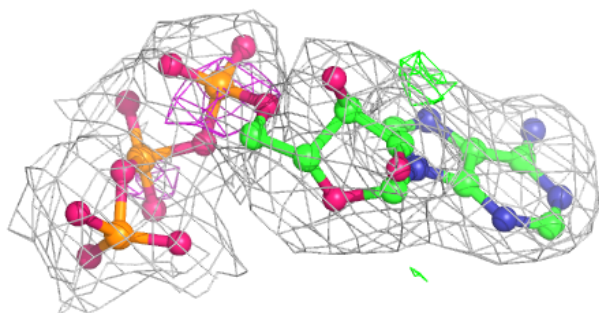
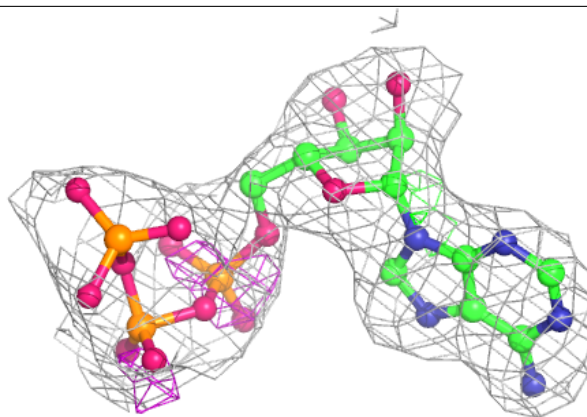
Electron density around ATP B 901:

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



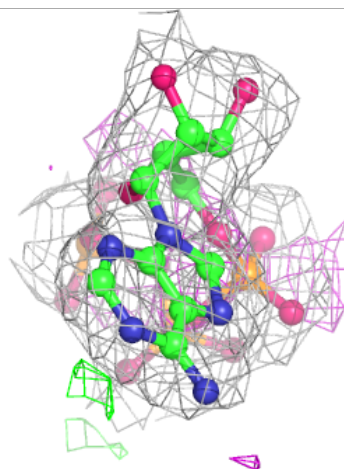
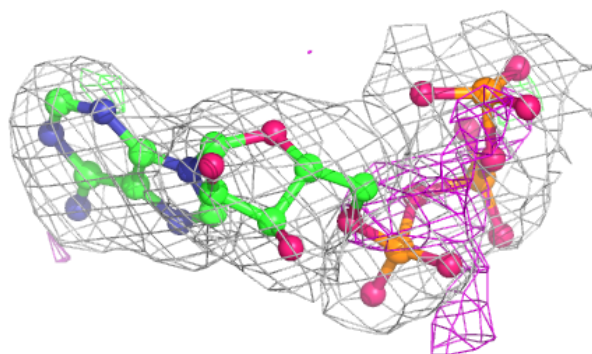
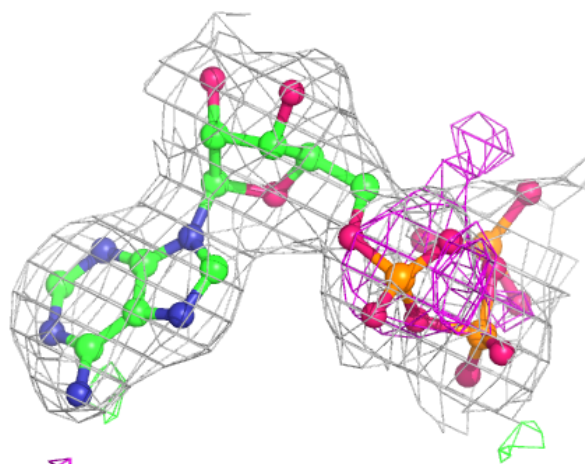
Electron density around ATP A 900:

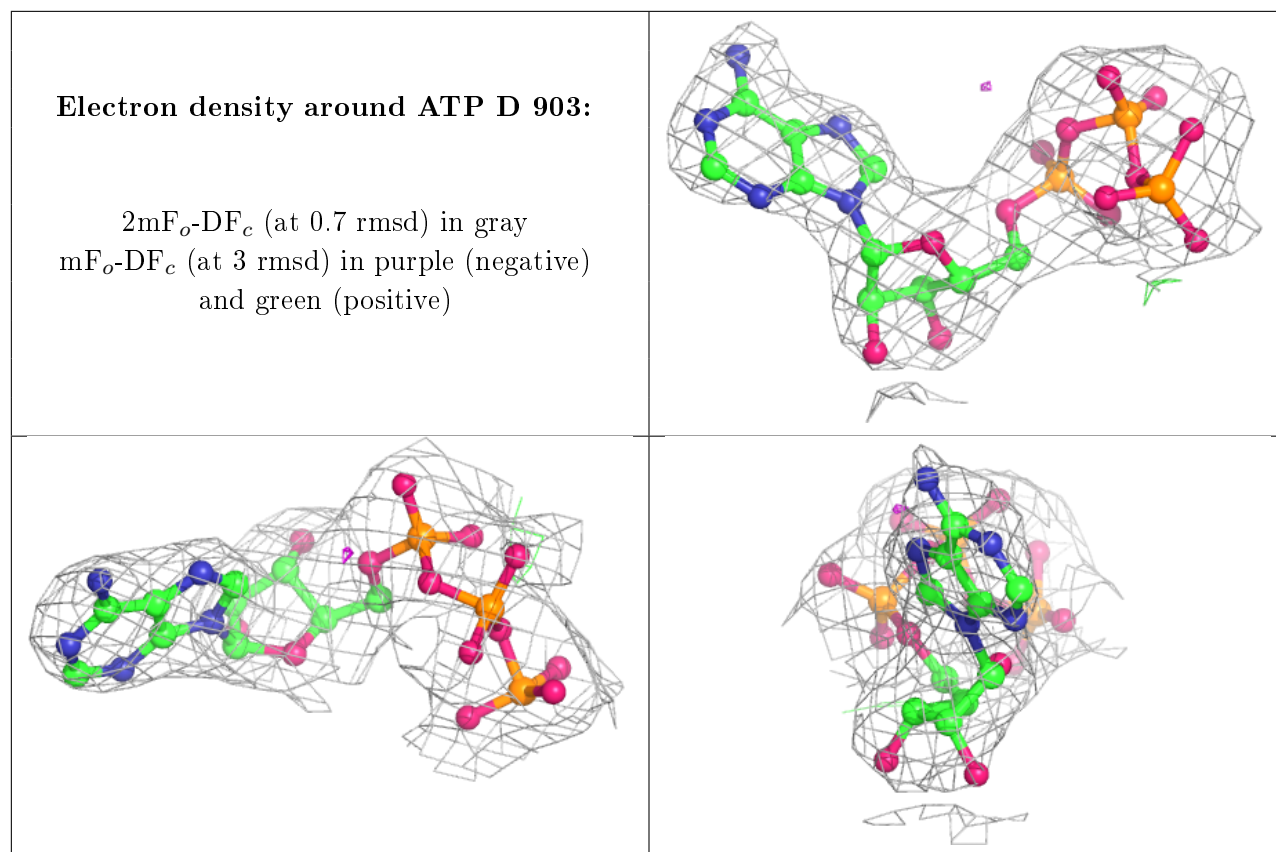
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ATP C 902:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.