



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:32 AM UTC

PDB ID : 2E89 / pdb_00002e89
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 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:

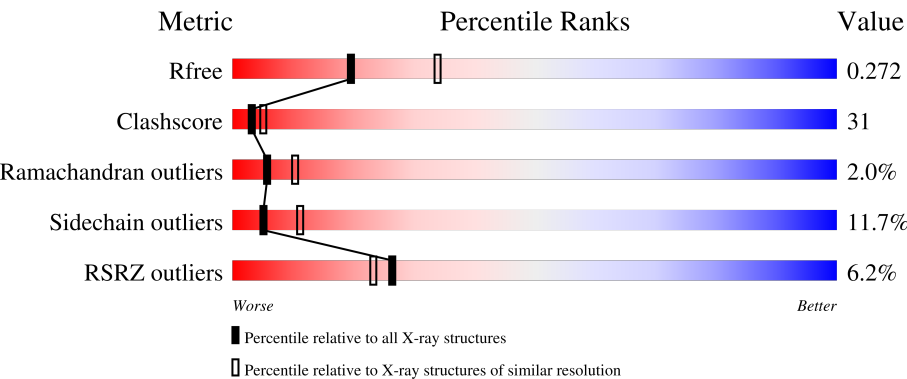
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 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	317	5% 51% 37% 9% .
1	B	317	4% 46% 44% 9% ..
1	C	317	2% 58% 34% 6% ..
1	D	317	14% 43% 40% 14% ..

2 Entry composition [i](#)

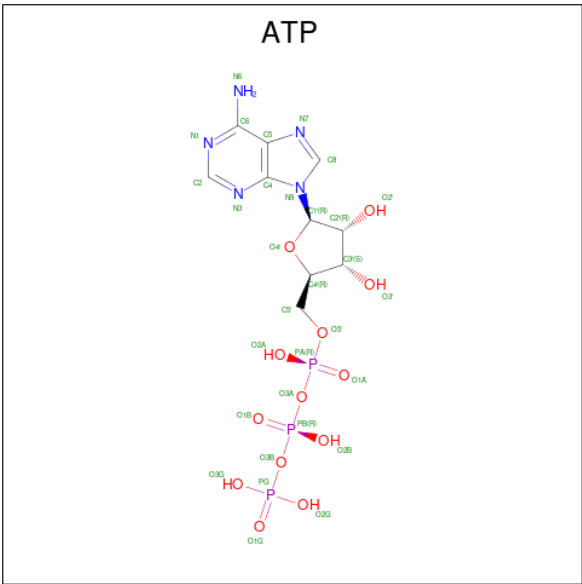
There are 5 unique types of molecules in this entry. The entry contains 10642 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



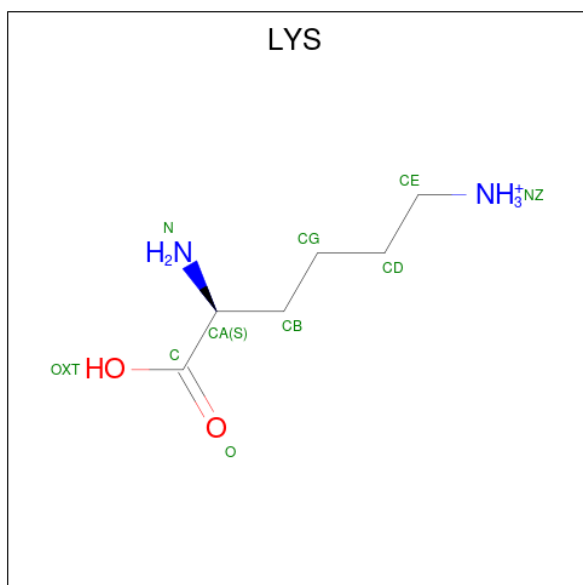
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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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 (CCD ID: 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 (CCD ID: 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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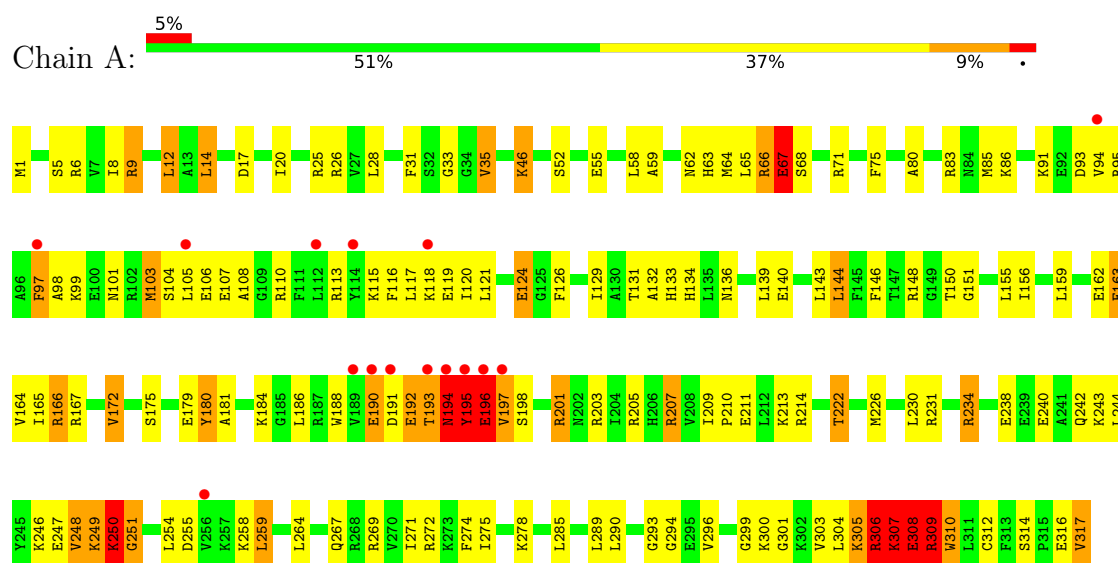
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	5	Total	O	0	0
			5	5		

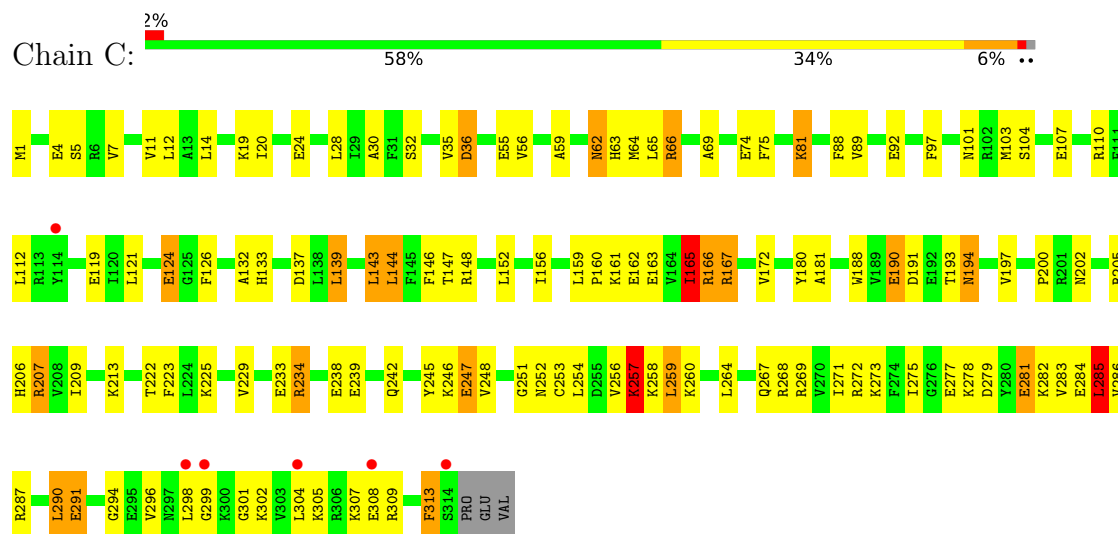
3 Residue-property plots

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.

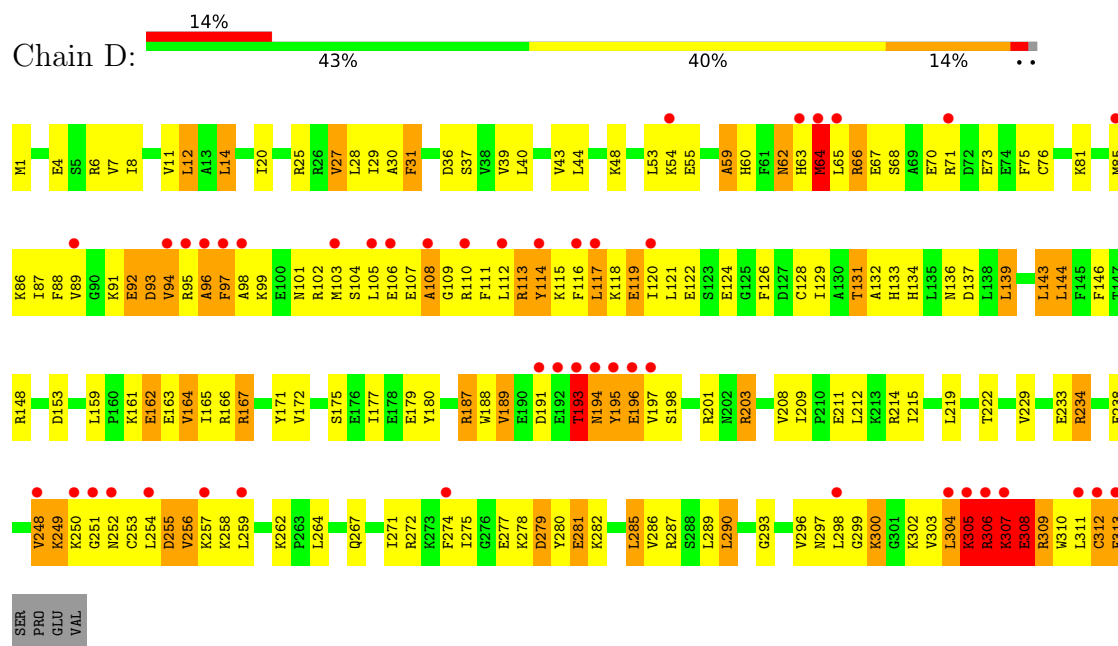
• Molecule 1: tRNA(Ile)-lysine synthase



• Molecule 1: tRNA(Ile)-lysine synthase



• Molecule 1: tRNA(Ile)-lysine synthase



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 – 2.50	Depositor EDS
% Data completeness (in resolution range)	91.8 (44.03-2.50) 91.8 (44.03-2.50)	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 0.227 , 0.272	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 , 39.2	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 [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.29	36/2672 (1.3%)	1.25	26/3569 (0.7%)
1	B	0.62	2/2647 (0.1%)	1.03	15/3535 (0.4%)
1	C	0.58	0/2647	1.00	11/3535 (0.3%)
1	D	0.73	5/2641 (0.2%)	1.28	31/3527 (0.9%)
All	All	0.85	43/10607 (0.4%)	1.15	83/14166 (0.6%)

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 (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	307	LYS	C-O	-18.18	1.03	1.24
1	A	250	LYS	CA-C	-15.11	1.33	1.53
1	A	248	VAL	C-O	-13.55	1.07	1.24
1	A	308	GLU	CA-C	-13.28	1.34	1.52
1	A	250	LYS	C-O	-12.50	1.09	1.24
1	A	310	TRP	C-O	-12.20	1.08	1.23
1	A	307	LYS	CA-C	-11.96	1.38	1.52
1	A	306	ARG	C-O	-11.83	1.10	1.23
1	A	308	GLU	C-O	-11.82	1.09	1.24
1	A	308	GLU	N-CA	-11.11	1.31	1.46
1	A	309	ARG	C-O	-9.97	1.11	1.24
1	D	96	ALA	N-CA	9.84	1.59	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	307	LYS	CA-CB	-9.51	1.38	1.53
1	A	307	LYS	C-N	-9.00	1.21	1.33
1	A	248	VAL	CB-CG1	-8.71	1.23	1.52
1	A	248	VAL	CB-CG2	-8.69	1.23	1.52
1	A	306	ARG	CA-C	-8.54	1.42	1.53
1	A	250	LYS	CA-CB	-8.08	1.39	1.53
1	D	96	ALA	CA-CB	-8.05	1.40	1.53
1	A	249	LYS	C-O	-7.68	1.14	1.23
1	A	163	GLU	CA-C	-7.60	1.46	1.53
1	A	249	LYS	CA-C	-7.52	1.43	1.52
1	A	310	TRP	CA-C	-7.52	1.43	1.52
1	A	250	LYS	C-N	-7.11	1.23	1.33
1	A	163	GLU	C-O	-7.10	1.17	1.24
1	A	310	TRP	CD2-CE2	-6.62	1.30	1.41
1	A	250	LYS	N-CA	-6.38	1.38	1.46
1	A	306	ARG	CZ-NH2	-6.35	1.25	1.33
1	A	249	LYS	CD-CE	-6.17	1.33	1.52
1	A	249	LYS	CE-NZ	-5.79	1.31	1.49
1	D	97	PHE	N-CA	5.72	1.53	1.46
1	A	309	ARG	CA-C	-5.60	1.45	1.52
1	D	209	ILE	CA-CB	5.58	1.57	1.53
1	A	310	TRP	CG-CD1	-5.50	1.23	1.36
1	B	163	GLU	CA-C	-5.49	1.45	1.52
1	D	95	ARG	C-O	-5.49	1.17	1.24
1	A	308	GLU	CA-CB	-5.44	1.44	1.53
1	A	308	GLU	C-N	-5.41	1.25	1.33
1	A	248	VAL	CA-CB	-5.38	1.47	1.54
1	A	163	GLU	C-N	-5.26	1.27	1.34
1	A	306	ARG	CB-CG	-5.09	1.37	1.52
1	B	163	GLU	C-O	-5.08	1.17	1.24
1	A	310	TRP	CD1-NE1	-5.00	1.27	1.37

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	306	ARG	N-CA-C	19.60	139.58	109.60
1	A	307	LYS	N-CA-C	18.09	130.69	110.97
1	A	193	THR	N-CA-C	-17.71	87.12	111.56
1	D	108	ALA	N-CA-C	-14.56	93.78	111.69
1	D	94	VAL	N-CA-C	14.25	126.87	110.62
1	A	309	ARG	N-CA-C	-13.95	94.73	114.12
1	D	98	ALA	N-CA-C	-11.47	97.58	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	307	LYS	CB-CA-C	-10.93	94.13	110.96
1	D	194	ASN	N-CA-C	-10.42	96.48	110.55
1	A	97	PHE	N-CA-C	-9.47	102.54	114.56
1	D	92	GLU	N-CA-C	-8.96	95.70	109.95
1	D	305	LYS	N-CA-C	8.94	124.08	109.96
1	D	117	LEU	N-CA-C	-8.71	101.72	111.82
1	A	307	LYS	CA-C-N	-7.51	107.20	121.54
1	A	307	LYS	C-N-CA	-7.51	107.20	121.54
1	D	93	ASP	CA-C-N	7.46	131.05	120.53
1	D	93	ASP	C-N-CA	7.46	131.05	120.53
1	D	193	THR	N-CA-C	-7.32	101.90	111.71
1	C	253	CYS	N-CA-C	7.31	120.52	109.41
1	A	307	LYS	O-C-N	-7.23	114.51	122.03
1	C	247	GLU	N-CA-C	-7.12	106.50	114.62
1	A	192	GLU	N-CA-C	6.95	121.70	112.25
1	A	248	VAL	N-CA-C	6.93	123.75	109.34
1	D	167	ARG	CA-C-N	6.91	126.53	119.56
1	D	167	ARG	C-N-CA	6.91	126.53	119.56
1	D	31	PHE	N-CA-C	6.83	119.88	108.20
1	C	313	PHE	N-CA-C	-6.82	101.73	110.53
1	A	167	ARG	CA-C-N	6.76	127.31	119.47
1	A	167	ARG	C-N-CA	6.76	127.31	119.47
1	A	163	GLU	CB-CA-C	-6.71	108.85	116.63
1	D	208	VAL	N-CA-C	6.70	117.32	110.82
1	D	312	CYS	N-CA-C	6.70	118.73	109.29
1	A	67	GLU	N-CA-C	-6.68	105.14	113.55
1	A	248	VAL	CG1-CB-CG2	-6.61	96.25	110.80
1	B	215	ILE	N-CA-C	-6.49	106.23	111.81
1	D	164	VAL	N-CA-C	6.39	122.63	109.34
1	C	137	ASP	N-CA-C	-6.38	104.25	111.07
1	B	215	ILE	CB-CA-C	-6.12	104.52	111.55
1	B	252	ASN	N-CA-C	-6.08	103.17	111.56
1	D	307	LYS	N-CA-C	-6.07	97.88	110.80
1	B	137	ASP	N-CA-C	-6.05	104.77	111.36
1	B	150	THR	N-CA-C	6.00	116.35	107.88
1	C	234	ARG	N-CA-C	-6.00	104.82	111.36
1	B	296	VAL	N-CA-C	5.99	117.32	108.45
1	C	294	GLY	N-CA-C	5.99	117.96	110.29
1	A	309	ARG	CG-CD-NE	5.94	125.07	112.00
1	D	203	ARG	N-CA-C	-5.93	104.72	111.07
1	A	118	LYS	N-CA-C	-5.93	104.82	111.28
1	C	290	LEU	N-CA-C	-5.92	105.89	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	106	GLU	N-CA-C	-5.85	105.63	112.89
1	D	97	PHE	N-CA-CB	5.79	120.14	110.41
1	A	172	VAL	N-CA-C	5.76	116.50	108.89
1	D	252	ASN	N-CA-C	-5.73	105.47	113.37
1	D	255	ASP	N-CA-C	-5.62	100.24	109.40
1	B	31	PHE	N-CA-C	5.61	117.45	108.41
1	C	165	ILE	N-CA-C	5.59	117.95	109.12
1	A	17	ASP	N-CA-C	5.57	117.35	111.28
1	B	172	VAL	N-CA-C	5.57	117.33	108.87
1	D	195	TYR	N-CA-C	-5.56	104.06	111.02
1	D	162	GLU	N-CA-C	5.53	116.47	107.23
1	C	172	VAL	N-CA-C	5.53	117.27	108.87
1	A	310	TRP	N-CA-C	5.49	118.52	109.85
1	D	113	ARG	N-CA-C	-5.45	104.56	111.11
1	A	33	GLY	N-CA-C	-5.43	107.86	114.92
1	B	281	GLU	N-CA-C	5.40	116.85	111.07
1	D	99	LYS	N-CA-C	5.37	117.21	111.36
1	D	163	GLU	CB-CA-C	-5.37	110.37	116.54
1	B	165	ILE	N-CA-C	5.35	116.68	108.71
1	B	220	GLU	N-CA-C	5.34	117.11	111.28
1	A	31	PHE	N-CA-C	5.30	116.89	108.67
1	D	137	ASP	N-CA-C	-5.29	105.59	111.36
1	A	307	LYS	CA-CB-CG	-5.21	103.68	114.10
1	B	262	LYS	CA-C-N	5.20	125.44	119.83
1	B	262	LYS	C-N-CA	5.20	125.44	119.83
1	D	172	VAL	N-CA-C	5.18	116.25	109.21
1	B	198	SER	N-CA-C	-5.15	105.78	111.71
1	C	285	LEU	N-CA-C	-5.13	104.66	112.04
1	C	246	LYS	N-CA-C	-5.07	107.60	112.97
1	A	294	GLY	N-CA-C	5.06	116.77	110.29
1	D	256	VAL	N-CA-C	-5.06	105.49	111.00
1	A	146	PHE	N-CA-C	-5.06	105.66	111.07
1	B	285	LEU	N-CA-C	-5.03	105.71	111.14
1	A	196	GLU	N-CA-C	-5.01	100.13	110.80

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	175	0
1	B	2606	0	2700	161	0
1	C	2606	0	2700	116	0
1	D	2600	0	2695	222	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	664	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 31.

All (664) 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:249:LYS:O	1:A:250:LYS:HD2	1.44	1.14
1:A:306:ARG:HH21	1:A:306:ARG:CG	1.52	1.14
1:A:307:LYS:O	1:A:308:GLU:HB2	1.51	1.10
1:A:306:ARG:HG2	1:A:306:ARG:NH2	1.46	1.06
1:D:66:ARG:HG2	1:D:66:ARG:HH11	1.22	1.01
1:A:66:ARG:HG3	1:A:66:ARG:HH11	1.26	1.00
1:A:64:MET:HE3	1:A:91:LYS:HE2	1.40	0.99
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:O	1:A:307:LYS:HG2	1.72	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD22	1:C:194:ASN:H	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:A:249:LYS:C	1:A:250:LYS:HD2	2.06	0.81
1:A:190:GLU:CD	1:A:190:GLU:H	1.88	0.80
1:C:20:ILE:HG23	1:C:166:ARG:HG3	1.63	0.80
1:D:308:GLU:O	1:D:308:GLU:HG2	1.81	0.80
1:A:65:LEU:HA	1:A:95:ARG:NH2	1.97	0.79
1:D:187:ARG:HG3	1:D:187:ARG:HH11	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:249:LYS:C	1:A:250:LYS:CD	2.57	0.76
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:C:190:GLU:CD	1:C:190:GLU:H	1.89	0.76
1:A:150:THR:O	1:B:226:MET:HG3	1.84	0.76
1:D:234:ARG:HD3	1:D:238:GLU:OE1	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:ASN:HD22	1:D:64:MET:H	1.35	0.75
1:D:66:ARG:HH11	1:D:66:ARG:CG	1.99	0.75
1:D:97:PHE:CE1	1:D:101:ASN:ND2	2.55	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:B:97:PHE:HE2	1:B:103:MET:HE1	1.52	0.73
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:D:248:VAL:O	1:D:249:LYS:C	2.30	0.73
1:B:64:MET:HE3	1:B:91:LYS:HE2	1.70	0.73
1:D:197:VAL:HG12	1:D:203:ARG:NH2	2.04	0.73
1:D:281:GLU:CD	1:D:281:GLU:H	1.93	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:HG3	1:A:66:ARG:NH1	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:HH11	1:D:187:ARG:CG	2.01	0.72
1:D:304:LEU:HD23	1:D:312:CYS:O	1.90	0.72
1:C:291:GLU:OE2	1:C:291:GLU:HA	1.89	0.72
2:C:902:ATP:O1G	2:C:902:ATP:H5'1	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1:MET:HE3	1:A:6:ARG:CZ	2.22	0.69
1:B:103:MET:HB3	1:B:107:GLU:HG3	1.74	0.69
1:D:114:TYR:O	1:D:118:LYS:HG3	1.93	0.69
1:D:134:HIS:HD2	1:D:136:ASN:H	1.38	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: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:62:ASN:C	1:C:62:ASN:HD22	2.01	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:251:GLY:C	1:D:253:CYS:H	2.00	0.67
1:D:308:GLU:O	1:D:308:GLU:CG	2.42	0.67
1:D:193:THR:C	1:D:196:GLU:HG3	2.19	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:114:TYR:C	1:D:118:LYS:HE2	2.21	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:A:192:GLU:HA	1:A:194:ASN:CG	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:VAL:O	1:D:250:LYS:HG2	1.95	0.65
1:B:62:ASN:HD22	1:B:62:ASN:C	2.04	0.65
1:A:191:ASP:O	1:A:194:ASN:CB	2.44	0.65
1:D:248:VAL:HG12	1:D:249:LYS:N	2.11	0.65
1:D:63:HIS:C	1:D:65:LEU:H	2.05	0.64
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:C:190:GLU:CD	1:C:190:GLU:N	2.56	0.64
1:B:25:ARG:HD2	1:B:54:LYS:HG3	1.80	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: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: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:HH21	1:A:306:ARG:HG2	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: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: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:C:97:PHE:HE2	1:C:103:MET:HE1	1.64	0.62
1:A:121:LEU:HD12	1:A:126:PHE:CB	2.29	0.61
1:A:113:ARG:HD3	2:A:900:ATP:C4	2.35	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
1:D:191:ASP:OD1	1:D:193:THR:HG23	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:VAL:HG22	1:D:112:LEU:HD13	1.82	0.60
1:D:108:ALA:O	1:D:112:LEU:HG	2.00	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:HG3	1:D:102:ARG:HH11	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: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: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:HH11	1:A:207:ARG:CG	2.14	0.59
1:A:269:ARG:HH21	1:B:233:GLU:CD	2.11	0.59
1:A:131:THR:HG22	1:A:133:HIS:H	1.66	0.59
1:B:102:ARG:HG3	1:B:102:ARG:HH11	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:HD2	1:B:300:LYS:O	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:A:249:LYS:C	1:A:250:LYS:HD3	2.27	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:A:196:GLU:C	1:A:198:SER:H	2.11	0.58
1:B:66:ARG:HD2	1:B:66:ARG:N	2.18	0.58
1:B:260:LYS:HE2	1:B:290:LEU:O	2.04	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:D:305:LYS:O	1:D:311:LEU:HD12	2.04	0.58
1:B:33:GLY:C	1:B:189:VAL:HG12	2.28	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
1:D:116:PHE:O	1:D:120:ILE:HG12	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:ND2	1:A:194:ASN:H	2.01	0.57
1:A:243:LYS:HG3	1:A:244:LEU:N	2.20	0.57
1:B:95:ARG:HG3	1:B:95:ARG:HH11	1.70	0.57
1:C:225:LYS:HG2	1:D:280:TYR:CD2	2.40	0.57
1:D:274:PHE:C	1:D:274:PHE:CD2	2.81	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:A:246:LYS:C	1:A:248:VAL:H	2.11	0.57
1:B:14:LEU:HD22	1:B:18:GLU:HG3	1.86	0.57
1:D:60:HIS:CD2	1:D:73:GLU:HA	2.39	0.57
1:D:128:CYS:HA	1:D:164:VAL:HG22	1.85	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:7:VAL:O	1:C:11:VAL:HG23	2.05	0.57
1:C:66:ARG:HG3	1:C:66:ARG:HH11	1.70	0.57
1:C:144:LEU:HD22	1:C:148:ARG:HD2	1.86	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:66:ARG:HG2	1:D:66:ARG:NH1	2.03	0.56
1:D:159:LEU:HB2	1:D:162:GLU:HG3	1.85	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:147:THR:OG1	1:D:212:LEU:HD22	2.05	0.56
1:C:242:GLN:OE1	1:C:242:GLN:HA	2.06	0.56
1:B:1:MET:HE3	1:B:6:ARG:HG3	1.86	0.56
1:C:35:VAL:HG23	1:C:36:ASP:N	2.18	0.56
1:C:272:ARG:HD3	1:C:278:LYS:NZ	2.20	0.56
1:B:242:GLN:HA	1:B:242:GLN:OE1	2.05	0.56
1:B:252:ASN:ND2	1:B:313:PHE:HB2	2.19	0.56
1:D:251:GLY:C	1:D:253:CYS:N	2.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:305:LYS:HG3	1:D:306:ARG:H	1.70	0.55
1:A:197:VAL:O	1:A:197:VAL:HG12	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:36:ASP:OD2	1:D:37:SER:N	2.38	0.55
1:D:287:ARG:HA	1:D:290:LEU:HD12	1.87	0.55
1:A:285:LEU:HD21	1:C:307:LYS:HE2	1.87	0.55
1:B:93:ASP:O	1:B:94:VAL:C	2.50	0.55
1:A:191:ASP:O	1:A:194:ASN:CG	2.49	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:26:ARG:NH1	1:A:55:GLU:OE1	2.40	0.55
1:A:209:ILE:HB	1:A:210:PRO:HD3	1.89	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:94:VAL:HG11	1:A:105:LEU:O	2.07	0.55
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:279:ASP:O	1:B:283:VAL:HG23	2.06	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:D:308:GLU:C	1:D:310:TRP:H	2.16	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:180:TYR:C	1:A:180:TYR:CD2	2.86	0.53
1:B:26:ARG:NH2	1:B:55:GLU:OE2	2.41	0.53
1:B:188:TRP:HE1	3:B:950:LYS:HE2	1.73	0.53
1:C:66:ARG:HG3	1:C:66:ARG:NH1	2.24	0.53
1:C:81:LYS:HD3	1:C:81:LYS:C	2.34	0.53
1:D:97:PHE:CG	1:D:97:PHE:O	2.62	0.53
1:A:192:GLU:HG2	1:A:194:ASN:OD1	2.09	0.53
1:A:248:VAL:O	1:A:248:VAL:CG1	2.56	0.53
1:B:240:GLU:HA	1:B:240:GLU:OE1	2.08	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:A:62:ASN:C	1:A:62:ASN:HD22	2.17	0.52
1:B:103:MET:C	1:B:104:SER:O	2.52	0.52
1:C:24:GLU:OE1	1:C:24:GLU:N	2.33	0.52
1:C:194:ASN:HA	1:C:206:HIS:CD2	2.44	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:O	1:D:257:LYS:CG	2.58	0.52
1:A:93:ASP:O	1:A:94:VAL:C	2.53	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:O	1:D:257:LYS:HG2	2.10	0.52
1:A:194:ASN:O	1:A:195:TYR:CB	2.56	0.51
1:A:35:VAL:HG23	5:A:912:HOH:O	2.10	0.51
1:A:134:HIS:HD2	1:A:136:ASN:H	1.58	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:A:175:SER:O	1:A:179:GLU:HG3	2.10	0.51
1:A:194:ASN:ND2	1:A:194:ASN:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:281:GLU:CD	1:B:281:GLU:H	2.18	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:D:63:HIS:O	1:D:65:LEU:N	2.43	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:C:62:ASN:ND2	1:C:69:ALA:HB1	2.26	0.50
1:D:62:ASN:HD22	1:D:62:ASN:C	2.20	0.50
1:D:88:PHE:CE2	1:D:124:GLU:HG3	2.47	0.50
1:B:281:GLU:CD	1:B:281:GLU:N	2.70	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:D:272:ARG:HG2	1:D:277:GLU:O	2.12	0.49
1:D:307:LYS:O	1:D:308:GLU:C	2.54	0.49
1:B:97:PHE:HE2	1:B:103:MET:CE	2.23	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:D:193:THR:O	1:D:196:GLU:HG3	2.12	0.49
1:A:65:LEU:CA	1:A:95:ARG:NH2	2.73	0.49
1:A:131:THR:HG22	1:A:132:ALA:N	2.26	0.49
1:B:25:ARG:CD	1:B:54:LYS:HG3	2.43	0.49
1:C:273:LYS:O	1:C:273:LYS:HD3	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:D:274:PHE:C	1:D:274:PHE:HD2	2.21	0.49
1:C:36:ASP:N	1:C:36:ASP:OD2	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:104:SER:H	1:B:107:GLU:CD	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:HA	1:B:66:ARG:NE	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:A:104:SER:O	1:A:105:LEU:C	2.55	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:14:LEU:HD13	1:A:20:ILE:HG13	1.96	0.48
1:A:75:PHE:CZ	1:A:188:TRP:HA	2.49	0.48
1:A:116:PHE:O	1:A:119:GLU:HB2	2.14	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:62:ASN:C	1:C:62:ASN:ND2	2.70	0.48
1:C:252:ASN:HD21	1:C:313:PHE:CB	2.23	0.48
1:C:284:GLU:CD	1:C:287:ARG:HE	2.22	0.48
1:D:73:GLU:O	1:D:76:CYS:HB2	2.13	0.48
1:C:275:ILE:HA	1:C:313:PHE:HZ	1.78	0.48
1:C:279:ASP:OD1	1:C:282:LYS:HD2	2.13	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:B:68:SER:O	1:B:69:ALA:C	2.56	0.48
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: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:B:62:ASN:ND2	1:B:62:ASN:C	2.72	0.47
1:D:296:VAL:HG23	1:D:296:VAL:O	2.14	0.47
1:C:139:LEU:HD23	1:C:223:PHE:CD1	2.50	0.47
1:D:272:ARG:NH2	1:D:278:LYS:HZ3	2.12	0.47
1:D:293:GLY:HA2	1:D:306:ARG:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:209:ILE:O	1:A:213:LYS:HG3	2.14	0.47
1:A:211:GLU:OE2	1:A:214:ARG:NH1	2.48	0.47
1:C:299:GLY:C	1:C:301:GLY:H	2.22	0.47
1:D:102:ARG:HG3	1:D:102:ARG:NH1	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:D:1:MET:HE3	1:D:6:ARG:HG3	1.96	0.47
1:A:205:ARG:HA	1:A:209:ILE:HD12	1.96	0.47
1:C:146:PHE:C	1:C:146:PHE:CD2	2.93	0.47
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:73:GLU:O	1:B:76:CYS:HB2	2.15	0.46
1:B:197:VAL:HG13	1:B:203:ARG:HA	1.97	0.46
1:C:279:ASP:O	1:C:283:VAL:HG23	2.15	0.46
1:D:146:PHE:C	1:D:146:PHE:CD2	2.92	0.46
1:B:38:VAL:HG13	1:B:79:PHE:CZ	2.50	0.46
1:D:249:LYS:O	1:D:249:LYS:HG2	2.13	0.46
1:A:250:LYS:CD	1:A:250:LYS:N	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:A:196:GLU:C	1:A:198:SER:N	2.72	0.46
1:C:309:ARG:O	1:C:309:ARG:HG2	2.15	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:A:307:LYS:C	1:A:307:LYS:CD	2.77	0.46
1:B:258:LYS:O	1:B:262:LYS:HD3	2.15	0.46
1:B:97:PHE:CE2	1:B:103:MET:HE1	2.41	0.46
1:B:242:GLN:OE1	1:B:273:LYS:HE3	2.16	0.46
1:D:194:ASN:O	1:D:195:TYR:C	2.54	0.46
1:D:201:ARG:HG2	1:D:201:ARG:NH1	2.30	0.46
1:D:281:GLU:O	1:D:285:LEU:HB2	2.16	0.46
1:C:62:ASN:HD21	1:C:69:ALA:HB1	1.81	0.46
1:C:194:ASN:N	1:C:194:ASN:ND2	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:TYR:O	1:D:118:LYS:HE2	2.15	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:30:ALA:HB2	1:D:117:LEU:HD11	1.98	0.45
1:D:300:LYS:HB2	1:D:300:LYS:HE3	1.58	0.45
1:A:194:ASN:N	1:A:194:ASN:HD22	2.14	0.45
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:63:HIS:C	1:D:65:LEU:N	2.71	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: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: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:A:131:THR:CG2	1:A:132:ALA:N	2.80	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:HD23	1:B:152:LEU:HA	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:61:PHE:CD2	1:B:63:HIS:CD2	3.05	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:D:104:SER:OG	1:D:105:LEU:N	2.50	0.45
1:B:8:ILE:HG22	1:B:12:LEU:HD22	1.99	0.45
1:B:26:ARG:CZ	1:B:55:GLU:OE2	2.65	0.45
1:D:305:LYS:CG	1:D:306:ARG:N	2.75	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:46:LYS:NZ	1:A:184:LYS:HZ3	2.15	0.44
1:A:110:ARG:HH21	1:A:201:ARG:NH2	2.15	0.44
1:A:110:ARG:HH21	1:A:201:ARG:HH22	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:THR:OG1	1:A:151:GLY:N	2.47	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:62:ASN:HB3	1:D:91:LYS:HG3	1.99	0.44
1:D:67:GLU:CG	1:D:68:SER:N	2.80	0.44
1:C:32:SER:HB3	2:C:902:ATP:N7	2.32	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:D:64:MET:C	1:D:66:ARG:N	2.75	0.44
1:A:194:ASN:O	1:A:195:TYR:CD1	2.70	0.44
1:A:195:TYR:C	1:A:196:GLU:OE1	2.61	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:D:8:ILE:HG22	1:D:12:LEU:HD22	1.99	0.44
1:D:29:ILE:HG23	1:D:40:LEU:HD23	1.98	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:D:308:GLU:C	1:D:310:TRP:N	2.75	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:C:245:TYR:C	1:C:247:GLU:H	2.25	0.44
1:B:250:LYS:HB2	1:B:310:TRP:CZ3	2.53	0.44
1:D:97:PHE:CD2	1:D:97:PHE:C	2.93	0.44
1:D:211:GLU:O	1:D:214:ARG:HB2	2.17	0.44
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:A:83:ARG:HB2	1:A:85:MET:HG3	1.99	0.43
1:A:267:GLN:O	1:A:271:ILE:HG12	2.18	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:B:109:GLY:O	1:B:110:ARG:C	2.61	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:D:110:ARG:O	1:D:111:PHE:C	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:ARG:HH11	1:A:309:ARG:HD2	1.60	0.43
1:D:85:MET:CG	1:D:86:LYS:N	2.80	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:B:255:ASP:O	1:B:256:VAL:C	2.62	0.43
1:C:269:ARG:HH21	1:D:233:GLU:CD	2.26	0.43
1:C:296:VAL:N	1:C:304:LEU:O	2.50	0.43
1:D:48:LYS:HE2	1:D:53:LEU:O	2.19	0.43
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: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:25:ARG:NH1	1:A:52:SER:O	2.52	0.42
1:A:307:LYS:C	1:A:307:LYS:HD3	2.44	0.42
1:B:15:GLN:OE1	1:B:15:GLN:HA	2.18	0.42
1:B:188:TRP:CD1	3:B:950:LYS:HE2	2.54	0.42
1:C:28:LEU:HD11	1:C:59:ALA:HB2	2.00	0.42
1:C:104:SER:N	1:C:107:GLU:OE2	2.44	0.42
1:A:156:ILE:HD11	1:A:230:LEU:CB	2.50	0.42
1:B:49:ASN:O	1:B:50:TYR:C	2.61	0.42
1:D:64:MET:O	1:D:64:MET:HG3	2.16	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:HD12	1:A:12:LEU:HA	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: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:62:ASN:HD22	1:D:64:MET:N	2.10	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:ALA:O	1:D:109:GLY:C	2.62	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:A:68:SER:O	1:A:71:ARG:N	2.53	0.42
1:A:201:ARG:HH11	1:A:201:ARG:HB2	1.85	0.42
1:A:242:GLN:O	1:A:243:LYS:C	2.63	0.42
1:B:114:TYR:CZ	1:B:118:LYS:NZ	2.74	0.42
1:A:98:ALA:HB2	1:A:108:ALA:HB3	2.02	0.41
1:A:193:THR:C	1:A:195:TYR:H	2.28	0.41
1:C:121:LEU:HD12	1:C:126:PHE:HB2	2.01	0.41
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:63:HIS:HB2	1:D:65:LEU:HG	2.02	0.41
1:D:193:THR:O	1:D:196:GLU:HB2	2.20	0.41
1:D:309:ARG:O	1:D:309:ARG:HG3	2.18	0.41
1:A:190:GLU:CD	1:A:190:GLU:N	2.66	0.41
1:A:197:VAL:O	1:A:197:VAL:CG1	2.68	0.41
1:A:247:GLU:C	1:A:248:VAL:HG23	2.46	0.41
1:B:1:MET:HE3	1:B:6:ARG:HE	1.85	0.41
1:B:197:VAL:HG12	1:B:203:ARG:CZ	2.50	0.41
1:C:194:ASN:H	1:C:194:ASN:ND2	1.99	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: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:1:MET:HE3	1:A:6:ARG:NH2	2.34	0.41
1:C:144:LEU:HD23	1:C:144:LEU:HA	1.89	0.41
1:D:307:LYS:O	1:D:309:ARG:N	2.53	0.41
1:D:14:LEU:HD13	1:D:20:ILE:HG13	2.01	0.41
1:A:180:TYR:C	1:A:180:TYR:HD2	2.29	0.41
1:B:42:ASP:OD1	1:B:180:TYR:OH	2.30	0.41
1:D:64:MET:O	1:D:65:LEU:C	2.63	0.41
1:A:62:ASN:ND2	1:A:64:MET:H	2.17	0.41
1:A:230:LEU:O	1:A:231:ARG:C	2.63	0.41
1:B:150:THR:OG1	1:B:151:GLY:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:LEU:HD23	1:B:266:LEU:HB3	2.03	0.41
1:B:305:LYS:HB3	1:B:305:LYS:HE2	1.83	0.41
1:D:4:GLU:O	1:D:8:ILE:HG12	2.21	0.41
1:D:30:ALA:HB1	2:D:903:ATP:H1'	2.03	0.41
1:D:44:LEU:HD23	1:D:44:LEU:HA	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:D:153:ASP:CA	1:D:234:ARG:HH21	2.23	0.41
1:D:164:VAL:HA	1:D:166:ARG:HH12	1.85	0.41
1:A:66:ARG:HB3	1:A:67:GLU:H	1.73	0.41
1:A:272:ARG:CG	1:A:278:LYS:HD2	2.51	0.41
1:B:226:MET:HE3	1:B:230:LEU:CD1	2.51	0.41
1:D:97:PHE:HE2	1:D:103:MET:HE2	1.86	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
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:A:234:ARG:HD3	1:A:238:GLU:CD	2.46	0.40
1:C:32:SER:HB3	2:C:902:ATP:C5	2.56	0.40
1:D:14:LEU:HD23	1:D:171:TYR:CE1	2.56	0.40
1:D:102:ARG:NH1	1:D:102:ARG:CG	2.84	0.40
1:A:299:GLY:C	1:A:301:GLY:N	2.79	0.40
1:B:284:GLU:CD	1:B:287:ARG:HE	2.29	0.40
1:D:94:VAL:C	1:D:96:ALA:N	2.77	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:B:69:ALA:O	1:B:70:GLU:C	2.64	0.40
1:C:97:PHE:HE2	1:C:103:MET:CE	2.31	0.40
1:C:97:PHE:CE2	1:C:101:ASN:ND2	2.89	0.40
1:C:162:GLU:O	1:C:163:GLU:C	2.64	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:39:VAL:HG13	1:D:180:TYR:CD2	2.57	0.40
1:D:112:LEU:O	1:D:115:LYS:HB3	2.21	0.40

There are no symmetry-related clashes.

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	315/317 (99%)	284 (90%)	24 (8%)	7 (2%)	5	9
1	B	312/317 (98%)	284 (91%)	20 (6%)	8 (3%)	4	7
1	C	312/317 (98%)	296 (95%)	14 (4%)	2 (1%)	21	38
1	D	311/317 (98%)	272 (88%)	31 (10%)	8 (3%)	4	7
All	All	1250/1268 (99%)	1136 (91%)	89 (7%)	25 (2%)	6	10

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	TYR
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

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Mol	Chain	Res	Type
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%)	252 (88%)	33 (12%)	5	11
1	B	282/285 (99%)	250 (89%)	32 (11%)	5	12
1	C	282/285 (99%)	249 (88%)	33 (12%)	5	11
1	D	281/285 (99%)	247 (88%)	34 (12%)	5	10
All	All	1130/1140 (99%)	998 (88%)	132 (12%)	5	11

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ILE
1	A	9	ARG
1	A	12	LEU
1	A	14	LEU
1	A	35	VAL
1	A	46	LYS
1	A	66	ARG
1	A	67	GLU
1	A	103	MET
1	A	124	GLU
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

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Mol	Chain	Res	Type
1	A	195	TYR
1	A	196	GLU
1	A	201	ARG
1	A	207	ARG
1	A	222	THR
1	A	234	ARG
1	A	250	LYS
1	A	259	LEU
1	A	264	LEU
1	A	290	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	66	ARG
1	B	81	LYS
1	B	83	ARG
1	B	92	GLU
1	B	113	ARG
1	B	124	GLU
1	B	131	THR
1	B	135	LEU
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	194	ASN
1	B	198	SER
1	B	201	ARG
1	B	222	THR
1	B	234	ARG
1	B	240	GLU
1	B	257	LYS
1	B	259	LEU
1	B	264	LEU

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Mol	Chain	Res	Type
1	B	272	ARG
1	B	281	GLU
1	B	285	LEU
1	B	303	VAL
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	89	VAL
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	165	ILE
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	234	ARG
1	C	239	GLU
1	C	254	LEU
1	C	257	LYS
1	C	259	LEU
1	C	264	LEU
1	C	281	GLU
1	C	285	LEU
1	C	291	GLU
1	C	305	LYS
1	D	12	LEU
1	D	14	LEU
1	D	27	VAL
1	D	55	GLU

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Mol	Chain	Res	Type
1	D	62	ASN
1	D	64	MET
1	D	66	ARG
1	D	71	ARG
1	D	81	LYS
1	D	89	VAL
1	D	92	GLU
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	187	ARG
1	D	189	VAL
1	D	193	THR
1	D	196	GLU
1	D	198	SER
1	D	234	ARG
1	D	279	ASP
1	D	281	GLU
1	D	285	LEU
1	D	290	LEU
1	D	303	VAL
1	D	304	LEU
1	D	305	LYS
1	D	306	ARG
1	D	307	LYS
1	D	308	GLU
1	D	313	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	63	HIS
1	A	134	HIS
1	A	202	ASN
1	B	62	ASN
1	B	134	HIS
1	B	202	ASN
1	B	218	ASN

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Mol	Chain	Res	Type
1	B	252	ASN
1	B	267	GLN
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	C	267	GLN
1	D	60	HIS
1	D	62	ASN
1	D	63	HIS
1	D	101	ASN
1	D	134	HIS
1	D	206	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 oligosaccharides 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	-	32,33,33	1.35	3 (9%)	48,52,52	2.34	19 (39%)
2	ATP	A	900	-	32,33,33	1.38	2 (6%)	48,52,52	2.27	19 (39%)
2	ATP	B	901	-	32,33,33	1.37	5 (15%)	48,52,52	2.33	18 (37%)
3	LYS	B	950	-	8,9,9	0.87	0	7,10,10	0.52	0
2	ATP	C	902	-	32,33,33	1.26	3 (9%)	48,52,52	2.31	18 (37%)

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	-	-	4/22/38/38	0/3/3/3
2	ATP	A	900	-	-	1/22/38/38	0/3/3/3
2	ATP	B	901	-	-	6/22/38/38	0/3/3/3
3	LYS	B	950	-	-	1/9/9/9	-
2	ATP	C	902	-	-	3/22/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	ATP	C5-N7	-4.08	1.31	1.39
2	D	903	ATP	C5-N7	-4.01	1.31	1.39
2	B	901	ATP	C5-N7	-3.52	1.32	1.39
2	B	901	ATP	C4-N9	-3.08	1.31	1.37
2	C	902	ATP	C4-N9	-2.68	1.32	1.37
2	C	902	ATP	C5-N7	-2.61	1.34	1.39
2	D	903	ATP	C8-N9	-2.49	1.33	1.37
2	D	903	ATP	C4-N9	-2.46	1.32	1.37
2	A	900	ATP	C8-N9	-2.44	1.33	1.37
2	B	901	ATP	C8-N9	-2.19	1.33	1.37
2	C	902	ATP	PA-O3A	2.15	1.61	1.59
2	B	901	ATP	PB-O3B	2.12	1.61	1.59
2	B	901	ATP	PB-O3A	2.01	1.61	1.59

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	ATP	C5-C4-N3	-5.83	118.69	126.72
2	C	902	ATP	C5-C4-N3	-5.68	118.90	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	903	ATP	C5-C4-N3	-5.41	119.26	126.72
2	C	902	ATP	O2G-PG-O3B	-4.64	89.09	104.64
2	A	900	ATP	C5-C4-N3	-4.58	120.41	126.72
2	C	902	ATP	O3A-PB-O1B	-4.54	97.05	110.70
2	C	902	ATP	N3-C2-N1	-4.53	121.73	128.58
2	D	903	ATP	N3-C2-N1	-4.50	121.76	128.58
2	A	900	ATP	O2G-PG-O3B	-4.47	89.64	104.64
2	A	900	ATP	N3-C2-N1	-4.46	121.83	128.58
2	B	901	ATP	O3A-PB-O1B	-4.39	97.49	110.70
2	D	903	ATP	O2G-PG-O3B	-4.38	89.94	104.64
2	A	900	ATP	O3A-PB-O1B	-4.36	97.59	110.70
2	D	903	ATP	O3A-PB-O1B	-4.35	97.63	110.70
2	B	901	ATP	N3-C2-N1	-4.21	122.22	128.58
2	D	903	ATP	N3-C4-N9	4.11	134.15	127.17
2	B	901	ATP	O2B-PB-O3B	4.07	118.26	107.27
2	D	903	ATP	O2B-PB-O3B	4.06	118.24	107.27
2	A	900	ATP	O2B-PB-O3B	4.02	118.15	107.27
2	A	900	ATP	O2B-PB-O3A	-3.95	96.60	107.27
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	N3-C4-N9	3.90	133.80	127.17
2	B	901	ATP	O3G-PG-O3B	-3.85	91.71	104.64
2	C	902	ATP	O2B-PB-O3A	-3.82	96.95	107.27
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	A	900	ATP	N3-C4-N9	3.74	133.54	127.17
2	D	903	ATP	O2B-PB-O3A	-3.73	97.20	107.27
2	D	903	ATP	C2-N3-C4	3.70	120.87	111.83
2	B	901	ATP	C2-N3-C4	3.64	120.73	111.83
2	C	902	ATP	O2B-PB-O3B	3.61	117.04	107.27
2	A	900	ATP	C2-N3-C4	3.59	120.59	111.83
2	B	901	ATP	O2B-PB-O3A	-3.56	97.66	107.27
2	B	901	ATP	N9-C8-N7	-3.53	108.93	113.94
2	C	902	ATP	C2-N3-C4	3.53	120.44	111.83
2	B	901	ATP	C4-C5-N7	-3.51	106.57	110.58
2	D	903	ATP	N9-C8-N7	-3.47	109.02	113.94
2	A	900	ATP	N9-C8-N7	-3.27	109.29	113.94
2	C	902	ATP	N3-C4-N9	3.25	132.69	127.17
2	C	902	ATP	C4-C5-N7	-3.19	106.93	110.58
2	C	902	ATP	N9-C8-N7	-3.18	109.42	113.94
2	B	901	ATP	C5-N7-C8	3.16	108.42	103.45
2	A	900	ATP	C5-N7-C8	3.09	108.31	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	ATP	O3G-PG-O1G	3.02	122.59	110.83
2	B	901	ATP	O3B-PG-O1G	-2.97	95.39	111.04
2	C	902	ATP	O3G-PG-O1G	2.96	122.36	110.83
2	D	903	ATP	C5-N7-C8	2.94	108.07	103.45
2	D	903	ATP	O3G-PG-O1G	2.93	122.26	110.83
2	A	900	ATP	O3G-PG-O1G	2.91	122.16	110.83
2	D	903	ATP	C2'-C3'-C4'	-2.89	97.02	102.61
2	D	903	ATP	C4-N9-C8	2.80	108.67	105.74
2	C	902	ATP	O3B-PG-O1G	-2.77	96.44	111.04
2	C	902	ATP	O2G-PG-O1G	2.77	121.62	110.83
2	D	903	ATP	O2B-PB-O1B	2.76	125.29	112.44
2	C	902	ATP	C5-N7-C8	2.76	107.78	103.45
2	D	903	ATP	O3B-PG-O1G	-2.75	96.59	111.04
2	B	901	ATP	C4-N9-C8	2.72	108.59	105.74
2	A	900	ATP	O2B-PB-O1B	2.71	125.05	112.44
2	B	901	ATP	O2B-PB-O1B	2.71	125.04	112.44
2	A	900	ATP	C4-N9-C8	2.69	108.57	105.74
2	C	902	ATP	O2B-PB-O1B	2.63	124.68	112.44
2	A	900	ATP	O3B-PG-O1G	-2.63	97.22	111.04
2	D	903	ATP	O2G-PG-O1G	2.63	121.07	110.83
2	A	900	ATP	O2G-PG-O1G	2.60	120.97	110.83
2	D	903	ATP	C4-C5-N7	-2.56	107.66	110.58
2	B	901	ATP	O2G-PG-O1G	2.53	120.68	110.83
2	A	900	ATP	C4-C5-N7	-2.45	107.78	110.58
2	C	902	ATP	C5-C4-N9	2.38	108.40	105.81
2	A	900	ATP	O3G-PG-O2G	2.20	116.05	107.80
2	D	903	ATP	O3G-PG-O2G	2.19	116.00	107.80
2	B	901	ATP	O3G-PG-O2G	2.15	115.87	107.80
2	A	900	ATP	C2'-C3'-C4'	-2.14	98.47	102.61
2	C	902	ATP	O3G-PG-O2G	2.05	115.47	107.80

There are no chirality outliers.

All (15) 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
3	B	950	LYS	OXT-C-CA-N
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

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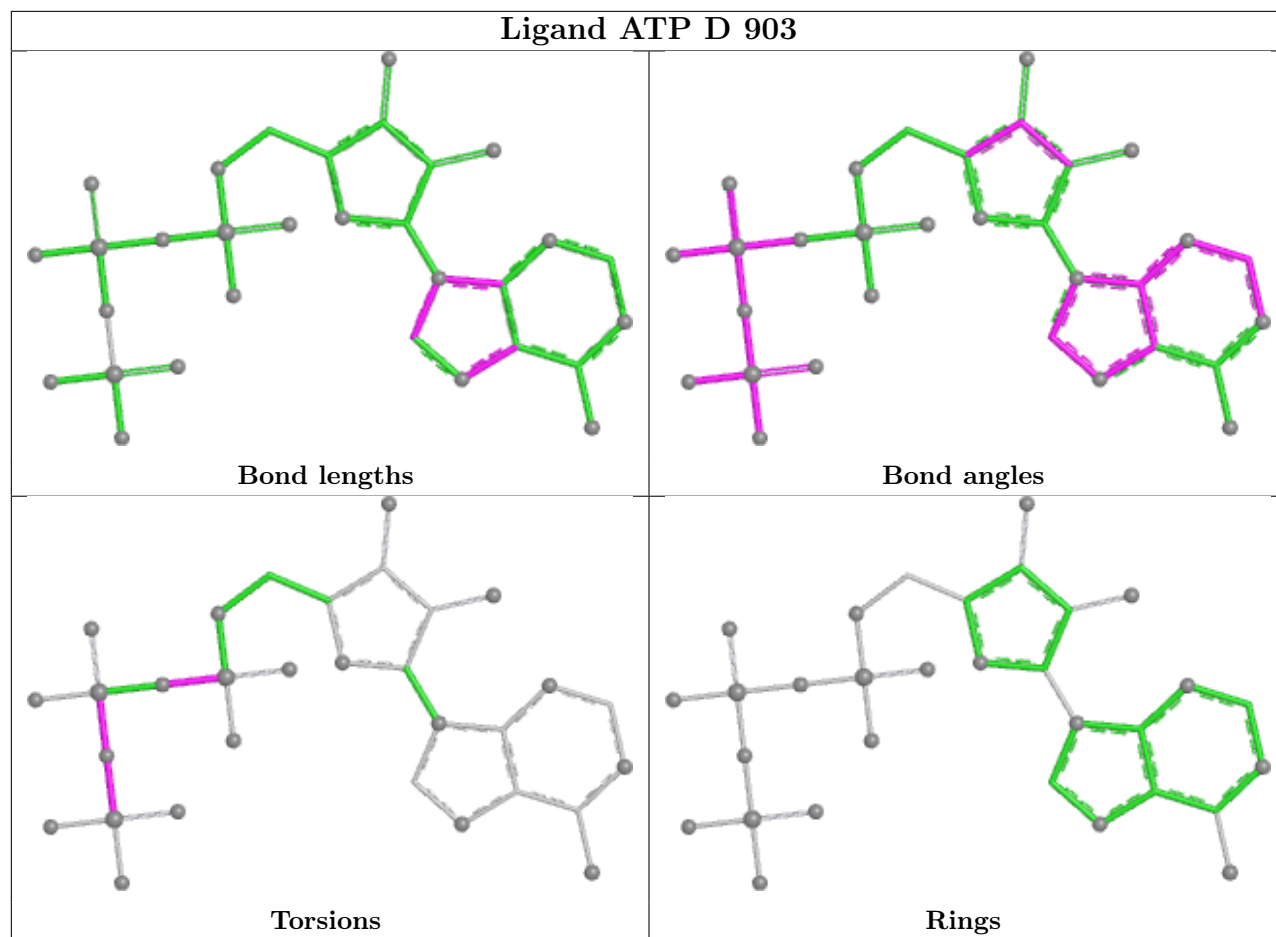
Mol	Chain	Res	Type	Atoms
2	C	902	ATP	PB-O3A-PA-O2A
2	D	903	ATP	PB-O3B-PG-O2G
2	B	901	ATP	PG-O3B-PB-O1B
2	B	901	ATP	PB-O3A-PA-O1A
2	C	902	ATP	PB-O3A-PA-O1A
2	D	903	ATP	PB-O3A-PA-O1A
2	D	903	ATP	PB-O3A-PA-O2A
2	D	903	ATP	PG-O3B-PB-O2B

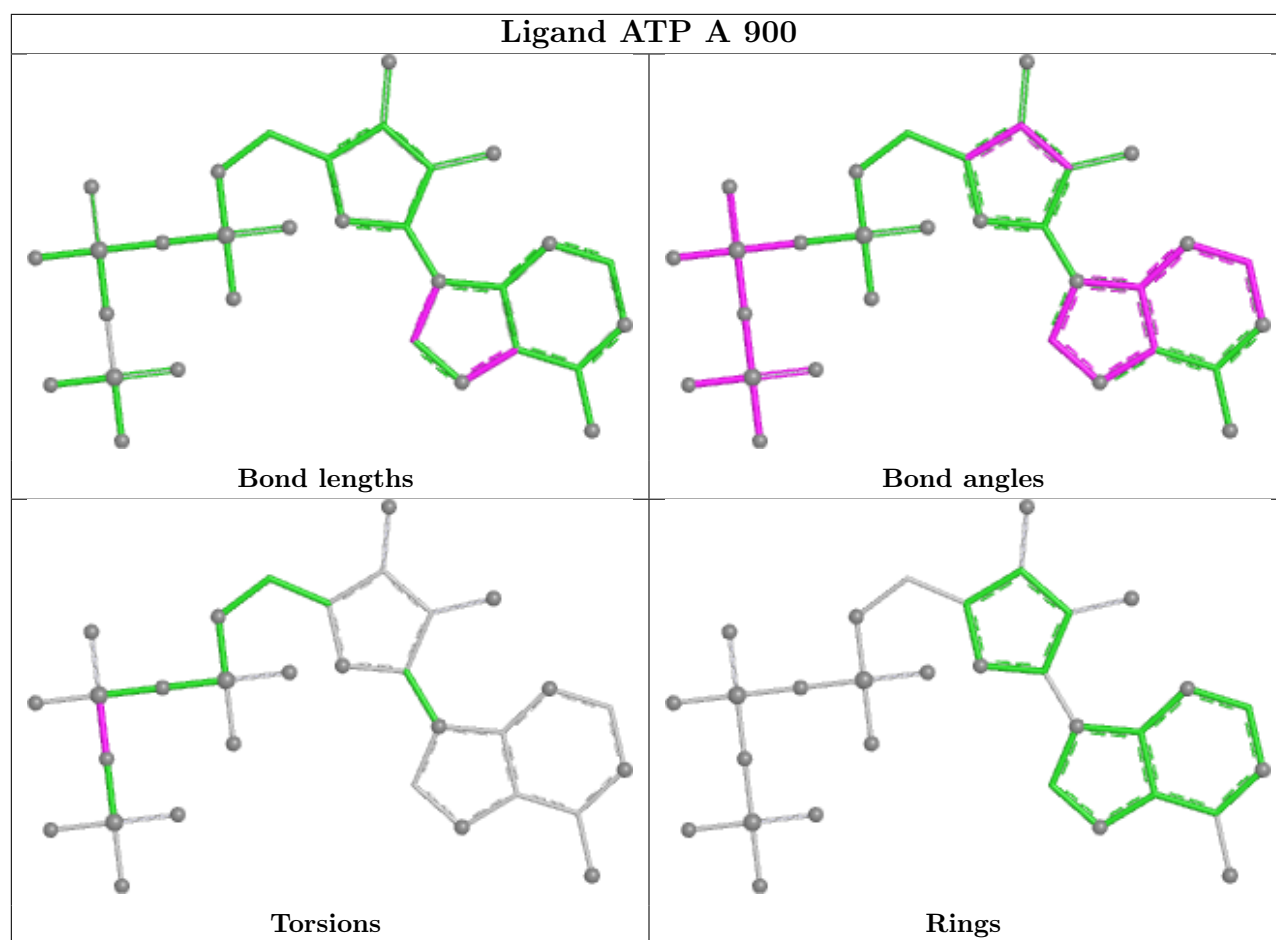
There are no ring outliers.

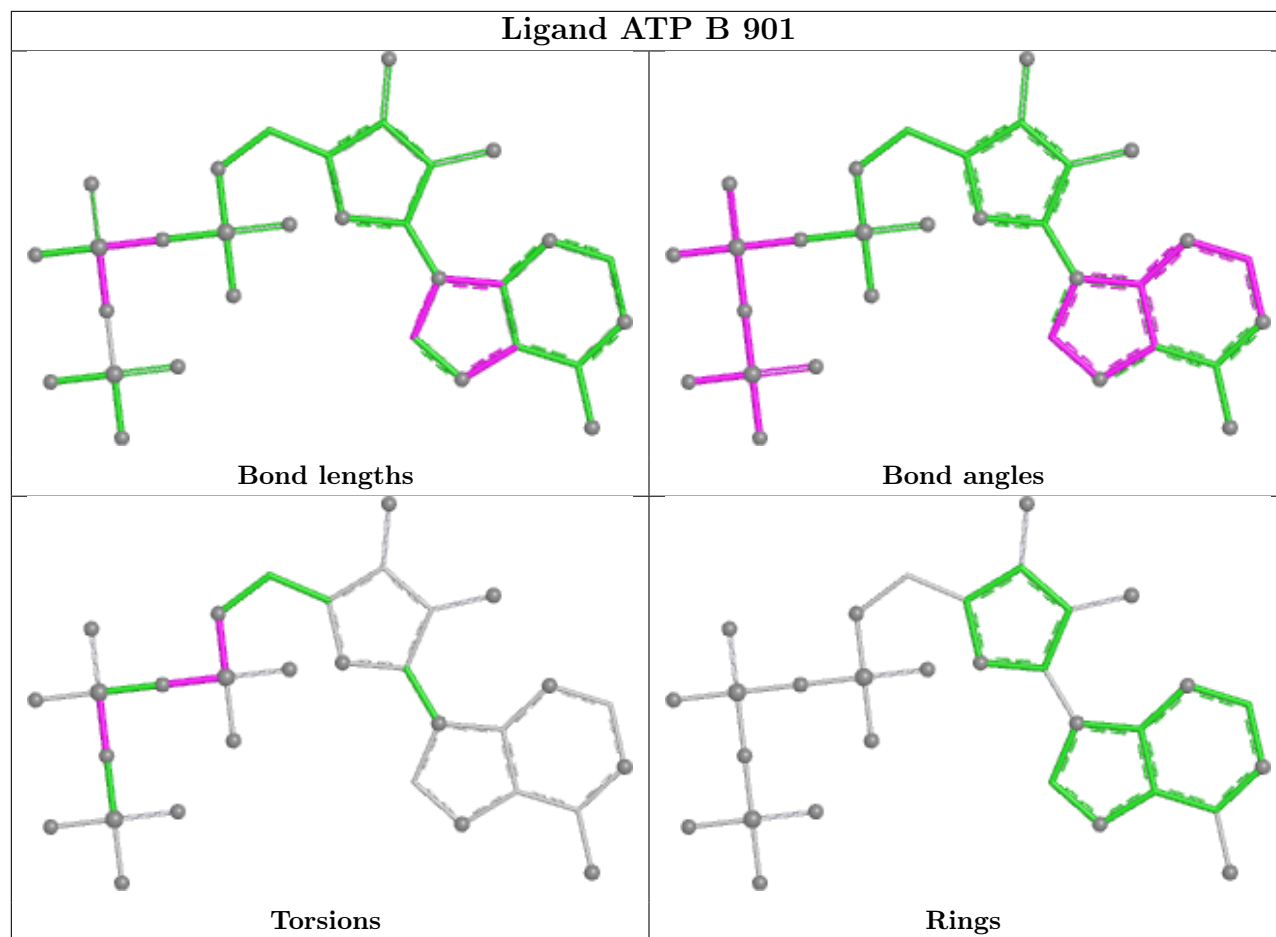
5 monomers are involved in 16 short contacts:

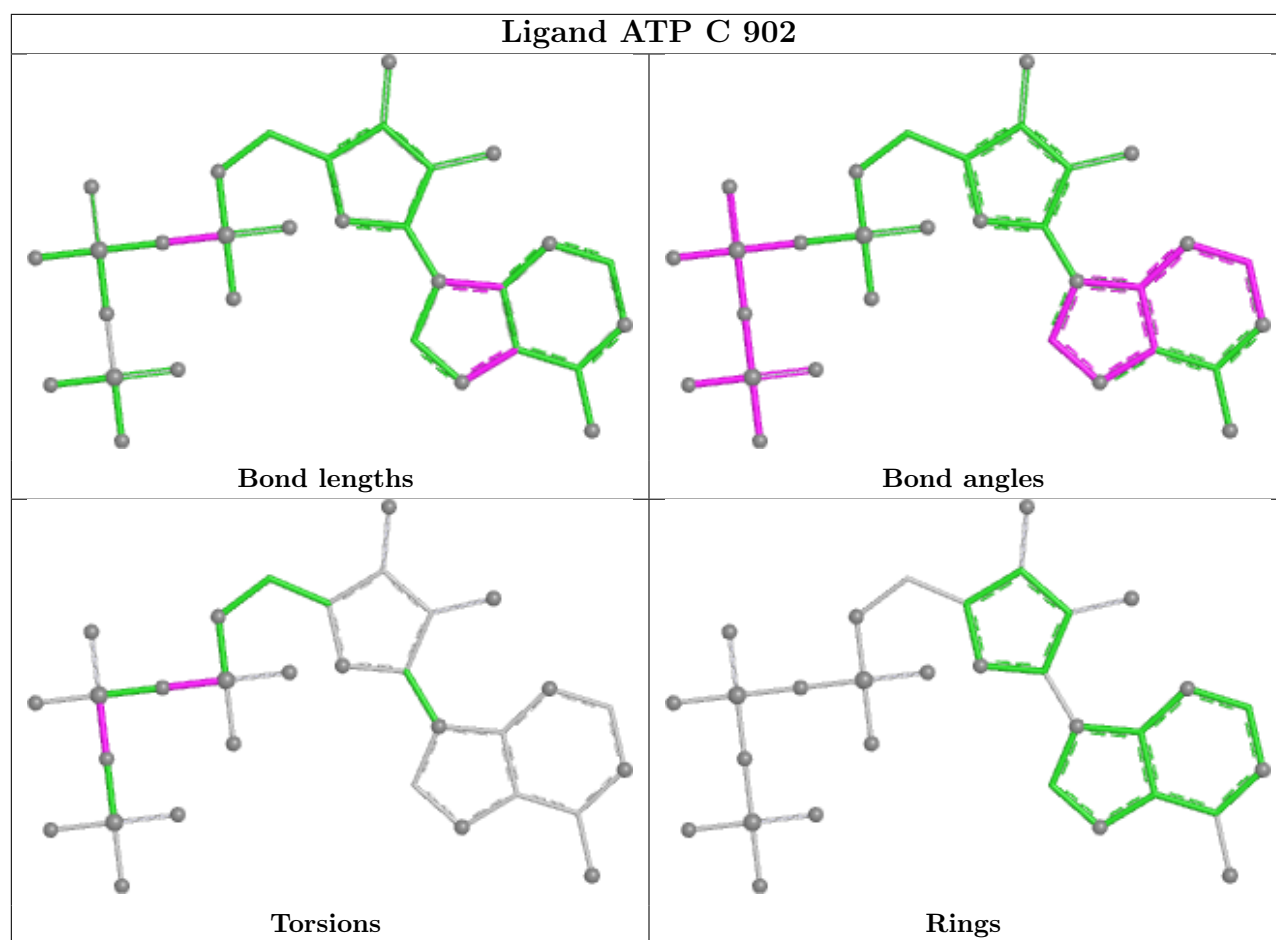
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	903	ATP	3	0
2	A	900	ATP	3	0
2	B	901	ATP	1	0
3	B	950	LYS	4	0
2	C	902	ATP	5	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	317/317 (100%)	0.29	15 (4%) 36 32	26, 46, 91, 110	0
1	B	314/317 (99%)	0.32	12 (3%) 44 39	22, 47, 88, 98	0
1	C	314/317 (99%)	-0.09	6 (1%) 66 62	21, 42, 79, 85	0
1	D	313/317 (98%)	0.78	45 (14%) 6 5	28, 60, 108, 116	0
All	All	1258/1268 (99%)	0.33	78 (6%) 26 23	21, 49, 94, 116	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	307	LYS	5.3
1	D	116	PHE	5.1
1	D	305	LYS	4.7
1	B	314	SER	4.4
1	A	193	THR	4.0
1	D	94	VAL	4.0
1	A	196	GLU	3.9
1	D	89	VAL	3.9
1	D	117	LEU	3.8
1	D	196	GLU	3.8
1	A	105	LEU	3.8
1	D	313	PHE	3.6
1	D	311	LEU	3.5
1	D	304	LEU	3.5
1	D	251	GLY	3.5
1	B	313	PHE	3.5
1	D	259	LEU	3.4
1	A	190	GLU	3.4
1	B	311	LEU	3.3
1	D	252	ASN	3.3
1	B	193	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	64	MET	3.3
1	D	195	TYR	3.2
1	D	106	GLU	3.1
1	D	194	ASN	3.1
1	D	114	TYR	3.1
1	A	195	TYR	3.0
1	D	274	PHE	3.0
1	D	97	PHE	3.0
1	D	254	LEU	3.0
1	D	110	ARG	3.0
1	C	314	SER	3.0
1	A	114	TYR	2.9
1	D	105	LEU	2.9
1	A	191	ASP	2.9
1	B	195	TYR	2.9
1	D	257	LYS	2.8
1	D	120	ILE	2.8
1	D	98	ALA	2.8
1	D	108	ALA	2.8
1	D	71	ARG	2.8
1	D	306	ARG	2.7
1	D	298	LEU	2.7
1	A	256	VAL	2.7
1	B	105	LEU	2.6
1	A	194	ASN	2.6
1	B	194	ASN	2.5
1	D	248	VAL	2.5
1	D	312	CYS	2.5
1	D	63	HIS	2.5
1	A	197	VAL	2.5
1	A	189	VAL	2.4
1	C	308	GLU	2.4
1	D	193	THR	2.4
1	B	82	GLU	2.3
1	C	299	GLY	2.3
1	D	65	LEU	2.2
1	D	112	LEU	2.2
1	D	192	GLU	2.2
1	D	197	VAL	2.2
1	A	94	VAL	2.2
1	D	191	ASP	2.2
1	B	259	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	95	ARG	2.2
1	A	97	PHE	2.2
1	C	304	LEU	2.1
1	C	114	TYR	2.1
1	D	250	LYS	2.1
1	B	190	GLU	2.1
1	A	118	LYS	2.1
1	D	54	LYS	2.1
1	D	103	MET	2.1
1	A	112	LEU	2.1
1	C	298	LEU	2.1
1	D	96	ALA	2.0
1	B	1	MET	2.0
1	B	250	LYS	2.0
1	D	85	MET	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.

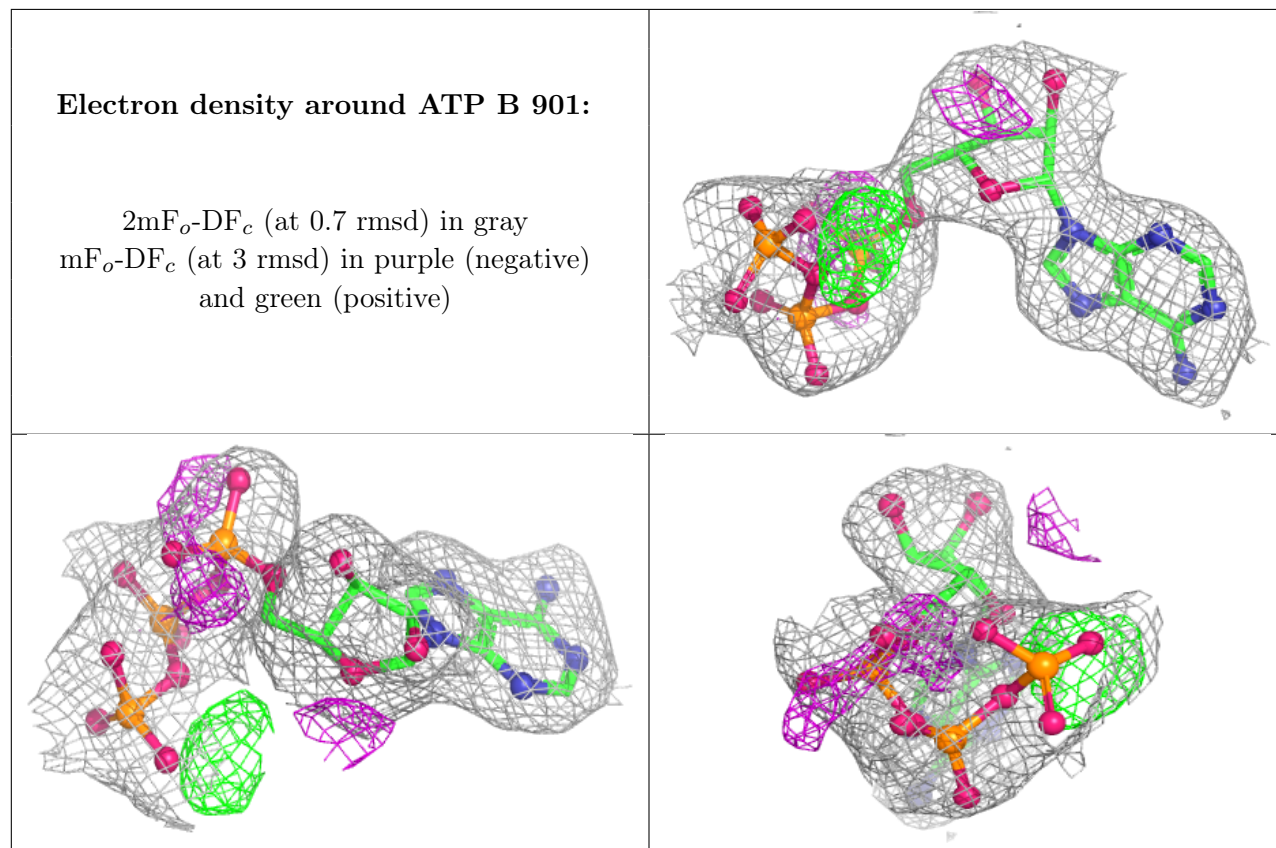
6.4 Ligands [i](#)

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	B	901	31/31	0.83	0.10	36,46,82,83	0
3	LYS	B	950	10/10	0.83	0.15	46,57,59,60	0
2	ATP	A	900	31/31	0.88	0.09	36,53,84,86	0
2	ATP	C	902	31/31	0.89	0.10	29,37,69,72	0
2	ATP	D	903	31/31	0.90	0.09	75,77,81,82	0
4	MG	C	601	1/1	0.91	0.10	59,59,59,59	0

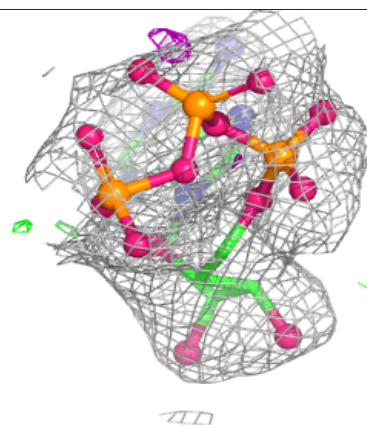
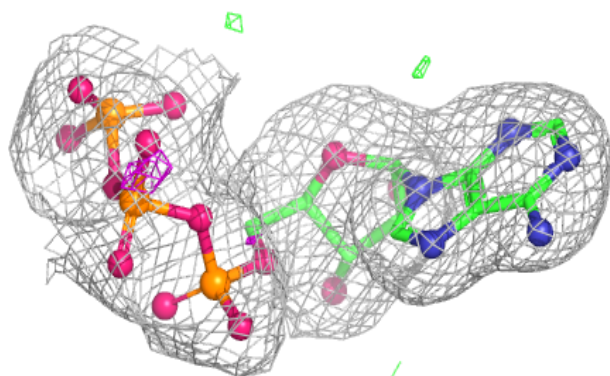
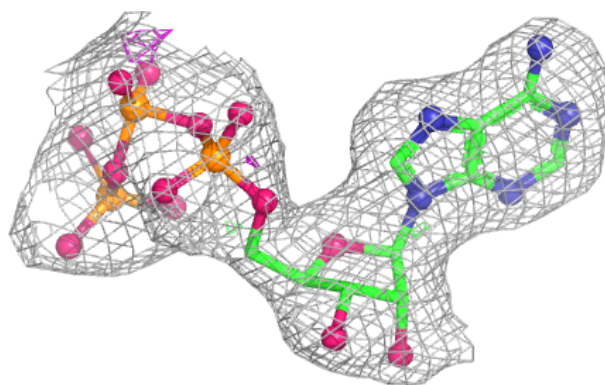
The following is a graphical depiction of the model fit to experimental electron density of all

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.



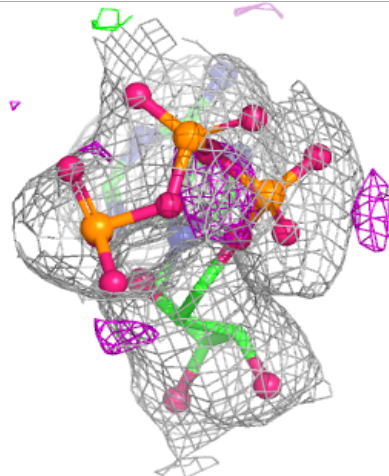
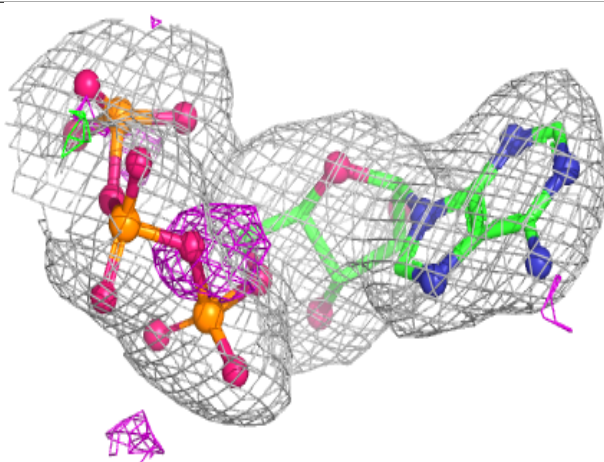
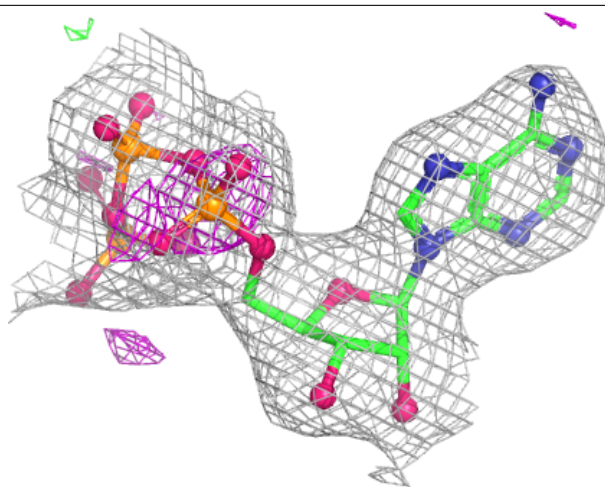
Electron density around ATP A 900:

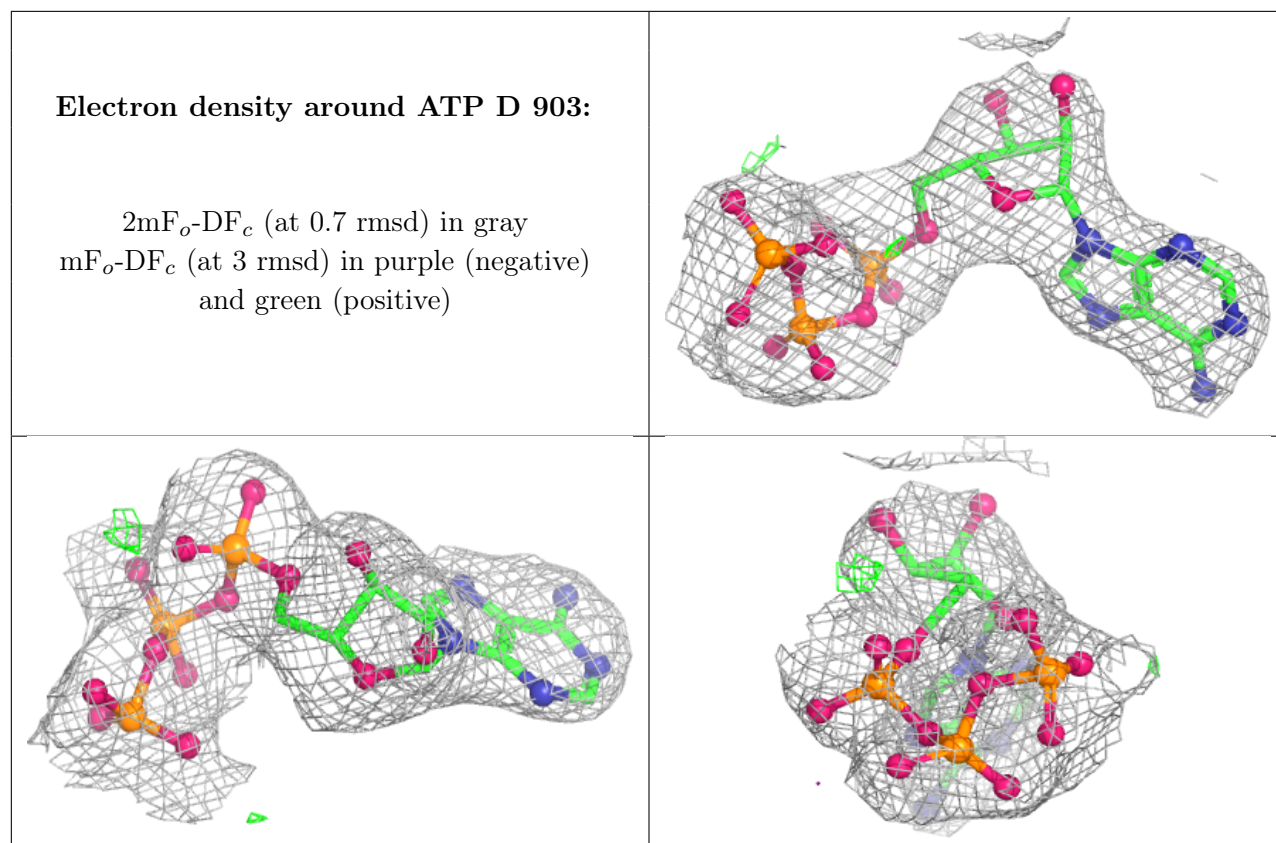
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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 [i](#)

There are no such residues in this entry.