



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:52 PM EDT

PDB ID : 3E9H / pdb_00003e9h
Title : Lysyl-tRNA synthetase from *Bacillus stearothermophilus* complexed with L-Lysylsulfamoyl adenosine
Authors : Sakurama, H.; Takita, T.; Mikami, B.; Itoh, T.; Yasukawa, K.; Inouye, K.
Deposited on : 2008-08-22
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

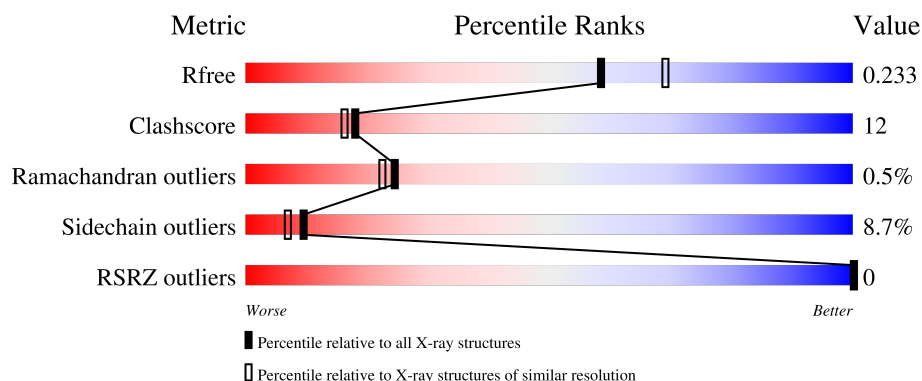
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	493	
1	B	493	
1	C	493	
1	D	493	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16420 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.

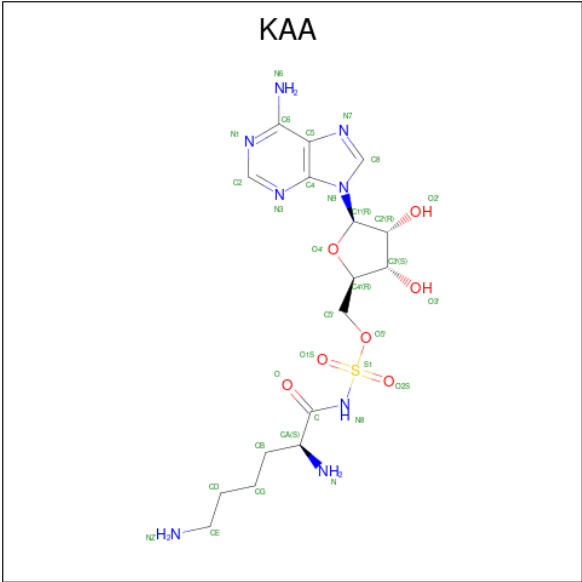
- Molecule 1 is a protein called Lysyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	484	Total	C	N	O	S	0	0	0
			3956	2509	690	739	18			
1	B	484	Total	C	N	O	S	0	0	0
			3956	2509	690	739	18			
1	C	484	Total	C	N	O	S	0	0	0
			3956	2509	690	739	18			
1	D	484	Total	C	N	O	S	0	0	0
			3956	2509	690	739	18			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is 5'-O-[(L-LYSYLAMINO)SULFONYL]ADENOSINE (CCD ID: KAA) (formula: C₁₆H₂₆N₈O₇S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			32	16	8	7	1		
3	B	1	Total	C	N	O	S	0	0
			32	16	8	7	1		
3	C	1	Total	C	N	O	S	0	0
			32	16	8	7	1		
3	D	1	Total	C	N	O	S	0	0
			32	16	8	7	1		

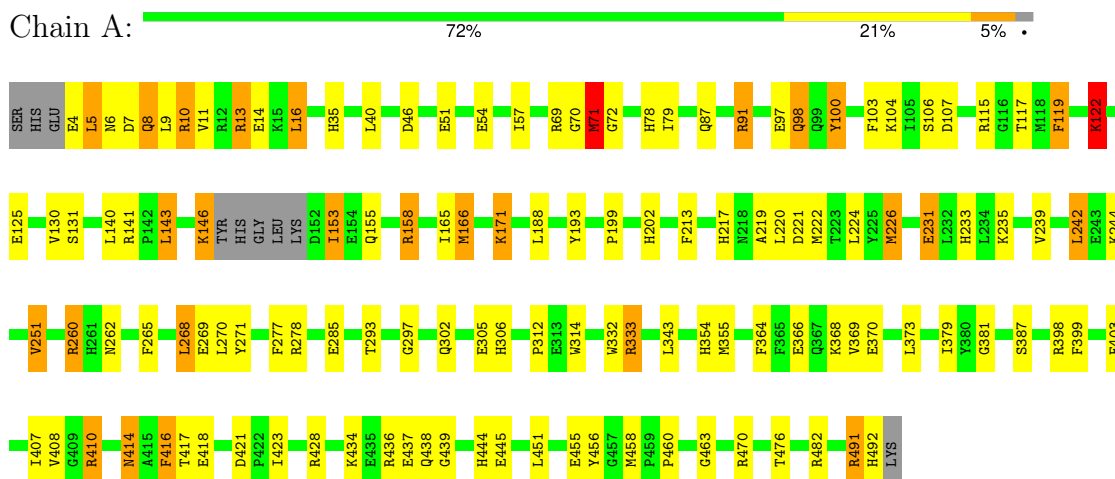
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	100	Total	O	0	0
			100	100		
4	B	113	Total	O	0	0
			113	113		
4	C	121	Total	O	0	0
			121	121		
4	D	130	Total	O	0	0
			130	130		

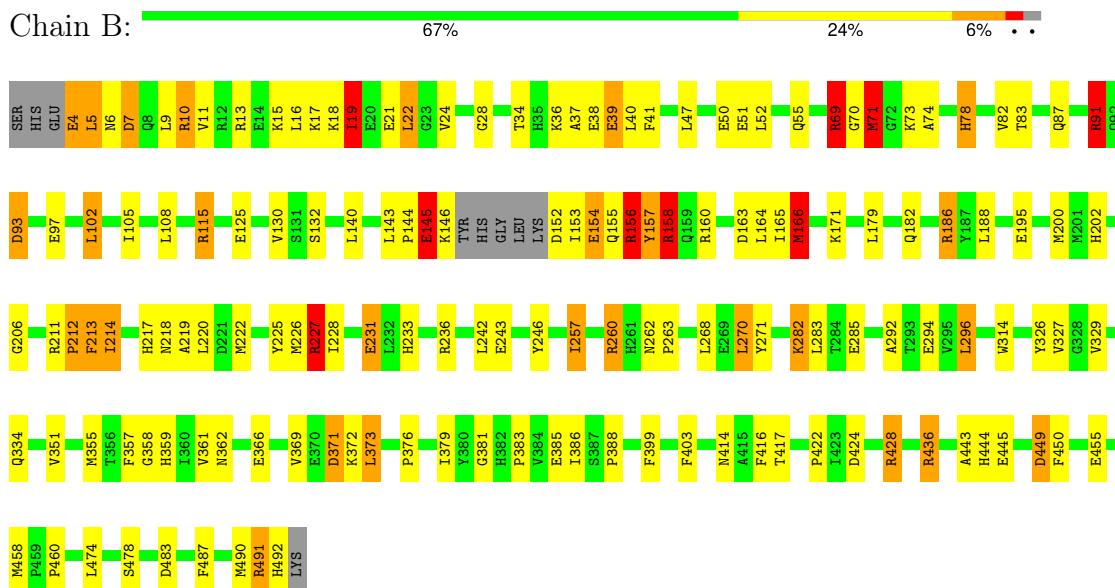
3 Residue-property plots

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: Lysyl-tRNA synthetase

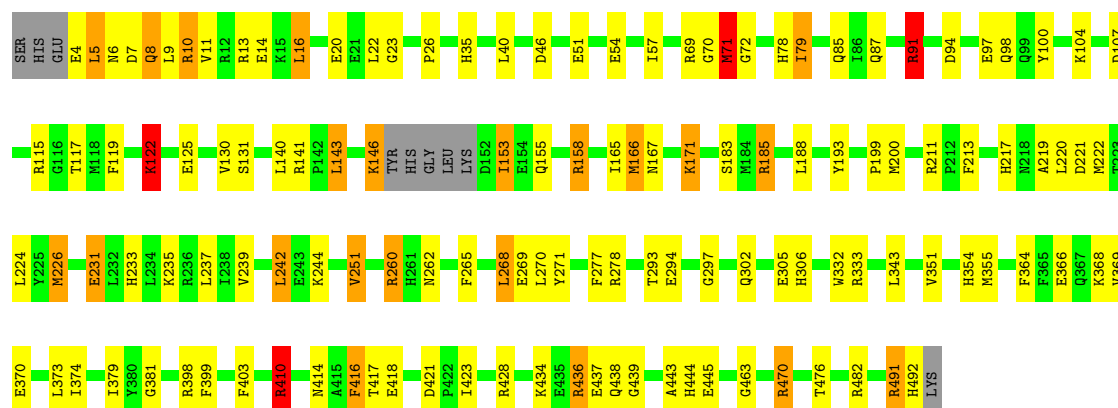


• Molecule 1: Lysyl-tRNA synthetase



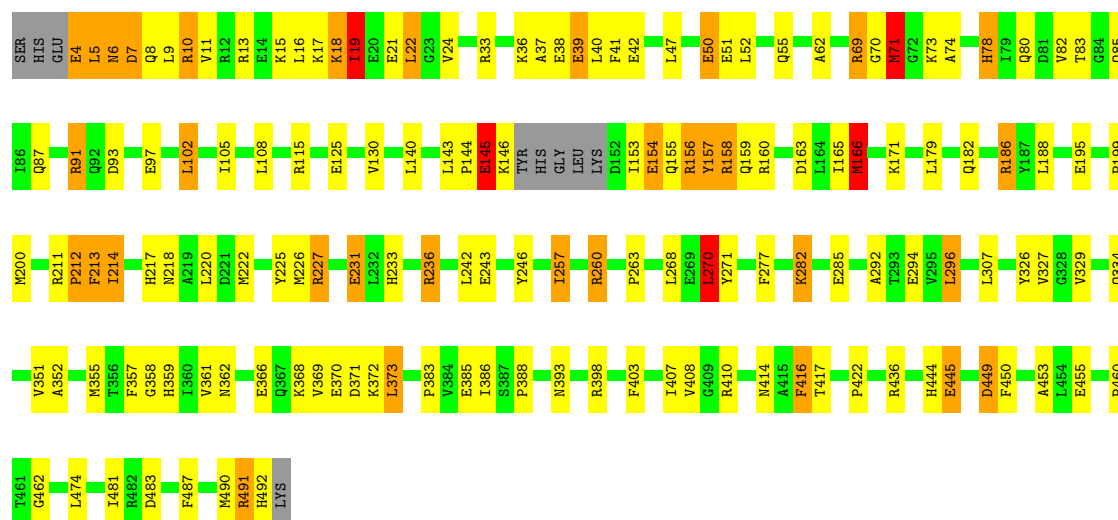
• Molecule 1: Lysyl-tRNA synthetase

Chain C:  71% 22% ..



• Molecule 1: Lysyl-tRNA synthetase

Chain D:  67% 24% 7% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.64Å 83.21Å 150.81Å 90.00° 89.95° 90.00°	Depositor
Resolution (Å)	14.97 – 2.10 14.97 – 2.10	Depositor EDS
% Data completeness (in resolution range)	89.0 (14.97-2.10) 89.9 (14.97-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.05Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.190 , 0.241 0.181 , 0.233	Depositor DCC
R_{free} test set	11100 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å ²)	22.7	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 14.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for k,h,-l 0.023 for -k,-h,-l 0.486 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16420	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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: KAA, MG

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	1.15	3/4035 (0.1%)	1.39	62/5433 (1.1%)
1	B	1.17	7/4035 (0.2%)	1.47	62/5433 (1.1%)
1	C	1.18	3/4035 (0.1%)	1.45	66/5433 (1.2%)
1	D	1.16	4/4035 (0.1%)	1.45	61/5433 (1.1%)
All	All	1.17	17/16140 (0.1%)	1.44	251/21732 (1.2%)

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	2
1	B	0	2
1	C	0	1
1	D	0	2
All	All	0	7

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	166	MET	SD-CE	-8.33	1.58	1.79
1	D	71	MET	SD-CE	7.36	1.98	1.79
1	B	166	MET	SD-CE	-7.22	1.61	1.79
1	D	19	ILE	CA-CB	7.03	1.64	1.54
1	B	71	MET	SD-CE	6.66	1.96	1.79
1	C	166	MET	SD-CE	6.10	1.94	1.79
1	B	19	ILE	CA-CB	5.92	1.63	1.54
1	B	283	LEU	CA-C	5.81	1.60	1.52
1	B	428	ARG	CD-NE	-5.73	1.38	1.46
1	C	185	ARG	CD-NE	-5.66	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	100	TYR	CA-C	5.41	1.59	1.52
1	A	458	MET	SD-CE	-5.38	1.66	1.79
1	B	228	ILE	CG1-CD1	5.25	1.72	1.51
1	D	462	GLY	CA-C	5.20	1.56	1.52
1	A	312	PRO	CA-C	5.13	1.58	1.52
1	C	71	MET	SD-CE	5.12	1.92	1.79
1	B	458	MET	SD-CE	-5.06	1.66	1.79

All (251) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	369	VAL	N-CA-C	15.12	123.56	111.62
1	D	369	VAL	N-CA-C	14.67	123.21	111.62
1	C	185	ARG	NE-CZ-NH2	-14.44	106.20	119.20
1	D	236	ARG	NE-CZ-NH1	-14.01	107.49	121.50
1	D	236	ARG	NE-CZ-NH2	13.97	131.77	119.20
1	B	428	ARG	NE-CZ-NH1	-12.77	108.73	121.50
1	B	428	ARG	NE-CZ-NH2	12.63	130.57	119.20
1	C	410	ARG	NE-CZ-NH2	12.29	130.26	119.20
1	C	185	ARG	NE-CZ-NH1	12.20	133.70	121.50
1	D	236	ARG	CD-NE-CZ	12.02	141.23	124.40
1	D	417	THR	N-CA-C	-11.18	92.14	109.25
1	B	91	ARG	NE-CZ-NH2	11.06	129.15	119.20
1	C	185	ARG	CD-NE-CZ	11.00	139.80	124.40
1	C	410	ARG	NE-CZ-NH1	-10.52	110.98	121.50
1	B	91	ARG	NE-CZ-NH1	-10.43	111.07	121.50
1	C	333	ARG	NE-CZ-NH1	-10.40	111.10	121.50
1	B	417	THR	N-CA-C	-10.29	93.51	109.25
1	B	227	ARG	NE-CZ-NH2	-10.18	110.04	119.20
1	C	333	ARG	NE-CZ-NH2	10.16	128.35	119.20
1	C	10	ARG	NE-CZ-NH2	9.90	128.11	119.20
1	D	7	ASP	N-CA-C	-9.85	100.63	111.36
1	D	436	ARG	NE-CZ-NH2	9.57	127.81	119.20
1	B	227	ARG	NE-CZ-NH1	9.57	131.07	121.50
1	D	436	ARG	NE-CZ-NH1	-9.54	111.96	121.50
1	A	13	ARG	NE-CZ-NH2	9.47	127.72	119.20
1	B	69	ARG	NE-CZ-NH1	-9.43	112.07	121.50
1	A	231	GLU	N-CA-C	9.40	122.39	111.11
1	B	7	ASP	N-CA-C	-9.28	101.05	111.82
1	D	186	ARG	NE-CZ-NH1	9.27	130.77	121.50
1	B	156	ARG	NE-CZ-NH2	9.27	127.54	119.20
1	C	470	ARG	NE-CZ-NH2	-9.26	110.86	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	10	ARG	NE-CZ-NH1	-9.25	112.25	121.50
1	C	231	GLU	N-CA-C	9.22	122.17	111.11
1	A	491	ARG	NE-CZ-NH2	8.99	127.29	119.20
1	A	491	ARG	NE-CZ-NH1	-8.68	112.83	121.50
1	B	156	ARG	NE-CZ-NH1	-8.64	112.86	121.50
1	D	186	ARG	CD-NE-CZ	8.61	136.45	124.40
1	C	436	ARG	NE-CZ-NH2	-8.51	111.54	119.20
1	C	410	ARG	CD-NE-CZ	8.49	136.29	124.40
1	A	333	ARG	NE-CZ-NH2	-8.46	111.59	119.20
1	B	69	ARG	NE-CZ-NH2	8.43	126.78	119.20
1	B	428	ARG	CD-NE-CZ	8.38	136.13	124.40
1	B	91	ARG	CD-NE-CZ	8.36	136.10	124.40
1	D	491	ARG	NE-CZ-NH2	8.34	126.70	119.20
1	A	13	ARG	NE-CZ-NH1	-8.22	113.28	121.50
1	C	470	ARG	CD-NE-CZ	8.21	135.90	124.40
1	D	491	ARG	NE-CZ-NH1	-8.14	113.36	121.50
1	D	186	ARG	NE-CZ-NH2	-8.12	111.89	119.20
1	A	333	ARG	CD-NE-CZ	8.09	135.73	124.40
1	A	130	VAL	N-CA-C	8.05	119.96	109.58
1	D	158	ARG	NE-CZ-NH2	8.03	126.42	119.20
1	C	91	ARG	NE-CZ-NH2	-8.00	112.00	119.20
1	C	69	ARG	NE-CZ-NH2	7.88	126.29	119.20
1	C	417	THR	N-CA-C	-7.83	97.26	109.25
1	C	69	ARG	NE-CZ-NH1	-7.80	113.70	121.50
1	A	417	THR	N-CA-C	-7.78	97.35	109.25
1	D	436	ARG	CD-NE-CZ	7.75	135.25	124.40
1	D	5	LEU	N-CA-C	7.70	120.87	109.24
1	D	236	ARG	CG-CD-NE	-7.67	95.14	112.00
1	B	428	ARG	CG-CD-NE	-7.66	95.15	112.00
1	C	333	ARG	CD-NE-CZ	7.64	135.10	124.40
1	C	115	ARG	N-CA-C	-7.62	97.46	109.50
1	A	69	ARG	NE-CZ-NH2	-7.58	112.38	119.20
1	B	5	LEU	N-CA-C	7.58	120.68	109.24
1	D	231	GLU	N-CA-C	7.57	123.85	111.37
1	A	91	ARG	NE-CZ-NH1	-7.56	113.94	121.50
1	A	410	ARG	CD-NE-CZ	7.54	134.95	124.40
1	D	158	ARG	NE-CZ-NH1	-7.50	114.00	121.50
1	A	470	ARG	NE-CZ-NH2	7.50	125.95	119.20
1	A	470	ARG	NE-CZ-NH1	-7.48	114.02	121.50
1	B	156	ARG	CD-NE-CZ	7.41	134.78	124.40
1	A	436	ARG	NE-CZ-NH1	-7.41	114.09	121.50
1	B	231	GLU	N-CA-C	7.23	123.30	111.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	416	PHE	N-CA-C	7.16	119.05	108.60
1	C	10	ARG	CD-NE-CZ	7.16	134.42	124.40
1	A	436	ARG	NE-CZ-NH2	7.11	125.60	119.20
1	A	91	ARG	NE-CZ-NH2	7.07	125.56	119.20
1	D	69	ARG	NE-CZ-NH2	-7.05	112.86	119.20
1	C	436	ARG	CD-NE-CZ	6.97	134.15	124.40
1	C	436	ARG	NE-CZ-NH1	6.93	128.44	121.50
1	B	491	ARG	NE-CZ-NH2	-6.93	112.97	119.20
1	A	13	ARG	CD-NE-CZ	6.89	134.05	124.40
1	A	268	LEU	N-CA-C	-6.89	98.01	109.24
1	B	491	ARG	CD-NE-CZ	6.88	134.03	124.40
1	A	10	ARG	NE-CZ-NH2	-6.87	113.02	119.20
1	C	130	VAL	N-CA-C	6.85	118.42	109.58
1	A	10	ARG	CD-NE-CZ	6.79	133.90	124.40
1	A	491	ARG	CD-NE-CZ	6.78	133.90	124.40
1	C	91	ARG	CD-NE-CZ	6.72	133.81	124.40
1	A	69	ARG	CD-NE-CZ	6.69	133.77	124.40
1	A	355	MET	N-CA-C	6.66	120.73	110.20
1	A	35	HIS	N-CA-C	6.62	119.13	109.07
1	A	115	ARG	N-CA-C	-6.59	99.17	109.72
1	D	243	GLU	N-CA-C	6.59	124.83	110.80
1	D	156	ARG	CD-NE-CZ	6.58	133.61	124.40
1	C	213	PHE	N-CA-C	-6.56	98.94	109.96
1	C	364	PHE	N-CA-C	-6.55	104.06	111.07
1	C	91	ARG	NE-CZ-NH1	6.53	128.03	121.50
1	A	416	PHE	N-CA-C	6.50	118.10	108.60
1	A	166	MET	N-CA-C	6.49	121.20	113.28
1	C	35	HIS	N-CA-C	6.47	118.91	109.07
1	C	268	LEU	N-CA-C	-6.47	98.70	109.24
1	B	449	ASP	N-CA-C	6.44	117.96	111.07
1	D	108	LEU	N-CA-C	-6.42	100.92	110.23
1	B	436	ARG	NE-CZ-NH2	-6.42	113.43	119.20
1	C	166	MET	N-CA-C	6.38	121.06	113.28
1	B	69	ARG	CD-NE-CZ	6.37	133.32	124.40
1	B	243	GLU	N-CA-C	6.34	124.30	110.80
1	D	78	HIS	N-CA-C	-6.31	98.61	108.90
1	C	239	VAL	N-CA-C	-6.30	104.19	110.62
1	B	115	ARG	N-CA-C	-6.30	99.13	109.40
1	B	186	ARG	CD-NE-CZ	6.30	133.22	124.40
1	B	236	ARG	CD-NE-CZ	6.30	133.22	124.40
1	A	72	GLY	N-CA-C	-6.27	101.50	112.53
1	D	55	GLN	N-CA-C	6.27	118.11	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	355	MET	N-CA-C	6.26	120.10	110.20
1	B	213	PHE	N-CA-C	-6.25	99.46	109.96
1	D	369	VAL	CB-CA-C	-6.24	105.50	111.05
1	C	119	PHE	N-CA-CB	-6.23	101.91	111.56
1	C	398	ARG	N-CA-C	-6.20	105.20	112.89
1	B	200	MET	N-CA-C	-6.20	105.50	114.12
1	C	72	GLY	N-CA-C	-6.19	101.63	112.53
1	A	379	ILE	N-CA-C	-6.19	99.67	108.58
1	D	491	ARG	CD-NE-CZ	6.18	133.06	124.40
1	A	69	ARG	NE-CZ-NH1	6.18	127.68	121.50
1	C	491	ARG	CD-NE-CZ	6.18	133.05	124.40
1	D	227	ARG	NE-CZ-NH1	-6.17	115.33	121.50
1	B	436	ARG	CD-NE-CZ	6.17	133.03	124.40
1	C	69	ARG	CD-NE-CZ	6.15	133.01	124.40
1	D	91	ARG	CD-NE-CZ	6.14	133.00	124.40
1	B	130	VAL	N-CA-C	6.11	117.18	108.93
1	C	470	ARG	NE-CZ-NH1	6.08	127.58	121.50
1	C	306	HIS	N-CA-C	6.08	119.73	109.76
1	A	364	PHE	N-CA-C	-6.07	104.57	111.07
1	B	369	VAL	CB-CA-C	-6.06	105.66	111.05
1	A	239	VAL	N-CA-C	-6.05	104.45	110.62
1	C	122	LYS	N-CA-C	-6.04	104.81	111.82
1	D	213	PHE	N-CA-C	-6.03	99.83	109.96
1	D	156	ARG	NE-CZ-NH2	-6.02	113.78	119.20
1	D	115	ARG	N-CA-C	-6.02	99.59	109.40
1	A	119	PHE	N-CA-CB	-6.01	102.24	111.56
1	C	167	ASN	CA-C-N	6.01	125.49	119.24
1	C	167	ASN	C-N-CA	6.01	125.49	119.24
1	D	97	GLU	N-CA-C	6.01	117.91	111.36
1	B	158	ARG	CD-NE-CZ	5.96	132.75	124.40
1	C	491	ARG	NE-CZ-NH2	-5.96	113.84	119.20
1	B	97	GLU	N-CA-C	5.95	117.85	111.36
1	D	334	GLN	N-CA-C	-5.90	101.55	110.28
1	B	186	ARG	NE-CZ-NH2	5.89	124.50	119.20
1	B	227	ARG	CB-CG-CD	5.88	124.83	111.30
1	C	379	ILE	N-CA-C	-5.87	100.12	108.58
1	B	388	PRO	N-CA-C	5.84	121.52	113.98
1	D	73	LYS	N-CA-C	5.84	120.02	113.02
1	B	186	ARG	NE-CZ-NH1	-5.81	115.69	121.50
1	C	131	SER	N-CA-C	-5.77	106.28	113.55
1	B	450	PHE	N-CA-C	-5.75	105.09	111.36
1	D	366	GLU	N-CA-C	5.74	117.54	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	332	TRP	N-CA-C	-5.72	105.18	111.82
1	A	333	ARG	NE-CZ-NH1	5.71	127.21	121.50
1	A	91	ARG	CD-NE-CZ	5.71	132.39	124.40
1	D	51	GLU	N-CA-C	-5.71	105.82	112.89
1	C	185	ARG	CG-CD-NE	-5.70	99.47	112.00
1	B	55	GLN	N-CA-C	5.68	117.47	111.28
1	D	352	ALA	CA-C-N	-5.67	113.83	119.56
1	D	352	ALA	C-N-CA	-5.67	113.83	119.56
1	C	13	ARG	NE-CZ-NH2	-5.67	114.10	119.20
1	D	368	LYS	CA-C-N	-5.66	117.16	123.16
1	D	368	LYS	C-N-CA	-5.66	117.16	123.16
1	A	213	PHE	N-CA-C	-5.64	100.48	109.96
1	D	157	TYR	N-CA-C	-5.61	105.55	112.90
1	B	143	LEU	N-CA-C	-5.61	102.34	110.08
1	C	269	GLU	N-CA-C	-5.60	99.88	109.24
1	B	218	ASN	N-CA-C	5.60	117.08	110.97
1	B	158	ARG	NE-CZ-NH2	-5.58	114.18	119.20
1	D	69	ARG	NE-CZ-NH1	5.57	127.07	121.50
1	D	158	ARG	CD-NE-CZ	5.56	132.18	124.40
1	A	333	ARG	CG-CD-NE	-5.55	99.80	112.00
1	A	398	ARG	N-CA-C	-5.53	106.04	112.89
1	B	78	HIS	N-CA-C	-5.53	100.17	109.07
1	B	34	THR	N-CA-C	-5.52	106.90	113.97
1	A	226	MET	N-CA-C	-5.52	102.11	110.28
1	B	334	GLN	N-CA-C	-5.50	102.25	110.23
1	B	73	LYS	N-CA-C	5.49	119.61	113.02
1	B	51	GLU	N-CA-C	-5.49	105.84	112.54
1	A	278	ARG	N-CA-C	-5.49	104.94	111.69
1	D	69	ARG	CD-NE-CZ	5.47	132.06	124.40
1	D	130	VAL	N-CA-C	5.47	116.76	109.37
1	A	306	HIS	N-CA-C	5.47	118.73	109.76
1	B	236	ARG	NE-CZ-NH2	-5.46	114.28	119.20
1	C	13	ARG	CD-NE-CZ	5.46	132.04	124.40
1	C	10	ARG	N-CA-C	-5.45	105.42	111.36
1	B	262	ASN	N-CA-C	-5.44	100.72	109.58
1	D	398	ARG	N-CA-C	-5.43	105.91	112.54
1	D	143	LEU	N-CA-C	-5.43	102.59	110.08
1	A	122	LYS	N-CA-C	-5.42	105.53	111.82
1	B	366	GLU	N-CA-C	5.42	117.19	111.28
1	A	410	ARG	NE-CZ-NH1	5.42	126.92	121.50
1	C	226	MET	N-CA-C	-5.40	102.28	110.28
1	D	393	ASN	N-CA-C	-5.40	102.97	109.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	436	ARG	NE-CZ-NH1	5.40	126.90	121.50
1	B	108	LEU	N-CA-C	-5.39	101.87	109.96
1	B	227	ARG	CD-NE-CZ	5.39	131.95	124.40
1	D	50	GLU	N-CA-C	5.39	119.02	112.23
1	D	449	ASP	N-CA-C	5.38	116.83	111.07
1	A	10	ARG	N-CA-C	-5.37	105.51	111.36
1	A	131	SER	N-CA-C	-5.36	106.79	113.55
1	A	460	PRO	N-CA-C	-5.36	102.68	111.15
1	B	491	ARG	NE-CZ-NH1	5.35	126.85	121.50
1	B	227	ARG	CG-CD-NE	5.34	123.76	112.00
1	A	202	HIS	N-CA-C	5.33	118.25	109.72
1	B	236	ARG	NE-CZ-NH1	5.33	126.83	121.50
1	C	200	MET	N-CA-C	-5.33	106.16	113.30
1	D	52	LEU	N-CA-C	-5.32	105.56	111.36
1	D	307	LEU	N-CA-C	-5.32	98.71	108.02
1	C	439	GLY	N-CA-C	5.31	122.65	115.32
1	D	460	PRO	N-CA-C	-5.30	102.87	111.14
1	D	218	ASN	N-CA-C	5.30	116.75	110.97
1	A	439	GLY	N-CA-C	5.29	122.62	115.32
1	D	481	ILE	N-CA-C	-5.28	104.45	111.05
1	D	416	PHE	N-CA-C	5.28	116.31	108.60
1	A	10	ARG	NE-CZ-NH1	5.27	126.77	121.50
1	B	52	LEU	N-CA-C	-5.26	105.62	111.36
1	D	156	ARG	NE-CZ-NH1	5.26	126.76	121.50
1	A	262	ASN	N-CA-C	-5.24	100.31	109.48
1	A	476	THR	N-CA-C	-5.24	105.75	113.61
1	D	199	PRO	N-CA-C	5.23	119.43	111.11
1	A	414	ASN	N-CA-C	-5.23	101.13	109.23
1	C	368	LYS	CA-C-N	-5.23	117.62	123.16
1	C	368	LYS	C-N-CA	-5.23	117.62	123.16
1	A	98	GLN	N-CA-C	5.22	116.65	111.07
1	C	9	LEU	N-CA-C	-5.21	105.78	111.82
1	C	369	VAL	CB-CA-C	-5.21	106.42	111.05
1	C	262	ASN	N-CA-C	-5.19	100.40	109.48
1	C	476	THR	N-CA-C	-5.18	105.85	113.61
1	B	157	TYR	N-CA-C	-5.17	106.12	112.90
1	A	369	VAL	CB-CA-C	-5.17	106.45	111.05
1	D	388	PRO	N-CA-C	5.16	120.63	113.98
1	C	22	LEU	N-CA-C	-5.15	106.83	113.01
1	C	13	ARG	NE-CZ-NH1	5.13	126.63	121.50
1	A	368	LYS	CA-C-N	-5.10	117.76	123.16
1	A	368	LYS	C-N-CA	-5.10	117.76	123.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	270	LEU	CA-CB-CG	5.10	134.14	116.30
1	C	332	TRP	N-CA-C	-5.08	105.93	111.82
1	A	369	VAL	N-CA-C	5.07	115.62	111.62
1	A	410	ARG	NE-CZ-NH2	-5.06	114.64	119.20
1	A	9	LEU	N-CA-C	-5.05	105.96	111.82
1	A	269	GLU	N-CA-C	-5.05	100.81	109.24
1	B	460	PRO	N-CA-C	-5.05	103.26	111.14
1	C	278	ARG	N-CA-C	-5.04	105.49	111.69
1	C	374	ILE	N-CA-C	5.03	116.12	111.45
1	B	371	ASP	CB-CA-C	5.01	120.40	110.17

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	271	TYR	Sidechain
1	A	456	TYR	Sidechain
1	B	271	TYR	Sidechain
1	B	326	TYR	Sidechain
1	C	271	TYR	Sidechain
1	D	271	TYR	Sidechain
1	D	326	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3956	0	3921	92	0
1	B	3956	0	3921	111	0
1	C	3956	0	3921	90	0
1	D	3956	0	3921	110	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	32	0	26	2	0
3	B	32	0	26	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	32	0	26	2	0
3	D	32	0	26	2	0
4	A	100	0	0	8	0
4	B	113	0	0	5	0
4	C	121	0	0	6	0
4	D	130	0	0	6	0
All	All	16420	0	15788	388	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 12.

All (388) 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:B:10:ARG:HB2	1:B:10:ARG:NH1	1.57	1.19
1:D:10:ARG:HB2	1:D:10:ARG:NH1	1.57	1.18
1:D:10:ARG:HH11	1:D:10:ARG:CB	1.60	1.14
1:C:260:ARG:NH2	1:C:410:ARG:HH21	1.43	1.14
1:B:10:ARG:HH11	1:B:10:ARG:CB	1.62	1.13
1:C:122:LYS:HD2	1:C:122:LYS:N	1.66	1.11
1:C:122:LYS:H	1:C:122:LYS:CD	1.56	1.10
1:D:145:GLU:HG2	1:D:146:LYS:H	0.97	1.10
1:A:122:LYS:HD2	1:A:122:LYS:N	1.67	1.09
1:B:145:GLU:HG2	1:B:146:LYS:H	0.98	1.09
1:A:122:LYS:H	1:A:122:LYS:CD	1.58	1.07
1:D:145:GLU:HG2	1:D:146:LYS:N	1.68	1.06
1:B:145:GLU:HG2	1:B:146:LYS:N	1.69	1.05
1:A:122:LYS:HD2	1:A:122:LYS:H	0.85	1.02
1:A:260:ARG:NH2	1:A:410:ARG:HE	1.57	1.02
1:C:260:ARG:HH22	1:C:410:ARG:NH2	1.59	0.99
1:C:122:LYS:HD2	1:C:122:LYS:H	0.83	0.99
1:B:153:ILE:HA	1:B:156:ARG:HH21	1.30	0.94
1:B:15:LYS:HD2	1:B:105:ILE:HG23	1.53	0.91
1:B:69:ARG:HH12	1:B:87:GLN:NE2	1.70	0.90
1:B:260:ARG:HH21	1:B:260:ARG:HB3	1.34	0.89
1:D:260:ARG:HB3	1:D:260:ARG:HH21	1.35	0.89
1:D:22:LEU:HD13	1:D:102:LEU:HD13	1.54	0.88
1:D:145:GLU:CG	1:D:146:LYS:H	1.84	0.87
1:B:22:LEU:HD13	1:B:102:LEU:HD13	1.57	0.86
1:B:145:GLU:CG	1:B:146:LYS:H	1.85	0.85
1:B:10:ARG:HB2	1:B:10:ARG:HH11	0.71	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ARG:HH22	1:A:410:ARG:HH21	1.21	0.85
1:D:15:LYS:HD2	1:D:105:ILE:HG23	1.59	0.84
1:C:260:ARG:HH22	1:C:410:ARG:HH21	0.84	0.82
1:D:71:MET:HG2	1:D:74:ALA:O	1.79	0.82
1:D:414:ASN:HD22	3:D:2005:KAA:HN8	1.27	0.82
1:D:4:GLU:O	1:D:5:LEU:HD22	1.80	0.81
1:C:260:ARG:HH21	1:C:410:ARG:HD3	1.45	0.81
1:B:4:GLU:O	1:B:5:LEU:HD22	1.81	0.80
1:D:38:GLU:HB2	1:D:83:THR:HB	1.63	0.80
1:A:260:ARG:HG2	1:A:260:ARG:HH21	1.45	0.79
1:B:71:MET:HG2	1:B:74:ALA:O	1.83	0.79
1:B:414:ASN:HD22	3:B:2003:KAA:HN8	1.29	0.79
1:D:10:ARG:HB2	1:D:10:ARG:HH11	0.71	0.79
1:B:15:LYS:CD	1:B:105:ILE:HG23	2.13	0.78
1:A:260:ARG:NH2	1:A:410:ARG:HH21	1.81	0.78
1:A:414:ASN:HD22	3:A:2002:KAA:HN8	1.31	0.78
1:D:153:ILE:HA	1:D:156:ARG:HH21	1.49	0.78
1:D:15:LYS:CD	1:D:105:ILE:HG23	2.13	0.78
1:B:38:GLU:HB2	1:B:83:THR:HB	1.65	0.77
1:A:260:ARG:HH21	1:A:410:ARG:HE	1.30	0.77
1:C:260:ARG:HH21	1:C:260:ARG:HG2	1.46	0.77
1:B:70:GLY:O	1:B:71:MET:HB3	1.83	0.76
1:D:145:GLU:O	1:D:146:LYS:HD2	1.87	0.75
1:B:145:GLU:O	1:B:146:LYS:HD2	1.87	0.74
1:D:70:GLY:O	1:D:71:MET:HB3	1.86	0.74
1:B:152:ASP:O	1:B:156:ARG:HD3	1.87	0.74
1:B:165:ILE:HG22	1:B:166:MET:HE3	1.70	0.73
1:C:414:ASN:HD22	3:C:2004:KAA:HN8	1.33	0.73
1:B:211:ARG:CZ	1:B:211:ARG:HB2	2.20	0.72
1:C:70:GLY:HA3	1:C:104:LYS:NZ	2.03	0.72
1:C:260:ARG:NH2	1:C:410:ARG:HD3	2.04	0.72
1:A:260:ARG:HH22	1:A:410:ARG:NH2	1.86	0.72
1:D:211:ARG:HB2	1:D:211:ARG:CZ	2.20	0.71
1:A:70:GLY:HA3	1:A:104:LYS:HZ2	1.55	0.71
1:B:157:TYR:OH	1:B:483:ASP:OD2	2.08	0.71
1:C:70:GLY:HA3	1:C:104:LYS:HZ2	1.54	0.71
1:B:260:ARG:HB3	1:B:260:ARG:NH2	2.06	0.71
1:B:214:ILE:HD13	1:B:214:ILE:N	2.07	0.70
1:A:71:MET:HE3	1:A:71:MET:HA	1.74	0.70
1:D:214:ILE:HD13	1:D:214:ILE:N	2.06	0.70
1:C:71:MET:HA	1:C:71:MET:HE3	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:ARG:HH21	1:B:260:ARG:CB	2.04	0.69
1:D:257:ILE:HG22	1:D:263:PRO:HD3	1.72	0.69
1:A:70:GLY:HA3	1:A:104:LYS:NZ	2.07	0.69
1:D:182:GLN:NE2	4:D:708:HOH:O	2.26	0.69
1:D:260:ARG:HB3	1:D:260:ARG:NH2	2.08	0.69
1:B:213:PHE:C	1:B:214:ILE:HD13	2.17	0.69
1:D:445:GLU:HG3	4:D:852:HOH:O	1.91	0.68
1:C:4:GLU:O	1:C:5:LEU:HB2	1.92	0.68
1:A:153:ILE:HD12	1:A:153:ILE:H	1.60	0.67
1:A:4:GLU:O	1:A:5:LEU:HB2	1.93	0.67
1:C:10:ARG:O	1:C:14:GLU:HG2	1.95	0.67
1:A:260:ARG:HH22	1:A:410:ARG:HE	1.42	0.67
1:D:260:ARG:HH21	1:D:260:ARG:CB	2.06	0.67
1:D:145:GLU:CG	1:D:146:LYS:N	2.48	0.67
1:C:260:ARG:NH2	1:C:410:ARG:NH2	2.26	0.66
1:C:8:GLN:HA	1:C:11:VAL:HG23	1.77	0.66
1:B:257:ILE:HG22	1:B:263:PRO:HD3	1.77	0.66
1:C:153:ILE:HD12	1:C:153:ILE:H	1.61	0.66
1:B:444:HIS:HD2	4:B:753:HOH:O	1.78	0.66
1:B:69:ARG:HH12	1:B:87:GLN:HE21	1.42	0.66
1:D:213:PHE:C	1:D:214:ILE:HD13	2.21	0.65
1:A:8:GLN:HA	1:A:11:VAL:HG23	1.78	0.65
1:A:10:ARG:O	1:A:14:GLU:HG2	1.97	0.65
1:B:355:MET:HB3	1:B:359:HIS:HB2	1.78	0.65
1:B:424:ASP:OD2	1:B:428:ARG:HD3	1.96	0.65
1:D:355:MET:HB3	1:D:359:HIS:HB2	1.79	0.65
1:A:8:GLN:NE2	1:A:8:GLN:C	2.54	0.65
1:B:7:ASP:O	1:B:10:ARG:HG2	1.96	0.65
1:D:7:ASP:O	1:D:10:ARG:HG2	1.96	0.65
1:B:145:GLU:CG	1:B:146:LYS:N	2.49	0.64
1:B:182:GLN:NE2	4:B:501:HOH:O	2.30	0.64
1:C:8:GLN:C	1:C:8:GLN:NE2	2.55	0.64
1:B:19:ILE:O	1:B:19:ILE:HD12	1.97	0.64
1:D:16:LEU:C	1:D:16:LEU:HD23	2.23	0.64
1:B:22:LEU:HD13	1:B:102:LEU:CD1	2.27	0.63
1:D:16:LEU:HD12	1:D:140:LEU:HD21	1.79	0.63
1:D:144:PRO:HG2	1:D:166:MET:SD	2.37	0.63
1:D:165:ILE:HG22	1:D:166:MET:HE3	1.79	0.63
1:C:260:ARG:NH2	1:C:260:ARG:HG2	2.13	0.63
1:B:16:LEU:HD23	1:B:16:LEU:C	2.24	0.63
1:D:22:LEU:HD13	1:D:102:LEU:CD1	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ARG:NH2	1:A:410:ARG:NE	2.39	0.62
1:B:144:PRO:HG2	1:B:166:MET:SD	2.38	0.62
1:C:146:LYS:HZ2	1:C:166:MET:HG2	1.64	0.62
1:B:16:LEU:HD12	1:B:140:LEU:HD21	1.79	0.62
1:C:98:GLN:H	1:C:98:GLN:NE2	1.98	0.62
1:D:157:TYR:OH	1:D:483:ASP:OD2	2.15	0.62
1:D:236:ARG:HD3	4:D:851:HOH:O	1.99	0.62
1:D:19:ILE:HD12	1:D:19:ILE:O	2.00	0.61
1:B:36:LYS:O	1:B:39:GLU:HG3	2.01	0.61
1:D:233:HIS:HD2	4:D:833:HOH:O	1.84	0.61
1:A:98:GLN:H	1:A:98:GLN:NE2	1.99	0.60
1:D:186:ARG:NH1	1:D:294:GLU:OE1	2.34	0.60
1:A:146:LYS:H	1:A:146:LYS:CD	2.13	0.60
1:C:146:LYS:H	1:C:146:LYS:CD	2.13	0.60
1:B:195:GLU:HB2	1:B:246:TYR:CZ	2.36	0.60
1:A:428:ARG:HD2	4:A:722:HOH:O	2.00	0.59
1:B:70:GLY:O	1:B:71:MET:CB	2.50	0.59
1:C:231:GLU:CD	3:C:2004:KAA:HNZ1	2.10	0.59
1:B:153:ILE:HA	1:B:156:ARG:NH2	2.10	0.59
1:D:8:GLN:HB3	4:D:889:HOH:O	2.01	0.59
1:A:260:ARG:NH2	1:A:260:ARG:HG2	2.13	0.58
1:B:212:PRO:HG2	1:B:214:ILE:HD11	1.84	0.58
1:D:70:GLY:O	1:D:71:MET:CB	2.51	0.58
1:C:217:HIS:HE1	1:C:219:ALA:HB3	1.69	0.58
1:B:206:GLY:HA3	4:B:924:HOH:O	2.04	0.58
1:D:444:HIS:HD2	4:D:831:HOH:O	1.85	0.58
1:C:423:ILE:CD1	1:D:13:ARG:NH2	2.67	0.57
1:A:217:HIS:HE1	1:A:219:ALA:HB3	1.69	0.57
1:A:16:LEU:C	1:A:16:LEU:HD23	2.30	0.57
1:B:15:LYS:HD2	1:B:105:ILE:CG2	2.32	0.57
1:D:212:PRO:HG2	1:D:214:ILE:HD11	1.85	0.57
1:A:260:ARG:HH21	1:A:260:ARG:CG	2.18	0.56
1:A:100:TYR:CZ	1:A:104:LYS:HE2	2.40	0.56
4:A:535:HOH:O	1:B:182:GLN:HG2	2.05	0.56
1:A:146:LYS:HZ2	1:A:166:MET:HG2	1.70	0.56
1:B:212:PRO:HG2	1:B:214:ILE:CD1	2.36	0.56
1:D:491:ARG:O	1:D:492:HIS:C	2.48	0.56
1:D:212:PRO:HG2	1:D:214:ILE:CD1	2.36	0.56
1:A:235:LYS:NZ	1:A:418:GLU:OE2	2.35	0.56
1:C:153:ILE:H	1:C:153:ILE:CD1	2.18	0.56
1:C:122:LYS:N	1:C:122:LYS:CD	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:LYS:H	1:C:146:LYS:HD2	1.71	0.55
1:D:257:ILE:CG2	1:D:263:PRO:HD3	2.36	0.55
1:A:251:VAL:HG22	1:A:265:PHE:CE1	2.41	0.55
1:C:146:LYS:NZ	1:C:166:MET:HG2	2.20	0.55
1:B:10:ARG:HG3	1:B:11:VAL:N	2.20	0.55
1:D:69:ARG:HH12	1:D:87:GLN:NE2	2.04	0.55
1:A:171:LYS:NZ	4:A:815:HOH:O	2.39	0.55
1:A:226:MET:HE2	1:B:226:MET:HE2	1.88	0.55
1:D:10:ARG:HG3	1:D:11:VAL:N	2.21	0.55
1:A:434:LYS:O	1:A:437:GLU:HB2	2.07	0.55
1:A:146:LYS:HD2	1:A:166:MET:HE3	1.88	0.55
1:A:231:GLU:CD	3:A:2002:KAA:HNZ1	2.15	0.55
1:C:146:LYS:HD2	1:C:166:MET:HE3	1.88	0.55
1:D:220:LEU:HB3	1:D:222:MET:HE3	1.89	0.55
1:B:155:GLN:OE1	1:B:158:ARG:HG2	2.07	0.54
1:A:251:VAL:HG22	1:A:265:PHE:CZ	2.42	0.54
1:D:36:LYS:O	1:D:39:GLU:HG3	2.08	0.54
1:C:226:MET:HE2	1:D:226:MET:HE2	1.89	0.54
4:C:590:HOH:O	1:D:182:GLN:HG2	2.08	0.54
1:D:231:GLU:CD	3:D:2005:KAA:HNZ1	2.16	0.54
1:C:436:ARG:NH1	1:C:443:ALA:O	2.41	0.54
1:D:195:GLU:HB2	1:D:246:TYR:CZ	2.43	0.54
1:C:434:LYS:O	1:C:437:GLU:HB2	2.09	0.53
1:B:19:ILE:HD12	1:B:19:ILE:C	2.33	0.53
1:B:202:HIS:CE1	1:B:227:ARG:HB2	2.44	0.53
1:D:15:LYS:HD2	1:D:105:ILE:CG2	2.35	0.53
1:A:260:ARG:NH2	1:A:260:ARG:CG	2.71	0.53
1:B:227:ARG:HG2	1:B:227:ARG:O	2.06	0.53
1:C:251:VAL:HG22	1:C:265:PHE:CE1	2.44	0.53
1:A:423:ILE:CD1	1:B:13:ARG:NH2	2.72	0.53
1:A:13:ARG:HG2	4:A:962:HOH:O	2.09	0.52
1:C:421:ASP:C	1:C:421:ASP:OD1	2.51	0.52
1:A:122:LYS:N	1:A:122:LYS:CD	2.41	0.52
1:A:146:LYS:NZ	1:A:166:MET:HG2	2.24	0.52
1:C:444:HIS:HD2	4:C:681:HOH:O	1.90	0.52
1:D:15:LYS:HD3	1:D:105:ILE:HG23	1.90	0.52
1:B:491:ARG:O	1:B:492:HIS:C	2.53	0.52
1:C:260:ARG:NH2	1:C:260:ARG:CG	2.72	0.52
1:A:51:GLU:O	1:A:54:GLU:HB3	2.10	0.52
1:B:444:HIS:CD2	4:B:753:HOH:O	2.58	0.52
1:C:100:TYR:CZ	1:C:104:LYS:HE2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:GLU:O	1:C:54:GLU:HB3	2.10	0.52
1:C:146:LYS:HD2	1:C:146:LYS:N	2.25	0.52
1:C:217:HIS:CE1	1:C:219:ALA:HB3	2.44	0.52
1:D:19:ILE:HD12	1:D:24:VAL:HB	1.91	0.52
1:A:146:LYS:H	1:A:146:LYS:HD2	1.73	0.52
1:C:16:LEU:C	1:C:16:LEU:HD23	2.35	0.52
1:A:293:THR:O	1:A:297:GLY:HA2	2.11	0.51
1:A:418:GLU:OE1	1:A:463:GLY:HA3	2.09	0.51
1:B:362:ASN:CG	1:B:386:ILE:HD13	2.35	0.51
1:A:217:HIS:CE1	1:A:219:ALA:HB3	2.45	0.51
1:A:421:ASP:OD1	1:A:421:ASP:C	2.53	0.51
1:D:357:PHE:O	1:D:361:VAL:HG23	2.11	0.51
1:A:146:LYS:HD2	1:A:146:LYS:N	2.26	0.51
1:A:491:ARG:O	1:A:492:HIS:O	2.29	0.51
1:C:78:HIS:HE1	1:C:125:GLU:OE1	1.94	0.51
1:A:140:LEU:HD12	1:B:422:PRO:HG2	1.93	0.51
1:A:153:ILE:H	1:A:153:ILE:CD1	2.18	0.51
1:B:4:GLU:OE1	1:B:5:LEU:N	2.44	0.50
1:D:4:GLU:OE1	1:D:5:LEU:N	2.44	0.50
1:A:100:TYR:OH	1:A:104:LYS:HE2	2.11	0.50
1:C:140:LEU:HD12	1:D:422:PRO:HG2	1.93	0.50
1:A:71:MET:HE2	1:D:42:GLU:CD	2.36	0.50
1:B:69:ARG:HH12	1:B:87:GLN:HE22	1.53	0.50
1:C:141:ARG:NH2	1:D:455:GLU:OE2	2.44	0.50
1:C:143:LEU:HD21	1:C:165:ILE:HG21	1.93	0.50
1:A:354:HIS:HB2	1:A:438:GLN:HE21	1.77	0.49
1:D:19:ILE:HD12	1:D:19:ILE:C	2.37	0.49
1:C:57:ILE:O	1:C:117:THR:HA	2.12	0.49
1:C:354:HIS:HB2	1:C:438:GLN:HE21	1.78	0.49
1:D:200:MET:HA	1:D:227:ARG:HD3	1.95	0.49
1:B:233:HIS:HD2	4:B:605:HOH:O	1.96	0.49
1:B:220:LEU:HB3	1:B:222:MET:HE3	1.94	0.49
1:C:293:THR:O	1:C:297:GLY:HA2	2.13	0.49
1:C:444:HIS:CD2	4:C:681:HOH:O	2.65	0.49
1:B:155:GLN:OE1	1:B:155:GLN:HA	2.13	0.49
1:D:19:ILE:CD1	1:D:24:VAL:HB	2.43	0.49
1:C:235:LYS:NZ	1:C:418:GLU:OE2	2.43	0.49
1:A:333:ARG:HD3	4:A:741:HOH:O	2.12	0.49
1:D:292:ALA:O	1:D:296:LEU:HB2	2.13	0.49
1:A:444:HIS:HD2	4:A:947:HOH:O	1.95	0.48
1:C:251:VAL:HG22	1:C:265:PHE:CZ	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:ILE:HD12	1:B:24:VAL:HB	1.94	0.48
1:B:231:GLU:CD	3:B:2003:KAA:HNZ1	2.21	0.48
1:C:491:ARG:O	1:C:492:HIS:O	2.31	0.48
1:D:153:ILE:CA	1:D:156:ARG:HH21	2.24	0.48
1:A:403:PHE:CD1	1:A:403:PHE:C	2.92	0.48
1:D:362:ASN:CG	1:D:386:ILE:HD13	2.38	0.48
1:C:70:GLY:CA	1:C:104:LYS:NZ	2.74	0.48
1:D:82:VAL:O	1:D:171:LYS:HE3	2.14	0.48
1:A:57:ILE:O	1:A:117:THR:HA	2.14	0.48
1:C:199:PRO:CG	1:D:487:PHE:HB2	2.44	0.48
1:A:260:ARG:NH2	1:A:410:ARG:NH2	2.53	0.48
1:B:82:VAL:O	1:B:171:LYS:HE3	2.14	0.47
1:B:292:ALA:O	1:B:296:LEU:HB2	2.14	0.47
1:A:199:PRO:CG	1:B:487:PHE:HB2	2.44	0.47
1:D:38:GLU:HB2	1:D:83:THR:CB	2.39	0.47
1:D:327:VAL:HG12	1:D:329:VAL:HG23	1.96	0.47
1:A:141:ARG:NH2	1:B:455:GLU:OE2	2.46	0.47
1:A:222:MET:HE2	1:A:224:LEU:HD21	1.96	0.47
1:C:403:PHE:CD1	1:C:403:PHE:C	2.93	0.47
1:A:5:LEU:O	1:A:8:GLN:HG3	2.15	0.47
1:B:153:ILE:CA	1:B:156:ARG:HH21	2.15	0.47
1:C:482:ARG:HG2	1:C:482:ARG:NH1	2.29	0.47
1:D:71:MET:CG	1:D:71:MET:O	2.61	0.47
1:C:428:ARG:HD2	4:C:771:HOH:O	2.15	0.47
1:D:69:ARG:HH12	1:D:87:GLN:HE21	1.62	0.47
1:D:6:ASN:OD1	1:D:6:ASN:N	2.43	0.47
1:A:220:LEU:O	1:A:221:ASP:C	2.57	0.47
1:B:38:GLU:HB2	1:B:83:THR:CB	2.39	0.47
1:A:143:LEU:HD21	1:A:165:ILE:HG21	1.97	0.47
1:B:153:ILE:HG13	1:B:154:GLU:N	2.30	0.47
1:C:185:ARG:HH22	1:D:195:GLU:CD	2.22	0.47
1:C:220:LEU:O	1:C:221:ASP:C	2.57	0.47
1:A:8:GLN:C	1:A:8:GLN:HE21	2.23	0.46
1:A:16:LEU:C	1:A:16:LEU:CD2	2.88	0.46
1:B:436:ARG:NH2	1:B:443:ALA:O	2.48	0.46
1:C:381:GLY:O	1:C:399:PHE:HB3	2.15	0.46
1:D:155:GLN:HA	1:D:155:GLN:OE1	2.15	0.46
1:A:78:HIS:HE1	1:A:125:GLU:OE1	1.97	0.46
1:C:158:ARG:HG2	1:C:158:ARG:HH11	1.79	0.46
1:A:260:ARG:HH22	1:A:410:ARG:NE	2.07	0.46
1:C:418:GLU:OE1	1:C:463:GLY:HA3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:450:PHE:O	1:D:453:ALA:HB3	2.15	0.46
1:B:257:ILE:CG2	1:B:263:PRO:HD3	2.43	0.46
1:C:5:LEU:O	1:C:8:GLN:HG3	2.16	0.46
1:D:16:LEU:HD23	1:D:16:LEU:O	2.16	0.45
1:D:156:ARG:HB3	1:D:163:ASP:HB2	1.98	0.45
1:D:217:HIS:CE1	1:D:220:LEU:HG	2.52	0.45
1:A:70:GLY:CA	1:A:104:LYS:NZ	2.77	0.45
1:D:195:GLU:HB2	1:D:246:TYR:CE2	2.51	0.45
1:D:257:ILE:H	1:D:257:ILE:HG12	1.59	0.45
1:B:71:MET:CG	1:B:71:MET:O	2.63	0.45
1:B:373:LEU:HD21	1:B:379:ILE:HD11	1.97	0.45
1:C:8:GLN:C	1:C:8:GLN:HE21	2.25	0.45
1:D:37:ALA:O	1:D:41:PHE:HD1	2.00	0.45
1:B:270:LEU:C	1:B:270:LEU:HD12	2.42	0.45
1:B:156:ARG:HB3	1:B:163:ASP:HB2	1.98	0.45
1:B:358:GLY:HA3	1:B:385:GLU:OE2	2.18	0.44
1:D:214:ILE:HD12	1:D:225:TYR:CD2	2.52	0.44
1:B:186:ARG:NH1	1:B:294:GLU:OE1	2.50	0.44
1:B:282:LYS:HE2	1:B:285:GLU:OE1	2.16	0.44
1:A:381:GLY:O	1:A:399:PHE:HB3	2.17	0.44
1:B:195:GLU:HB2	1:B:246:TYR:CE2	2.51	0.44
1:B:217:HIS:CE1	1:B:220:LEU:HG	2.53	0.44
1:C:233:HIS:HD2	4:C:678:HOH:O	2.00	0.44
1:B:424:ASP:O	1:B:428:ARG:HG2	2.17	0.44
1:D:407:ILE:C	1:D:408:VAL:HG22	2.42	0.44
1:A:71:MET:HE2	1:D:42:GLU:OE2	2.18	0.44
1:B:314:TRP:CD2	1:B:376:PRO:HB2	2.52	0.44
1:B:214:ILE:HD12	1:B:225:TYR:CD2	2.52	0.44
1:C:171:LYS:NZ	4:C:913:HOH:O	2.50	0.44
1:A:366:GLU:HG2	1:A:370:GLU:OE2	2.17	0.44
1:B:164:LEU:HD23	1:B:164:LEU:HA	1.86	0.44
1:C:366:GLU:HG2	1:C:370:GLU:OE2	2.17	0.44
1:A:158:ARG:HH11	1:A:158:ARG:HG2	1.83	0.44
1:B:217:HIS:HE1	1:B:219:ALA:HB3	1.82	0.44
1:B:19:ILE:CD1	1:B:24:VAL:HB	2.48	0.43
1:B:91:ARG:NH2	1:B:93:ASP:OD1	2.46	0.43
1:D:78:HIS:HE1	1:D:125:GLU:OE2	2.00	0.43
1:D:166:MET:HE2	1:D:166:MET:HA	2.00	0.43
1:D:270:LEU:C	1:D:270:LEU:HD12	2.43	0.43
1:A:285:GLU:HA	1:A:314:TRP:CH2	2.52	0.43
1:B:357:PHE:O	1:B:361:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:TYR:OH	1:C:104:LYS:HE2	2.19	0.43
1:D:153:ILE:HG13	1:D:154:GLU:N	2.33	0.43
1:B:37:ALA:O	1:B:41:PHE:HD1	2.01	0.43
1:C:20:GLU:O	1:C:23:GLY:N	2.47	0.43
1:D:370:GLU:HA	1:D:373:LEU:HD22	1.99	0.43
1:B:155:GLN:OE1	1:B:155:GLN:CA	2.67	0.43
1:C:78:HIS:NE2	1:C:87:GLN:HB2	2.34	0.43
1:C:16:LEU:C	1:C:16:LEU:CD2	2.92	0.43
1:B:78:HIS:HE1	1:B:125:GLU:OE2	2.01	0.43
1:B:102:LEU:HD12	1:B:102:LEU:HA	1.88	0.42
1:C:193:TYR:CD2	1:C:244:LYS:HB3	2.54	0.42
1:A:260:ARG:HH22	1:A:410:ARG:CZ	2.31	0.42
1:A:444:HIS:CD2	4:A:947:HOH:O	2.71	0.42
1:B:15:LYS:HD3	1:B:105:ILE:HG23	1.96	0.42
1:B:115:ARG:HB2	1:B:132:SER:HB3	2.00	0.42
1:C:423:ILE:HD13	1:D:13:ARG:NH2	2.34	0.42
1:C:71:MET:HA	1:C:71:MET:CE	2.44	0.42
1:D:33:ARG:HD3	1:D:62:ALA:HB3	2.00	0.42
1:D:160:ARG:HA	1:D:160:ARG:HD3	1.83	0.42
1:C:237:LEU:O	1:C:242:LEU:HB2	2.20	0.42
1:C:438:GLN:HE21	1:C:438:GLN:HB2	1.60	0.42
1:A:146:LYS:CD	1:A:146:LYS:N	2.82	0.42
1:B:403:PHE:CD1	1:B:403:PHE:C	2.97	0.42
1:C:185:ARG:NH2	1:D:195:GLU:OE1	2.47	0.42
1:A:71:MET:HA	1:A:71:MET:CE	2.45	0.42
1:B:160:ARG:HA	1:B:160:ARG:HD3	1.82	0.42
1:C:79:ILE:O	1:C:85:GLN:HA	2.20	0.42
1:C:146:LYS:CD	1:C:146:LYS:N	2.82	0.42
1:C:351:VAL:O	1:C:351:VAL:HG23	2.20	0.42
1:C:222:MET:HE2	1:C:224:LEU:HD21	2.01	0.42
1:D:158:ARG:HB2	1:D:490:MET:HE2	2.02	0.42
1:B:16:LEU:HD23	1:B:16:LEU:O	2.19	0.42
1:B:17:LYS:O	1:B:21:GLU:HG3	2.20	0.42
1:B:166:MET:HE2	1:B:166:MET:HA	2.02	0.42
1:B:327:VAL:HG12	1:B:329:VAL:HG23	2.01	0.42
1:C:104:LYS:HD3	1:C:104:LYS:HA	1.83	0.42
1:B:24:VAL:HG21	1:B:102:LEU:HD21	2.02	0.41
1:D:158:ARG:HG3	1:D:159:GLN:HG3	2.02	0.41
1:D:282:LYS:HE2	1:D:285:GLU:OE1	2.20	0.41
1:A:451:LEU:O	1:A:455:GLU:HG3	2.20	0.41
1:C:100:TYR:CE2	1:C:104:LYS:HE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:LYS:O	1:D:21:GLU:HG3	2.21	0.41
1:D:214:ILE:N	1:D:214:ILE:CD1	2.79	0.41
1:A:233:HIS:HD2	4:A:804:HOH:O	2.02	0.41
1:B:69:ARG:NH1	1:B:87:GLN:HE21	2.15	0.41
1:D:407:ILE:O	1:D:408:VAL:CG2	2.68	0.41
1:A:242:LEU:HD12	1:A:242:LEU:HA	1.95	0.41
1:C:143:LEU:HA	1:C:143:LEU:HD12	1.82	0.41
1:D:156:ARG:CZ	1:D:156:ARG:HB2	2.51	0.41
1:D:260:ARG:NH2	1:D:410:ARG:HE	2.18	0.41
1:A:100:TYR:CE2	1:A:104:LYS:HE2	2.55	0.41
1:A:143:LEU:HA	1:A:143:LEU:HD12	1.81	0.41
1:A:407:ILE:O	1:A:408:VAL:C	2.64	0.41
1:C:183:SER:OG	1:C:294:GLU:OE1	2.34	0.41
1:B:156:ARG:CZ	1:B:156:ARG:HB2	2.49	0.41
1:C:91:ARG:HG3	1:C:94:ASP:OD1	2.21	0.41
1:D:155:GLN:OE1	1:D:155:GLN:CA	2.69	0.41
1:A:193:TYR:CD2	1:A:244:LYS:HB3	2.57	0.40
1:D:24:VAL:HG21	1:D:102:LEU:HD21	2.04	0.40
1:D:358:GLY:HA3	1:D:385:GLU:OE2	2.22	0.40
1:D:80:GLN:HB2	1:D:85:GLN:HG2	2.03	0.40
1:A:482:ARG:NH1	1:A:482:ARG:HG2	2.36	0.40
1:C:71:MET:H	1:C:104:LYS:HZ2	1.69	0.40
1:D:403:PHE:CD1	1:D:403:PHE:C	2.99	0.40
1:A:78:HIS:NE2	1:A:87:GLN:HB2	2.36	0.40
1:A:103:PHE:O	1:A:106:SER:HB2	2.22	0.40
1:A:104:LYS:HD3	1:A:104:LYS:HA	1.85	0.40
1:B:158:ARG:HB2	1:B:490:MET:HE2	2.04	0.40
1:B:381:GLY:O	1:B:399:PHE:HB3	2.21	0.40
1:C:211:ARG:CZ	1:C:211:ARG:HB2	2.48	0.40
1:A:438:GLN:HE21	1:A:438:GLN:HB2	1.60	0.40
1:B:211:ARG:HB2	1:B:211:ARG:NH2	2.35	0.40
1:B:478:SER:HB3	1:B:483:ASP:HB2	2.02	0.40
1:D:18:LYS:NZ	1:D:18:LYS:HB2	2.36	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	480/493 (97%)	465 (97%)	13 (3%)	2 (0%)	30	28
1	B	480/493 (97%)	461 (96%)	16 (3%)	3 (1%)	21	18
1	C	480/493 (97%)	464 (97%)	14 (3%)	2 (0%)	30	28
1	D	480/493 (97%)	461 (96%)	17 (4%)	2 (0%)	30	28
All	All	1920/1972 (97%)	1851 (96%)	60 (3%)	9 (0%)	24	22

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	B	71	MET
1	B	145	GLU
1	C	5	LEU
1	D	71	MET
1	D	145	GLU
1	A	71	MET
1	C	71	MET
1	B	28	GLY

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	425/433 (98%)	392 (92%)	33 (8%)	11	9
1	B	425/433 (98%)	383 (90%)	42 (10%)	7	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	425/433 (98%)	391 (92%)	34 (8%)	11	8
1	D	425/433 (98%)	386 (91%)	39 (9%)	8	6
All	All	1700/1732 (98%)	1552 (91%)	148 (9%)	9	7

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	7	ASP
1	A	8	GLN
1	A	16	LEU
1	A	40	LEU
1	A	46	ASP
1	A	71	MET
1	A	79	ILE
1	A	91	ARG
1	A	97	GLU
1	A	107	ASP
1	A	119	PHE
1	A	122	LYS
1	A	143	LEU
1	A	146	LYS
1	A	153	ILE
1	A	155	GLN
1	A	158	ARG
1	A	171	LYS
1	A	188	LEU
1	A	242	LEU
1	A	251	VAL
1	A	260	ARG
1	A	268	LEU
1	A	270	LEU
1	A	277	PHE
1	A	302	GLN
1	A	305	GLU
1	A	343	LEU
1	A	373	LEU
1	A	387	SER
1	A	416	PHE
1	A	445	GLU
1	B	4	GLU

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Mol	Chain	Res	Type
1	B	6	ASN
1	B	9	LEU
1	B	10	ARG
1	B	18	LYS
1	B	19	ILE
1	B	22	LEU
1	B	39	GLU
1	B	40	LEU
1	B	47	LEU
1	B	50	GLU
1	B	69	ARG
1	B	71	MET
1	B	91	ARG
1	B	93	ASP
1	B	102	LEU
1	B	145	GLU
1	B	154	GLU
1	B	156	ARG
1	B	158	ARG
1	B	166	MET
1	B	179	LEU
1	B	188	LEU
1	B	212	PRO
1	B	214	ILE
1	B	227	ARG
1	B	242	LEU
1	B	257	ILE
1	B	260	ARG
1	B	268	LEU
1	B	270	LEU
1	B	282	LYS
1	B	296	LEU
1	B	351	VAL
1	B	371	ASP
1	B	372	LYS
1	B	373	LEU
1	B	383	PRO
1	B	416	PHE
1	B	445	GLU
1	B	449	ASP
1	B	474	LEU
1	C	6	ASN

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Mol	Chain	Res	Type
1	C	7	ASP
1	C	8	GLN
1	C	16	LEU
1	C	26	PRO
1	C	40	LEU
1	C	46	ASP
1	C	71	MET
1	C	79	ILE
1	C	91	ARG
1	C	97	GLU
1	C	107	ASP
1	C	122	LYS
1	C	143	LEU
1	C	146	LYS
1	C	153	ILE
1	C	155	GLN
1	C	158	ARG
1	C	171	LYS
1	C	188	LEU
1	C	242	LEU
1	C	251	VAL
1	C	260	ARG
1	C	268	LEU
1	C	270	LEU
1	C	277	PHE
1	C	302	GLN
1	C	305	GLU
1	C	343	LEU
1	C	373	LEU
1	C	410	ARG
1	C	416	PHE
1	C	445	GLU
1	C	470	ARG
1	D	4	GLU
1	D	6	ASN
1	D	9	LEU
1	D	10	ARG
1	D	18	LYS
1	D	19	ILE
1	D	22	LEU
1	D	39	GLU
1	D	40	LEU

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Mol	Chain	Res	Type
1	D	47	LEU
1	D	50	GLU
1	D	71	MET
1	D	91	ARG
1	D	93	ASP
1	D	102	LEU
1	D	145	GLU
1	D	154	GLU
1	D	166	MET
1	D	179	LEU
1	D	188	LEU
1	D	212	PRO
1	D	214	ILE
1	D	242	LEU
1	D	257	ILE
1	D	260	ARG
1	D	268	LEU
1	D	270	LEU
1	D	277	PHE
1	D	282	LYS
1	D	296	LEU
1	D	351	VAL
1	D	371	ASP
1	D	372	LYS
1	D	373	LEU
1	D	383	PRO
1	D	416	PHE
1	D	445	GLU
1	D	449	ASP
1	D	474	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	55	GLN
1	A	78	HIS
1	A	98	GLN
1	A	216	HIS
1	A	218	ASN
1	A	233	HIS
1	A	286	ASN

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Mol	Chain	Res	Type
1	A	290	HIS
1	A	354	HIS
1	A	427	GLN
1	A	438	GLN
1	A	444	HIS
1	A	489	GLN
1	B	55	GLN
1	B	78	HIS
1	B	80	GLN
1	B	85	GLN
1	B	87	GLN
1	B	98	GLN
1	B	233	HIS
1	B	286	ASN
1	B	414	ASN
1	B	438	GLN
1	B	444	HIS
1	B	489	GLN
1	B	492	HIS
1	C	6	ASN
1	C	55	GLN
1	C	78	HIS
1	C	87	GLN
1	C	98	GLN
1	C	216	HIS
1	C	218	ASN
1	C	233	HIS
1	C	286	ASN
1	C	290	HIS
1	C	354	HIS
1	C	427	GLN
1	C	438	GLN
1	C	444	HIS
1	D	55	GLN
1	D	78	HIS
1	D	87	GLN
1	D	98	GLN
1	D	233	HIS
1	D	286	ASN
1	D	414	ASN
1	D	438	GLN
1	D	444	HIS

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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	KAA	D	2005	-	34,34,34	2.74	8 (23%)	46,49,49	2.08	13 (28%)
3	KAA	C	2004	-	34,34,34	2.70	6 (17%)	46,49,49	2.09	11 (23%)
3	KAA	B	2003	-	34,34,34	2.76	8 (23%)	46,49,49	2.12	13 (28%)
3	KAA	A	2002	-	34,34,34	2.75	6 (17%)	46,49,49	2.18	13 (28%)

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
3	KAA	D	2005	-	-	3/23/40/40	0/3/3/3
3	KAA	C	2004	-	-	1/23/40/40	0/3/3/3
3	KAA	B	2003	-	-	2/23/40/40	0/3/3/3
3	KAA	A	2002	-	-	2/23/40/40	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2003	KAA	O2S-S1	9.19	1.50	1.42
3	D	2005	KAA	O2S-S1	8.98	1.50	1.42
3	A	2002	KAA	O1S-S1	8.95	1.50	1.42
3	A	2002	KAA	O2S-S1	8.93	1.50	1.42
3	D	2005	KAA	O1S-S1	8.87	1.50	1.42
3	B	2003	KAA	O1S-S1	8.80	1.50	1.42
3	C	2004	KAA	O1S-S1	8.77	1.50	1.42
3	C	2004	KAA	O2S-S1	8.75	1.50	1.42
3	B	2003	KAA	O5'-S1	-7.94	1.44	1.60
3	A	2002	KAA	O5'-S1	-7.87	1.44	1.60
3	D	2005	KAA	O5'-S1	-7.86	1.44	1.60
3	C	2004	KAA	O5'-S1	-7.84	1.44	1.60
3	C	2004	KAA	C5-N7	-3.07	1.33	1.39
3	A	2002	KAA	C5-N7	-3.06	1.33	1.39
3	D	2005	KAA	C5-N7	-3.03	1.33	1.39
3	B	2003	KAA	C5-N7	-3.02	1.33	1.39
3	D	2005	KAA	C-N8	-2.46	1.33	1.37
3	B	2003	KAA	C-N8	-2.42	1.33	1.37
3	C	2004	KAA	C-N8	-2.40	1.33	1.37
3	A	2002	KAA	C8-N9	-2.37	1.33	1.37
3	A	2002	KAA	C-N8	-2.37	1.33	1.37
3	C	2004	KAA	C8-N9	-2.34	1.33	1.37
3	B	2003	KAA	C8-N9	-2.29	1.33	1.37
3	D	2005	KAA	C8-N9	-2.25	1.33	1.37
3	D	2005	KAA	S1-N8	2.19	1.63	1.59
3	B	2003	KAA	C4-N9	-2.03	1.33	1.37
3	D	2005	KAA	C4-N9	-2.03	1.33	1.37
3	B	2003	KAA	S1-N8	2.03	1.63	1.59

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2003	KAA	O2S-S1-O1S	-6.91	110.50	120.85
3	A	2002	KAA	O2S-S1-O1S	-6.79	110.68	120.85
3	C	2004	KAA	O2S-S1-O1S	-6.36	111.33	120.85
3	D	2005	KAA	O2S-S1-O1S	-5.95	111.94	120.85
3	C	2004	KAA	C5-C4-N3	-5.48	119.17	126.72
3	A	2002	KAA	C5-C4-N3	-5.38	119.30	126.72
3	A	2002	KAA	N1-C2-N3	-5.28	120.59	128.58
3	D	2005	KAA	N1-C2-N3	-5.03	120.97	128.58
3	B	2003	KAA	N1-C2-N3	-4.99	121.02	128.58
3	C	2004	KAA	N1-C2-N3	-4.95	121.08	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2005	KAA	C5-C4-N3	-4.64	120.33	126.72
3	B	2003	KAA	C5-C4-N3	-4.53	120.48	126.72
3	A	2002	KAA	O5'-C5'-C4'	4.27	115.18	107.57
3	D	2005	KAA	O5'-C5'-C4'	4.02	114.72	107.57
3	C	2004	KAA	N3-C4-N9	3.98	133.94	127.17
3	A	2002	KAA	C2-N3-C4	3.91	121.39	111.83
3	A	2002	KAA	N3-C4-N9	3.81	133.64	127.17
3	C	2004	KAA	C2-N3-C4	3.79	121.08	111.83
3	B	2003	KAA	C2-N3-C4	3.56	120.52	111.83
3	D	2005	KAA	C2-N3-C4	3.55	120.50	111.83
3	B	2003	KAA	N9-C8-N7	-3.52	108.94	113.94
3	C	2004	KAA	O5'-C5'-C4'	3.48	113.77	107.57
3	B	2003	KAA	O5'-C5'-C4'	3.46	113.74	107.57
3	D	2005	KAA	O5'-S1-N8	3.42	114.55	105.69
3	D	2005	KAA	N3-C4-N9	3.39	132.93	127.17
3	A	2002	KAA	N9-C8-N7	-3.27	109.29	113.94
3	D	2005	KAA	N9-C8-N7	-3.23	109.36	113.94
3	C	2004	KAA	N9-C8-N7	-3.23	109.36	113.94
3	B	2003	KAA	C5-N7-C8	3.21	108.49	103.45
3	B	2003	KAA	C4-C5-N7	-3.12	107.02	110.58
3	B	2003	KAA	N3-C4-N9	3.11	132.45	127.17
3	A	2002	KAA	C5-N7-C8	2.96	108.10	103.45
3	C	2004	KAA	C5-N7-C8	2.95	108.08	103.45
3	B	2003	KAA	O5'-S1-N8	2.92	113.24	105.69
3	A	2002	KAA	C4-C5-N7	-2.89	107.28	110.58
3	D	2005	KAA	C5-N7-C8	2.86	107.95	103.45
3	C	2004	KAA	C4-C5-N7	-2.78	107.40	110.58
3	D	2005	KAA	C4-C5-N7	-2.67	107.53	110.58
3	B	2003	KAA	C4-N9-C8	2.62	108.49	105.74
3	D	2005	KAA	C4-N9-C8	2.56	108.43	105.74
3	A	2002	KAA	O5'-S1-N8	2.49	112.14	105.69
3	C	2004	KAA	O5'-S1-N8	2.45	112.03	105.69
3	C	2004	KAA	C4-N9-C8	2.42	108.28	105.74
3	A	2002	KAA	C4-N9-C8	2.41	108.27	105.74
3	B	2003	KAA	CB-CA-C	-2.37	105.91	110.76
3	B	2003	KAA	O5'-S1-O2S	2.34	112.56	105.48
3	A	2002	KAA	CB-CA-C	-2.31	106.05	110.76
3	D	2005	KAA	O5'-S1-O2S	2.26	112.31	105.48
3	A	2002	KAA	O5'-S1-O2S	2.07	111.74	105.48
3	D	2005	KAA	CB-CA-C	-2.05	106.58	110.76

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	2005	KAA	O-C-N8-S1
3	B	2003	KAA	O-C-CA-CB
3	D	2005	KAA	O-C-CA-CB
3	A	2002	KAA	O-C-CA-N
3	B	2003	KAA	O-C-CA-N
3	D	2005	KAA	O-C-CA-N
3	A	2002	KAA	C4'-C5'-O5'-S1
3	C	2004	KAA	C4'-C5'-O5'-S1

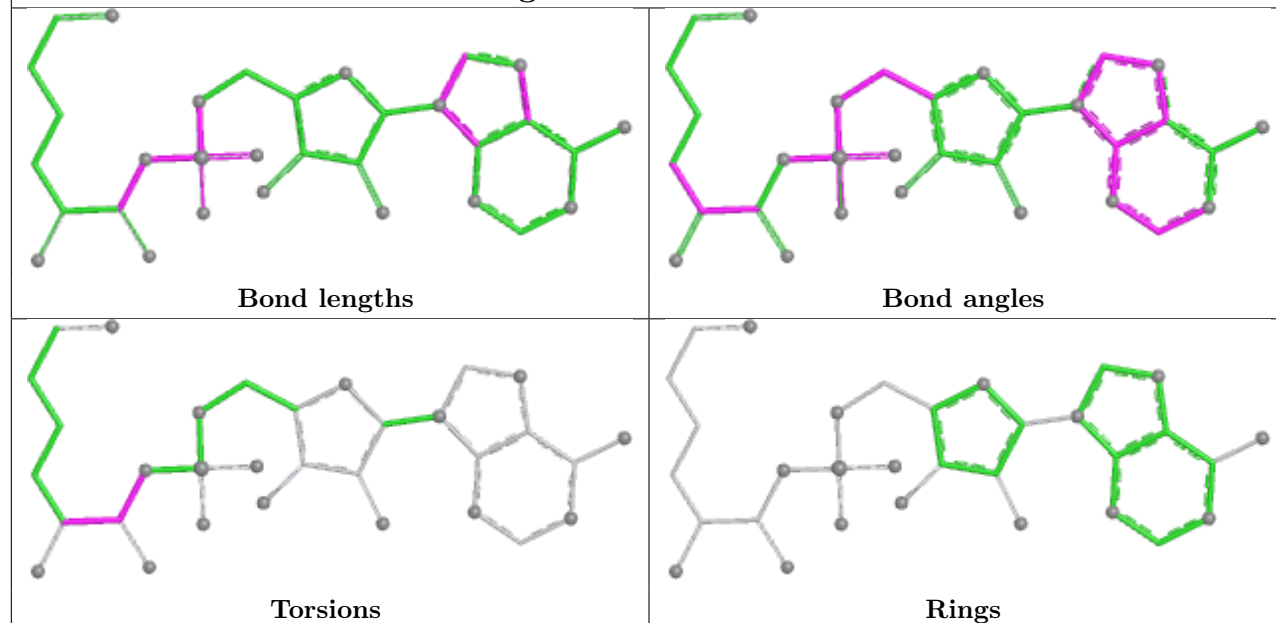
There are no ring outliers.

4 monomers are involved in 8 short contacts:

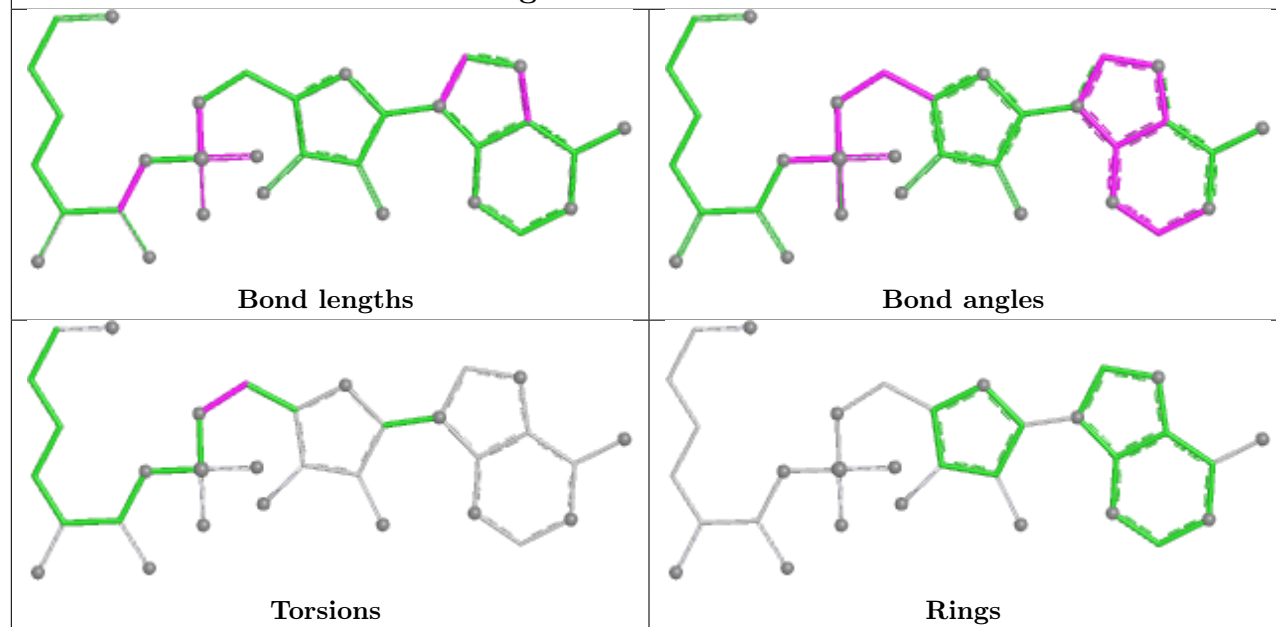
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2005	KAA	2	0
3	C	2004	KAA	2	0
3	B	2003	KAA	2	0
3	A	2002	KAA	2	0

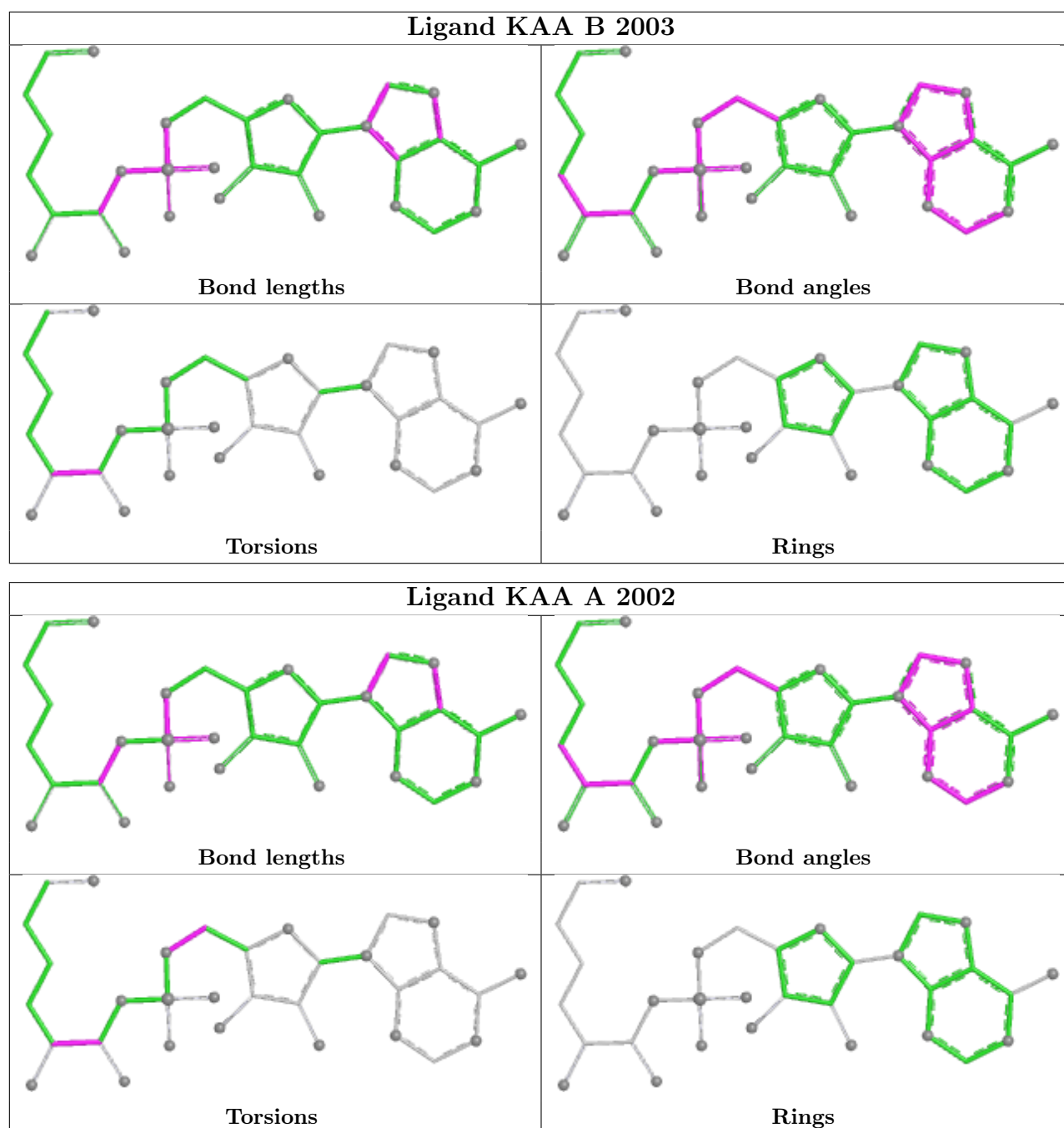
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand KAA D 2005



Ligand KAA C 2004





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	484/493 (98%)	-1.48	0 100 100	12, 22, 45, 72	0
1	B	484/493 (98%)	-1.45	0 100 100	14, 23, 52, 75	0
1	C	484/493 (98%)	-1.48	0 100 100	12, 22, 45, 72	0
1	D	484/493 (98%)	-1.46	0 100 100	13, 23, 51, 74	0
All	All	1936/1972 (98%)	-1.47	0 100 100	12, 22, 49, 75	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	A	2001	1/1	0.98	0.07	40,40,40,40	0
2	MG	C	2003	1/1	0.98	0.08	45,45,45,45	0
2	MG	B	2002	1/1	0.99	0.04	34,34,34,34	0
2	MG	D	2004	1/1	0.99	0.03	31,31,31,31	0

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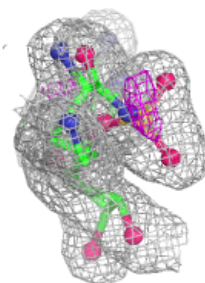
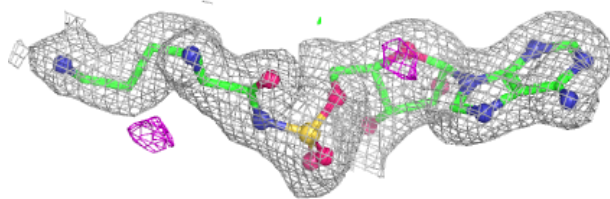
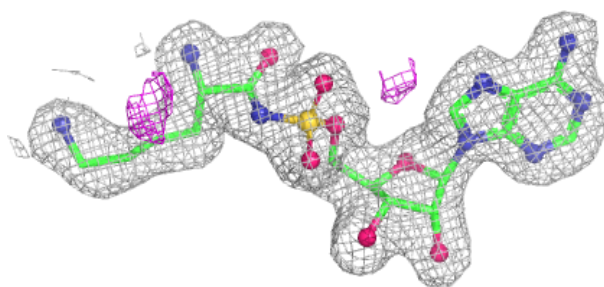
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	KAA	B	2003	32/32	0.99	0.03	7,17,25,26	0
3	KAA	A	2002	32/32	1.00	0.02	9,17,21,25	0
3	KAA	C	2004	32/32	1.00	0.02	10,15,20,24	0
3	KAA	D	2005	32/32	1.00	0.02	10,18,22,25	0

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.

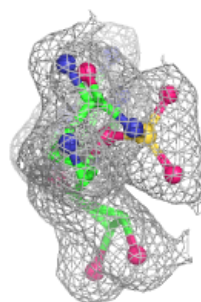
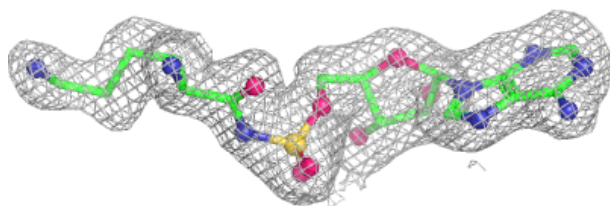
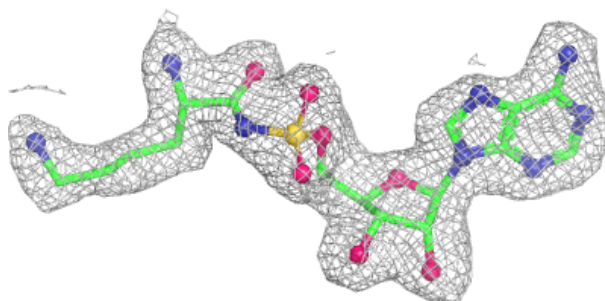
Electron density around KAA B 2003:

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

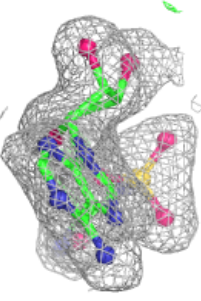
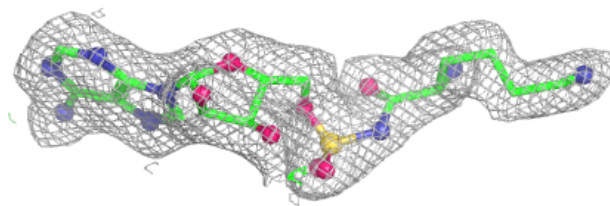
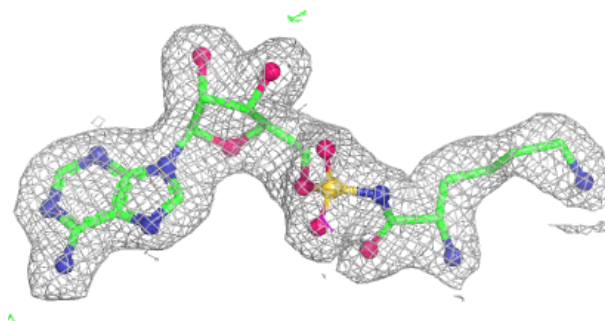


Electron density around KAA A 2002:

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

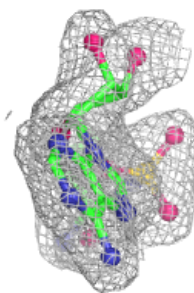
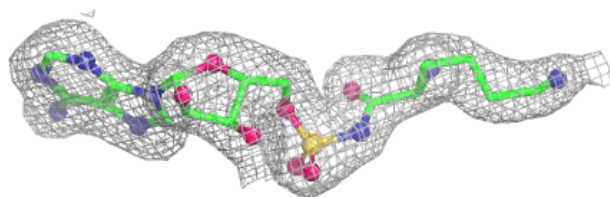
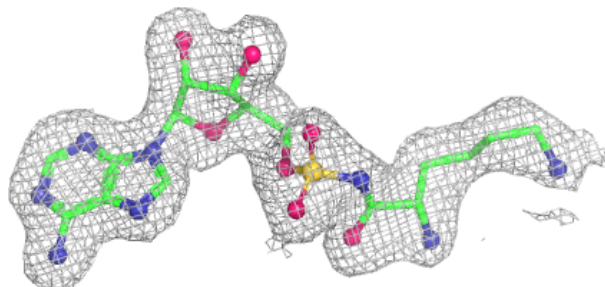
**Electron density around KAA C 2004:**

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



Electron density around KAA D 2005:

$2mF_o-DF_c$ (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.