



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:20 AM GMT

PDB ID : 3E9H
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

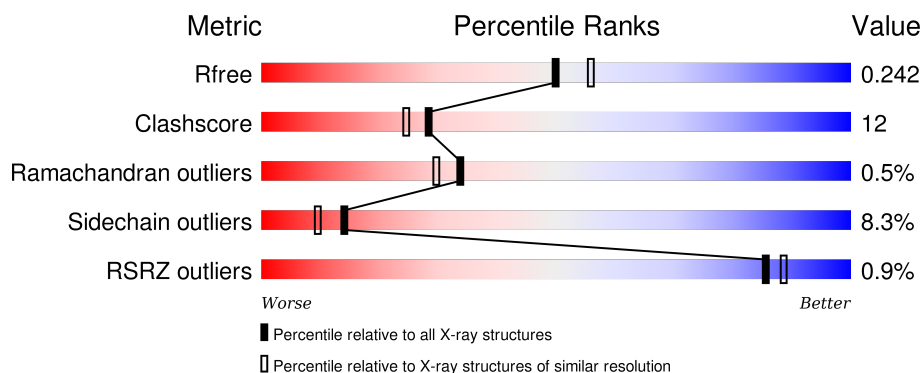
1 Overall quality at a glance

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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>17%</div> <div>• •</div> </div> </div>
1	B	493	<div> <div>%</div> <div> <div></div> <div>72%</div> <div>19%</div> <div>5%</div> <div>• •</div> </div> </div>
1	C	493	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>18%</div> <div>• • •</div> </div> </div>
1	D	493	<div> <div>%</div> <div> <div></div> <div>72%</div> <div>20%</div> <div>6%</div> <div>• •</div> </div> </div>

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.

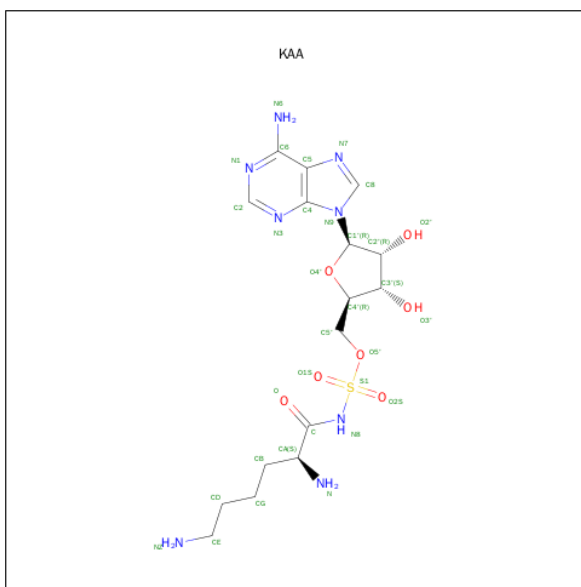
- Molecule 1 is a protein called Lysyl-tRNA synthetase.

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 (three-letter code: MG) (formula: Mg).

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

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



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

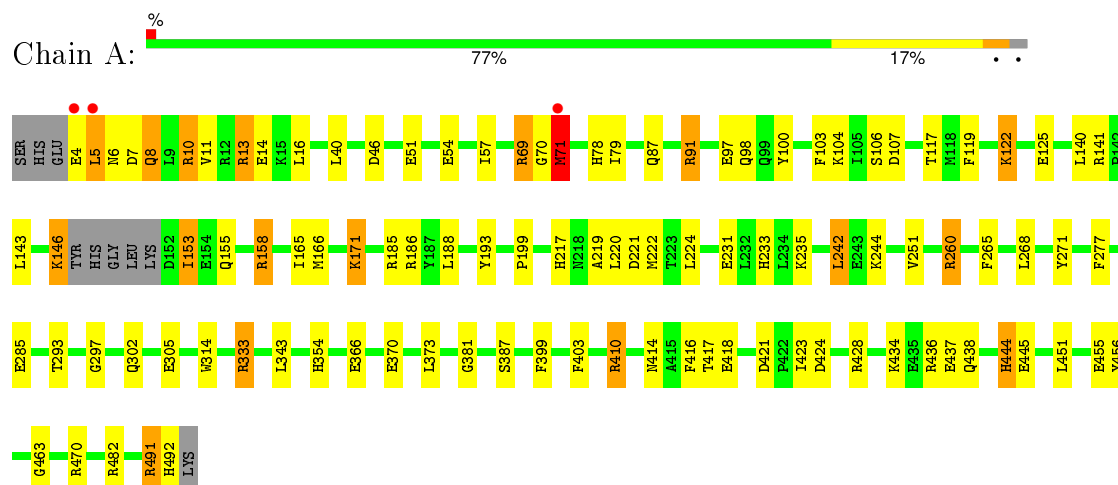
- Molecule 4 is water.

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

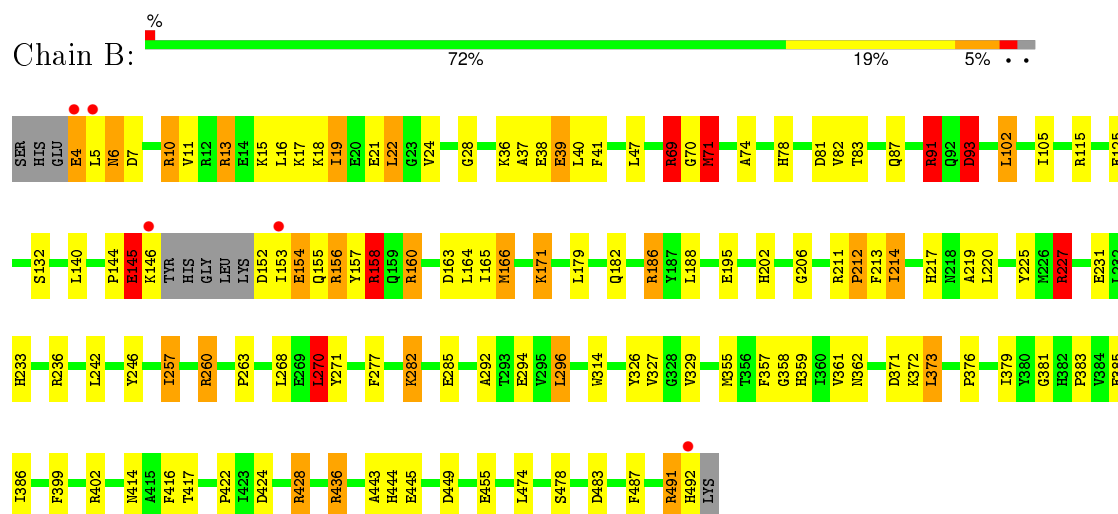
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

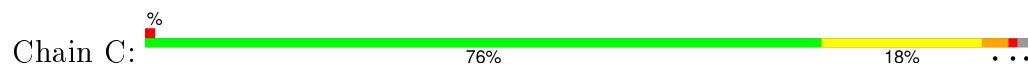
• Molecule 1: Lysyl-tRNA synthetase

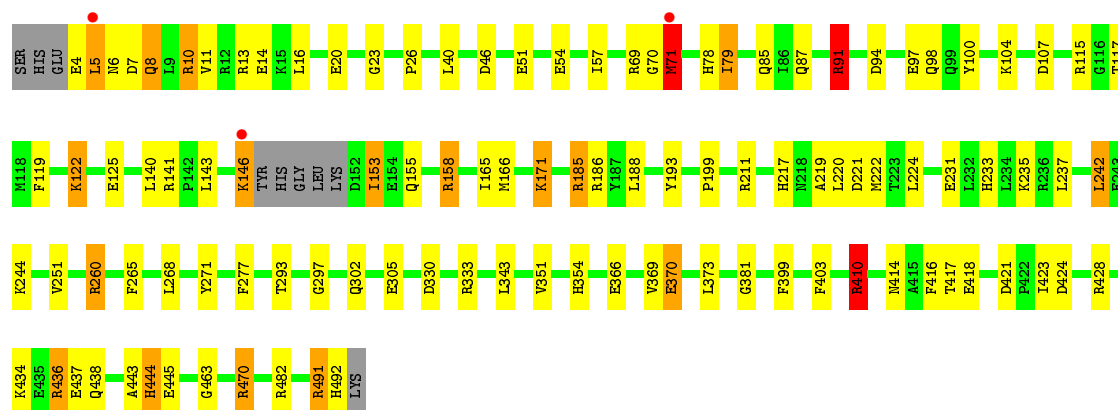


• Molecule 1: Lysyl-tRNA synthetase

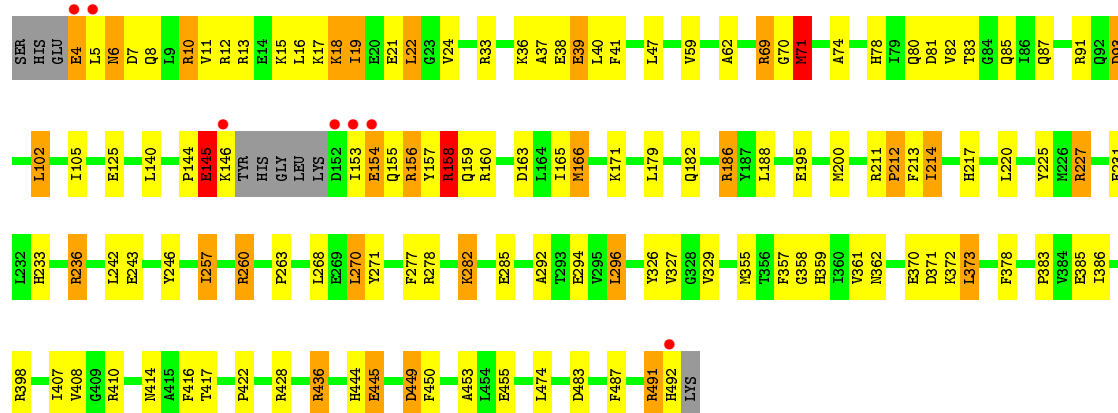


• Molecule 1: Lysyl-tRNA synthetase





● Molecule 1: Lysyl-tRNA synthetase



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 45.75 – 2.05	Depositor EDS
% Data completeness (in resolution range)	89.0 (14.97-2.10) 89.5 (45.75-2.05)	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 0.191 , 0.242	Depositor DCC
R_{free} test set	10356 reflections (10.01%)	DCC
Wilson B-factor (Å ²)	22.7	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.025 for k,h,-l 0.023 for -k,-h,-l 0.486 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 110887 reflections	Xtriage
F_o, F_c correlation	0.95	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.*

¹ Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.96	0/4035	1.30	32/5433 (0.6%)
1	B	0.99	0/4035	1.42	39/5433 (0.7%)
1	C	0.99	2/4035 (0.0%)	1.48	36/5433 (0.7%)
1	D	0.98	3/4035 (0.1%)	1.37	38/5433 (0.7%)
All	All	0.98	5/16140 (0.0%)	1.39	145/21732 (0.7%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	59	VAL	CB-CG1	5.62	1.64	1.52
1	C	370	GLU	CB-CG	-5.50	1.41	1.52
1	D	378	PHE	CD2-CE2	5.24	1.49	1.39
1	C	369	VAL	CB-CG1	-5.10	1.42	1.52
1	D	449	ASP	CB-CG	-5.08	1.41	1.51

All (145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	185	ARG	NE-CZ-NH2	-28.20	106.20	120.30
1	C	185	ARG	NE-CZ-NH1	26.80	133.70	120.30
1	D	236	ARG	NE-CZ-NH1	-25.63	107.49	120.30
1	B	428	ARG	NE-CZ-NH1	-23.14	108.73	120.30
1	D	236	ARG	NE-CZ-NH2	22.95	131.77	120.30
1	B	227	ARG	NE-CZ-NH1	21.53	131.07	120.30
1	D	186	ARG	NE-CZ-NH1	20.94	130.77	120.30
1	B	428	ARG	NE-CZ-NH2	20.54	130.57	120.30
1	B	227	ARG	NE-CZ-NH2	-20.51	110.04	120.30
1	C	410	ARG	NE-CZ-NH2	19.92	130.26	120.30
1	C	470	ARG	NE-CZ-NH2	-18.87	110.86	120.30
1	C	410	ARG	NE-CZ-NH1	-18.64	110.98	120.30
1	B	91	ARG	NE-CZ-NH1	-18.46	111.07	120.30
1	C	333	ARG	NE-CZ-NH1	-18.41	111.10	120.30
1	B	91	ARG	NE-CZ-NH2	17.70	129.15	120.30
1	C	436	ARG	NE-CZ-NH2	-17.52	111.54	120.30
1	A	333	ARG	NE-CZ-NH2	-17.42	111.59	120.30
1	D	186	ARG	NE-CZ-NH2	-16.82	111.89	120.30
1	D	436	ARG	NE-CZ-NH1	-16.67	111.96	120.30
1	C	91	ARG	NE-CZ-NH2	-16.60	112.00	120.30
1	B	69	ARG	NE-CZ-NH1	-16.46	112.07	120.30
1	C	436	ARG	NE-CZ-NH1	16.27	128.44	120.30
1	C	333	ARG	NE-CZ-NH2	16.09	128.35	120.30
1	C	10	ARG	NE-CZ-NH1	-16.09	112.25	120.30
1	A	69	ARG	NE-CZ-NH2	-15.84	112.38	120.30
1	C	10	ARG	NE-CZ-NH2	15.61	128.11	120.30
1	C	91	ARG	NE-CZ-NH1	15.46	128.03	120.30
1	D	436	ARG	NE-CZ-NH2	15.03	127.81	120.30
1	A	491	ARG	NE-CZ-NH1	-14.95	112.83	120.30
1	D	69	ARG	NE-CZ-NH2	-14.88	112.86	120.30
1	B	156	ARG	NE-CZ-NH1	-14.88	112.86	120.30
1	A	13	ARG	NE-CZ-NH2	14.84	127.72	120.30
1	A	69	ARG	NE-CZ-NH1	14.76	127.68	120.30
1	B	491	ARG	NE-CZ-NH2	-14.67	112.97	120.30
1	A	10	ARG	NE-CZ-NH2	-14.57	113.02	120.30
1	C	470	ARG	NE-CZ-NH1	14.56	127.58	120.30
1	B	156	ARG	NE-CZ-NH2	14.48	127.54	120.30
1	A	13	ARG	NE-CZ-NH1	-14.05	113.28	120.30
1	A	491	ARG	NE-CZ-NH2	13.98	127.29	120.30
1	D	491	ARG	NE-CZ-NH1	-13.88	113.36	120.30
1	A	333	ARG	NE-CZ-NH1	13.82	127.21	120.30
1	B	436	ARG	NE-CZ-NH2	-13.75	113.43	120.30
1	D	69	ARG	NE-CZ-NH1	13.54	127.07	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	410	ARG	NE-CZ-NH1	13.24	126.92	120.30
1	C	69	ARG	NE-CZ-NH1	-13.21	113.70	120.30
1	B	436	ARG	NE-CZ-NH1	13.20	126.90	120.30
1	B	491	ARG	NE-CZ-NH1	13.10	126.85	120.30
1	B	236	ARG	NE-CZ-NH1	13.05	126.83	120.30
1	D	156	ARG	NE-CZ-NH2	-13.04	113.78	120.30
1	B	69	ARG	NE-CZ-NH2	12.97	126.78	120.30
1	A	10	ARG	NE-CZ-NH1	12.95	126.77	120.30
1	C	491	ARG	NE-CZ-NH2	-12.93	113.84	120.30
1	D	156	ARG	NE-CZ-NH1	12.91	126.76	120.30
1	D	491	ARG	NE-CZ-NH2	12.80	126.70	120.30
1	A	91	ARG	NE-CZ-NH1	-12.72	113.94	120.30
1	C	13	ARG	NE-CZ-NH1	12.65	126.63	120.30
1	D	158	ARG	NE-CZ-NH1	-12.61	114.00	120.30
1	D	236	ARG	CD-NE-CZ	12.59	141.23	123.60
1	A	470	ARG	NE-CZ-NH1	-12.55	114.02	120.30
1	A	436	ARG	NE-CZ-NH1	-12.42	114.09	120.30
1	C	13	ARG	NE-CZ-NH2	-12.40	114.10	120.30
1	D	158	ARG	NE-CZ-NH2	12.25	126.42	120.30
1	B	158	ARG	NE-CZ-NH2	-12.24	114.18	120.30
1	B	236	ARG	NE-CZ-NH2	-12.03	114.28	120.30
1	C	69	ARG	NE-CZ-NH2	11.99	126.29	120.30
1	B	158	ARG	NE-CZ-NH1	11.72	126.16	120.30
1	C	185	ARG	CD-NE-CZ	11.57	139.80	123.60
1	D	91	ARG	NE-CZ-NH1	11.47	126.03	120.30
1	A	410	ARG	NE-CZ-NH2	-11.31	114.64	120.30
1	A	470	ARG	NE-CZ-NH2	11.31	125.95	120.30
1	C	491	ARG	NE-CZ-NH1	10.95	125.78	120.30
1	D	91	ARG	NE-CZ-NH2	-10.87	114.86	120.30
1	A	436	ARG	NE-CZ-NH2	10.60	125.60	120.30
1	A	91	ARG	NE-CZ-NH2	10.53	125.56	120.30
1	D	227	ARG	NE-CZ-NH1	-9.94	115.33	120.30
1	B	186	ARG	NE-CZ-NH1	-9.22	115.69	120.30
1	D	186	ARG	CD-NE-CZ	9.18	136.45	123.60
1	C	410	ARG	CD-NE-CZ	9.07	136.29	123.60
1	B	428	ARG	CD-NE-CZ	8.95	136.13	123.60
1	B	91	ARG	CD-NE-CZ	8.93	136.10	123.60
1	C	470	ARG	CD-NE-CZ	8.78	135.90	123.60
1	A	333	ARG	CD-NE-CZ	8.66	135.73	123.60
1	B	186	ARG	NE-CZ-NH2	8.40	124.50	120.30
1	D	436	ARG	CD-NE-CZ	8.32	135.25	123.60
1	C	333	ARG	CD-NE-CZ	8.21	135.10	123.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	270	LEU	CA-CB-CG	8.19	134.14	115.30
1	A	410	ARG	CD-NE-CZ	8.11	134.95	123.60
1	B	156	ARG	CD-NE-CZ	7.99	134.78	123.60
1	B	270	LEU	CA-CB-CG	7.97	133.62	115.30
1	D	236	ARG	CG-CD-NE	-7.93	95.14	111.80
1	B	428	ARG	CG-CD-NE	-7.93	95.15	111.80
1	D	93	ASP	CB-CG-OD2	-7.79	111.29	118.30
1	C	10	ARG	CD-NE-CZ	7.73	134.42	123.60
1	B	93	ASP	CB-CG-OD2	-7.60	111.46	118.30
1	C	436	ARG	CD-NE-CZ	7.54	134.15	123.60
1	A	13	ARG	CD-NE-CZ	7.46	134.05	123.60
1	D	428	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	B	491	ARG	CD-NE-CZ	7.45	134.03	123.60
1	A	10	ARG	CD-NE-CZ	7.36	133.90	123.60
1	A	491	ARG	CD-NE-CZ	7.35	133.90	123.60
1	C	91	ARG	CD-NE-CZ	7.29	133.81	123.60
1	A	69	ARG	CD-NE-CZ	7.26	133.77	123.60
1	D	156	ARG	CD-NE-CZ	7.15	133.61	123.60
1	D	417	THR	N-CA-C	-6.98	92.14	111.00
1	B	69	ARG	CD-NE-CZ	6.94	133.32	123.60
1	B	186	ARG	CD-NE-CZ	6.87	133.22	123.60
1	B	236	ARG	CD-NE-CZ	6.87	133.22	123.60
1	D	491	ARG	CD-NE-CZ	6.75	133.06	123.60
1	C	491	ARG	CD-NE-CZ	6.75	133.05	123.60
1	B	436	ARG	CD-NE-CZ	6.74	133.03	123.60
1	C	69	ARG	CD-NE-CZ	6.72	133.01	123.60
1	D	91	ARG	CD-NE-CZ	6.71	133.00	123.60
1	B	158	ARG	CD-NE-CZ	6.53	132.75	123.60
1	B	417	THR	N-CA-C	-6.48	93.51	111.00
1	A	91	ARG	CD-NE-CZ	6.28	132.39	123.60
1	D	158	ARG	CD-NE-CZ	6.13	132.18	123.60
1	D	69	ARG	CD-NE-CZ	6.05	132.06	123.60
1	D	449	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	C	13	ARG	CD-NE-CZ	6.03	132.04	123.60
1	B	227	ARG	CD-NE-CZ	5.96	131.95	123.60
1	A	185	ARG	NE-CZ-NH1	-5.95	117.33	120.30
1	A	186	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	C	185	ARG	CG-CD-NE	-5.87	99.47	111.80
1	A	333	ARG	CG-CD-NE	-5.71	99.80	111.80
1	B	227	ARG	CG-CD-NE	5.70	123.76	111.80
1	D	278	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	B	402	ARG	NE-CZ-NH2	-5.62	117.49	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	81	ASP	CB-CG-OD1	5.54	123.29	118.30
1	A	185	ARG	NE-CZ-NH2	5.50	123.05	120.30
1	A	436	ARG	CD-NE-CZ	5.48	131.27	123.60
1	B	81	ASP	CB-CG-OD1	5.47	123.22	118.30
1	D	12	ARG	NE-CZ-NH2	5.44	123.02	120.30
1	D	428	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	B	160	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	D	398	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	D	398	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	C	186	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	C	424	ASP	CB-CG-OD2	5.16	122.94	118.30
1	C	330	ASP	CB-CG-OD2	5.16	122.94	118.30
1	D	243	GLU	N-CA-C	5.12	124.83	111.00
1	B	227	ARG	CB-CG-CD	5.09	124.83	111.60
1	C	417	THR	N-CA-C	-5.09	97.26	111.00
1	A	417	THR	N-CA-C	-5.05	97.35	111.00
1	A	424	ASP	CB-CG-OD2	5.03	122.83	118.30
1	C	115	ARG	N-CA-C	-5.02	97.46	111.00

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 ⓘ

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	87	0
1	B	3956	0	3921	107	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3956	0	3921	85	0
1	D	3956	0	3921	101	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
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	369	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 (369) 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:NH1	1:B:10:ARG:HB2	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:CB	1:B:10:ARG:HH11	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:H	1:C:122:LYS:HD2	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH21	1:D:260:ARG:HB3	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:HH11	1:B:10:ARG:HB2	0.71	0.85
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:HH21	1:A:260:ARG:HG2	1.45	0.79
1:B:71:MET:HG2	1:B:74:ALA:O	1.83	0.79
1:D:10:ARG:HH11	1:D:10:ARG:HB2	0.71	0.79
1:B:414:ASN:HD22	3:B:2003:KAA:HN8	1.29	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:D:153:ILE:HA	1:D:156:ARG:HH21	1.49	0.78
1:A:414:ASN:HD22	3:A:2002:KAA:HN8	1.31	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:HG2	1:C:260:ARG:HH21	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: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:CZ	1:D:211:ARG:HB2	2.20	0.71
1:A:70:GLY:HA3	1:A:104:LYS:HZ2	1.55	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:GLY:HA3	1:C:104:LYS:HZ2	1.54	0.71
1:B:157:TYR:OH	1:B:483:ASP:OD2	2.08	0.71
1:B:260:ARG:NH2	1:B:260:ARG:HB3	2.06	0.71
1:B:214:ILE:N	1:B:214:ILE:HD13	2.07	0.70
1:D:214:ILE:HD13	1:D:214:ILE:N	2.06	0.70
1:B:260:ARG:CB	1:B:260:ARG:HH21	2.04	0.69
1:D:257:ILE:HG22	1:D:263:PRO:HD3	1.72	0.69
1:D:260:ARG:NH2	1:D:260:ARG:HB3	2.08	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: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:CB	1:D:260:ARG:HH21	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:H	1:C:153:ILE:HD12	1.61	0.66
1:B:444:HIS:HD2	4:B:753:HOH:O	1.78	0.66
1:A:71:MET:HE2	1:A:71:MET:HA	1.78	0.66
1:B:69:ARG:HH12	1:B:87:GLN:HE21	1.42	0.66
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: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:B:213:PHE:C	1:B:214:ILE:HD13	2.17	0.64
1:B:19:ILE:O	1:B:19:ILE:HD12	1.97	0.64
1:B:22:LEU:HD13	1:B:102:LEU:CD1	2.27	0.63
1:D:144:PRO:HG2	1:D:166:MET:SD	2.37	0.63
1:D:16:LEU:HD12	1:D:140:LEU:HD21	1.79	0.63
1:C:260:ARG:NH2	1:C:260:ARG:HG2	2.13	0.63
1:D:22:LEU:HD13	1:D:102:LEU:CD1	2.28	0.63

Continued on next page...

Continued from previous page...

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:B:16:LEU:HD12	1:B:140:LEU:HD21	1.79	0.62
1:B:165:ILE:HG22	1:B:166:MET:HE3	1.80	0.62
1:D:236:ARG:HD3	4:D:851:HOH:O	1.99	0.62
1:C:98:GLN:NE2	1:C:98:GLN:H	1.98	0.62
1:D:157:TYR:OH	1:D:483:ASP:OD2	2.15	0.62
1:D:19:ILE:O	1:D:19:ILE:HD12	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:D:213:PHE:C	1:D:214:ILE:HD13	2.21	0.60
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:8:GLN:C	1:A:8:GLN:NE2	2.54	0.60
1:A:146:LYS:H	1:A:146:LYS:CD	2.13	0.60
1:C:146:LYS:CD	1:C:146:LYS:H	2.13	0.60
1:B:195:GLU:HB2	1:B:246:TYR:CZ	2.36	0.60
1:B:70:GLY:O	1:B:71:MET:CB	2.50	0.59
1:A:428:ARG:HD2	4:A:722:HOH:O	2.00	0.59
1:C:8:GLN:C	1:C:8:GLN:NE2	2.55	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:HG2	1:A:260:ARG:NH2	2.13	0.58
1:B:212:PRO:HG2	1:B:214:ILE:HD11	1.84	0.58
1:D:16:LEU:HD23	1:D:16:LEU:C	2.23	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:D:444:HIS:HD2	4:D:831:HOH:O	1.85	0.58
1:B:206:GLY:HA3	4:B:924:HOH:O	2.04	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:B:15:LYS:HD2	1:B:105:ILE:CG2	2.32	0.57
1:B:16:LEU:C	1:B:16:LEU:HD23	2.24	0.57
1:D:212:PRO:HG2	1:D:214:ILE:HD11	1.85	0.57
1:A:260:ARG:CG	1:A:260:ARG:HH21	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:B:212:PRO:HG2	1:B:214:ILE:CD1	2.36	0.56
1:B:10:ARG:HG3	1:B:11:VAL:N	2.20	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:ARG:HG3	1:D:11:VAL:N	2.21	0.56
1:C:153:ILE:CD1	1:C:153:ILE:H	2.18	0.56
1:C:122:LYS:CD	1:C:122:LYS:N	2.40	0.55
1:D:257:ILE:CG2	1:D:263:PRO:HD3	2.36	0.55
1:C:146:LYS:H	1:C:146:LYS:HD2	1.71	0.55
1:C:146:LYS:NZ	1:C:166:MET:HG2	2.20	0.55
1:A:251:VAL:HG22	1:A:265:PHE:CE1	2.41	0.55
1:D:69:ARG:HH12	1:D:87:GLN:NE2	2.04	0.55
1:B:227:ARG:HG2	1:B:227:ARG:O	2.06	0.55
1:A:171:LYS:NZ	4:A:815:HOH:O	2.39	0.55
1:A:434:LYS:O	1:A:437:GLU:HB2	2.07	0.55
1:C:231:GLU:CD	3:C:2004:KAA:HNZ1	2.10	0.54
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
4:C:590:HOH:O	1:D:182:GLN:HG2	2.08	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: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:CG	1:A:260:ARG:NH2	2.71	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:16:LEU:HD23	1:A:16:LEU:C	2.30	0.53
1:A:13:ARG:HG2	4:A:962:HOH:O	2.09	0.52
1:A:122:LYS:CD	1:A:122:LYS:N	2.41	0.52
1:A:146:LYS:NZ	1:A:166:MET:HG2	2.24	0.52
1:D:15:LYS:HD3	1:D:105:ILE:HG23	1.90	0.52
1:C:444:HIS:HD2	4:C:681:HOH:O	1.90	0.52
1:C:260:ARG:NH2	1:C:260:ARG:CG	2.72	0.52
1:C:100:TYR:CZ	1:C:104:LYS:HE2	2.44	0.52
1:B:444:HIS:CD2	4:B:753:HOH:O	2.58	0.52
1:A:51:GLU:O	1:A:54:GLU:HB3	2.10	0.52
1:D:165:ILE:HG22	1:D:166:MET:HE3	1.90	0.52
1:C:146:LYS:N	1:C:146:LYS:HD2	2.25	0.52
1:C:217:HIS:CE1	1:C:219:ALA:HB3	2.44	0.52
1:C:51:GLU:O	1:C:54:GLU:HB3	2.10	0.52
1:D:19:ILE:HD12	1:D:24:VAL:HB	1.91	0.52
1:A:146:LYS:HD2	1:A:146:LYS:H	1.73	0.52
1:A:293:THR:O	1:A:297:GLY:HA2	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:491:ARG:O	1:D:492:HIS:C	2.48	0.51
1:A:418:GLU:OE1	1:A:463:GLY:HA3	2.09	0.51
1:A:217:HIS:CE1	1:A:219:ALA:HB3	2.45	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:153:ILE:H	1:A:153:ILE:CD1	2.18	0.51
1:A:140:LEU:HD12	1:B:422:PRO:HG2	1.93	0.51
1:D:4:GLU:OE1	1:D:5:LEU:N	2.44	0.50
1:B:4:GLU:OE1	1:B: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:B:69:ARG:HH12	1:B:87:GLN:HE22	1.53	0.50
1:A:231:GLU:CD	3:A:2002:KAA:HNZ1	2.15	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:C:354:HIS:HB2	1:C:438:GLN:HE21	1.78	0.49
1:C:57:ILE:O	1:C:117:THR:HA	2.12	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:C:444:HIS:CD2	4:C:681:HOH:O	2.65	0.49
1:C:293:THR:O	1:C:297:GLY:HA2	2.13	0.49
1:D:231:GLU:CD	3:D:2005:KAA:HNZ1	2.16	0.49
1:D:19:ILE:CD1	1:D:24:VAL:HB	2.43	0.49
1:B:155:GLN:HA	1:B:155:GLN:OE1	2.13	0.49
1:C:235:LYS:NZ	1:C:418:GLU:OE2	2.43	0.49
1:B:19:ILE:HD12	1:B:19:ILE:C	2.33	0.49
1:D:292:ALA:O	1:D:296:LEU:HB2	2.13	0.49
1:A:333:ARG:HD3	4:A:741:HOH:O	2.12	0.49
1:C:251:VAL:HG22	1:C:265:PHE:CZ	2.48	0.48
1:A:444:HIS:HD2	4:A:947:HOH:O	1.95	0.48
1:B:19:ILE:HD12	1:B:24:VAL:HB	1.94	0.48
1:D:153:ILE:CA	1:D:156:ARG:HH21	2.24	0.48
1:C:491:ARG:O	1:C:492:HIS:O	2.31	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:C:199:PRO:CG	1:D:487:PHE:HB2	2.44	0.48
1:A:57:ILE:O	1:A:117:THR:HA	2.14	0.48
1:A:260:ARG:NH2	1:A:410:ARG:NH2	2.53	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:421:ASP:C	1:C:421:ASP:OD1	2.51	0.48
1:B:362:ASN:CG	1:B:386:ILE:HD13	2.35	0.48
1:B:292:ALA:O	1:B:296:LEU:HB2	2.14	0.47
1:B:82:VAL:O	1:B:171:LYS:HE3	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:C:71:MET:CE	1:C:71:MET:HA	2.44	0.47
1:A:141:ARG:NH2	1:B:455:GLU:OE2	2.46	0.47
1:B:491:ARG:O	1:B:492:HIS:C	2.53	0.47
1:B:153:ILE:CA	1:B:156:ARG:HH21	2.15	0.47
1:A:5:LEU:O	1:A:8:GLN:HG3	2.15	0.47
1:D:71:MET:O	1:D:71:MET:CG	2.61	0.47
1:C:482:ARG:HG2	1:C:482:ARG:NH1	2.29	0.47
1:A:71:MET:CE	1:A:71:MET:HA	2.45	0.47
1:D:69:ARG:HH12	1:D:87:GLN:HE21	1.62	0.47
1:C:428:ARG:HD2	4:C:771:HOH:O	2.15	0.47
1:C:16:LEU:C	1:C:16:LEU:HD23	2.35	0.47
1:D:6:ASN:OD1	1:D:6:ASN:N	2.43	0.47
1:B:38:GLU:HB2	1:B:83:THR:CB	2.39	0.47
1:B:153:ILE:HG13	1:B:154:GLU:N	2.30	0.47
1:A:143:LEU:HD21	1:A:165:ILE:HG21	1.97	0.47
1:B:436:ARG:NH2	1:B:443:ALA:O	2.48	0.46
1:D:155:GLN:OE1	1:D:155:GLN:HA	2.15	0.46
1:C:381:GLY:O	1:C:399:PHE:HB3	2.15	0.46
1:A:421:ASP:C	1:A:421:ASP:OD1	2.53	0.46
1:C:158:ARG:HG2	1:C:158:ARG:HH11	1.79	0.46
1:A:78:HIS:HE1	1:A:125:GLU:OE1	1.97	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
1:D:450:PHE:O	1:D:453:ALA:HB3	2.15	0.46
1:C:5:LEU:O	1:C:8:GLN:HG3	2.16	0.46
1:B:257:ILE:CG2	1:B:263:PRO:HD3	2.43	0.46
1:D:16:LEU:HD23	1:D:16:LEU:O	2.16	0.45
1:C:146:LYS:HZ3	1:C:166:MET:HG2	1.79	0.45
1:B:6:ASN:OD1	1:B:6:ASN:N	2.45	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:257:ILE:HG12	1:D:257:ILE:H	1.59	0.45
1:D:195:GLU:HB2	1:D:246:TYR:CE2	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:MET:O	1:B:71:MET:CG	2.63	0.45
1:B:373:LEU:HD21	1:B:379:ILE:HD11	1.97	0.45
1:D:37:ALA:O	1:D:41:PHE:HD1	2.00	0.45
1:D:19:ILE:C	1:D:19:ILE:HD12	2.37	0.45
1:B:156:ARG:HB3	1:B:163:ASP:HB2	1.98	0.45
1:D:214:ILE:HD12	1:D:225:TYR:CD2	2.52	0.44
1:B:358:GLY:HA3	1:B:385:GLU:OE2	2.18	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:B:195:GLU:HB2	1:B:246:TYR:CE2	2.51	0.44
1:A:381:GLY:O	1:A:399:PHE:HB3	2.17	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:362:ASN:CG	1:D:386:ILE:HD13	2.38	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:A:146:LYS:HZ3	1:A:166:MET:HG2	1.82	0.44
1:C:366:GLU:HG2	1:C:370:GLU:OE2	2.17	0.44
1:B:164:LEU:HA	1:B:164:LEU:HD23	1.86	0.44
1:B:231:GLU:CD	3:B:2003:KAA:HNZ1	2.21	0.44
1:B:217:HIS:HE1	1:B:219:ALA:HB3	1.82	0.44
1:A:158:ARG:HG2	1:A:158:ARG:HH11	1.83	0.44
1:B:19:ILE:CD1	1:B:24:VAL:HB	2.48	0.43
1:A:403:PHE:CD1	1:A:403:PHE:C	2.92	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:A:285:GLU:HA	1:A:314:TRP:CH2	2.52	0.43
1:D:153:ILE:HG13	1:D:154:GLU:N	2.33	0.43
1:C:100:TYR:OH	1:C:104:LYS:HE2	2.19	0.43
1:B:357:PHE:O	1:B:361:VAL:HG23	2.18	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:A:222:MET:HE2	1:A:224:LEU:HD21	2.00	0.43
1:D:370:GLU:HA	1:D:373:LEU:HD22	1.99	0.43
1:B:155:GLN:CA	1:B:155:GLN:OE1	2.67	0.43
1:C:78:HIS:NE2	1:C:87:GLN:HB2	2.34	0.43
1:B:78:HIS:HE1	1:B:125:GLU:OE2	2.01	0.43
1:B:102:LEU:HA	1:B:102:LEU:HD12	1.88	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:TYR:CD2	1:C:244:LYS:HB3	2.54	0.42
1:C:403:PHE:CD1	1:C:403:PHE:C	2.93	0.42
1:A:260:ARG:HH22	1:A:410:ARG:CZ	2.31	0.42
1:B:15:LYS:HD3	1:B:105:ILE:HG23	1.96	0.42
1:C:423:ILE:HD13	1:D:13:ARG:NH2	2.34	0.42
1:A:444:HIS:CD2	4:A:947:HOH:O	2.71	0.42
1:B:115:ARG:HB2	1:B:132:SER:HB3	2.00	0.42
1:D:160:ARG:HA	1:D:160:ARG:HD3	1.83	0.42
1:D:33:ARG:HD3	1:D:62:ALA:HB3	2.00	0.42
1:C:438:GLN:HE21	1:C:438:GLN:HB2	1.60	0.42
1:C:237:LEU:O	1:C:242:LEU:HB2	2.20	0.42
1:A:146:LYS:CD	1:A:146:LYS:N	2.82	0.42
1:C:185:ARG:NH2	1:D:195:GLU:OE1	2.47	0.42
1:C:146:LYS:N	1:C:146:LYS:CD	2.82	0.42
1:B:160:ARG:HA	1:B:160:ARG:HD3	1.82	0.42
1:C:351:VAL:O	1:C:351:VAL:HG23	2.20	0.42
1:A:220:LEU:O	1:A:221:ASP:C	2.57	0.42
1:C:79:ILE:O	1:C:85:GLN:HA	2.20	0.42
1:C:185:ARG:HH22	1:D:195:GLU:CD	2.22	0.42
1:C:220:LEU:O	1:C:221:ASP:C	2.57	0.42
1:C:222:MET:HE2	1:C:224:LEU:HD21	2.01	0.42
1:C:104:LYS:HA	1:C:104:LYS:HD3	1.83	0.42
1:A:8:GLN:C	1:A:8:GLN:HE21	2.23	0.42
1:B:16:LEU:HD23	1:B:16:LEU:O	2.19	0.42
1:A:16:LEU:C	1:A:16:LEU:CD2	2.88	0.42
1:B:17:LYS:O	1:B:21:GLU:HG3	2.20	0.42
1:B:327:VAL:HG12	1:B:329:VAL:HG23	2.01	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:C:100:TYR:CE2	1:C:104:LYS:HE2	2.55	0.41
1:D:214:ILE:N	1:D:214:ILE:CD1	2.79	0.41
1:A:451:LEU:O	1:A:455:GLU:HG3	2.20	0.41
1:D:17:LYS:O	1:D:21:GLU:HG3	2.21	0.41
1:B:69:ARG:NH1	1:B:87:GLN:HE21	2.15	0.41
1:A:233:HIS:HD2	4:A:804:HOH:O	2.02	0.41
1:D:407:ILE:O	1:D:408:VAL:CG2	2.68	0.41
1:D:156:ARG:CZ	1:D:156:ARG:HB2	2.51	0.41
1:C:143:LEU:HD12	1:C:143:LEU:HA	1.82	0.41
1:A:242:LEU:HA	1:A:242:LEU:HD12	1.95	0.41
1:D:260:ARG:NH2	1:D:410:ARG:HE	2.18	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:TYR:CE2	1:A:104:LYS:HE2	2.55	0.41
1:A:143:LEU:HD12	1:A:143:LEU:HA	1.81	0.41
1:B:156:ARG:CZ	1:B:156:ARG:HB2	2.49	0.41
1:D:155:GLN:CA	1:D:155:GLN:OE1	2.69	0.41
1:C:91:ARG:HG3	1:C:94:ASP:OD1	2.21	0.41
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:A:193:TYR:CD2	1:A:244:LYS:HB3	2.57	0.40
1:D:80:GLN:HB2	1:D:85:GLN:HG2	2.03	0.40
1:C:71:MET:H	1:C:104:LYS:HZ2	1.69	0.40
1:C:8:GLN:C	1:C:8:GLN:HE21	2.25	0.40
1:A:482:ARG:HG2	1:A:482:ARG:NH1	2.36	0.40
1:A:104:LYS:HA	1:A:104:LYS:HD3	1.85	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: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:B:211:ARG:NH2	1:B:211:ARG:HB2	2.35	0.40
1:B:478:SER:HB3	1:B:483:ASP:HB2	2.02	0.40
1:A:438:GLN:HB2	1:A:438:GLN:HE21	1.60	0.40
1:B:270:LEU:C	1:B:270:LEU:HD12	2.42	0.40
1:D:18:LYS:HB2	1:D:18:LYS:NZ	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	480/493 (97%)	465 (97%)	13 (3%)	2 (0%)	39	37
1	B	480/493 (97%)	461 (96%)	16 (3%)	3 (1%)	30	24
1	C	480/493 (97%)	464 (97%)	14 (3%)	2 (0%)	39	37

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	480/493 (97%)	461 (96%)	17 (4%)	2 (0%)	39	37
All	All	1920/1972 (97%)	1851 (96%)	60 (3%)	9 (0%)	34	30

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%)	394 (93%)	31 (7%)	17	13
1	B	425/433 (98%)	384 (90%)	41 (10%)	10	6
1	C	425/433 (98%)	393 (92%)	32 (8%)	17	13
1	D	425/433 (98%)	388 (91%)	37 (9%)	13	8
All	All	1700/1732 (98%)	1559 (92%)	141 (8%)	14	9

All (141) 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	40	LEU
1	A	46	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	69	ARG
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	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	260	ARG
1	A	268	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	444	HIS
1	A	445	GLU
1	B	4	GLU
1	B	6	ASN
1	B	10	ARG
1	B	13	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	69	ARG
1	B	71	MET
1	B	91	ARG
1	B	93	ASP
1	B	102	LEU
1	B	145	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	154	GLU
1	B	158	ARG
1	B	166	MET
1	B	171	LYS
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	277	PHE
1	B	282	LYS
1	B	296	LEU
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
1	C	7	ASP
1	C	8	GLN
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	119	PHE
1	C	122	LYS
1	C	146	LYS
1	C	153	ILE
1	C	155	GLN
1	C	158	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	171	LYS
1	C	188	LEU
1	C	242	LEU
1	C	260	ARG
1	C	268	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	444	HIS
1	C	445	GLU
1	C	470	ARG
1	D	4	GLU
1	D	6	ASN
1	D	10	ARG
1	D	18	LYS
1	D	19	ILE
1	D	22	LEU
1	D	39	GLU
1	D	40	LEU
1	D	47	LEU
1	D	71	MET
1	D	93	ASP
1	D	102	LEU
1	D	145	GLU
1	D	154	GLU
1	D	158	ARG
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	296	LEU
1	D	371	ASP
1	D	372	LYS
1	D	373	LEU
1	D	383	PRO
1	D	416	PHE
1	D	436	ARG
1	D	445	GLU
1	D	449	ASP
1	D	474	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	78	HIS
1	A	98	GLN
1	A	159	GLN
1	A	216	HIS
1	A	218	ASN
1	A	233	HIS
1	A	286	ASN
1	A	354	HIS
1	A	427	GLN
1	A	438	GLN
1	A	444	HIS
1	B	55	GLN
1	B	78	HIS
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	C	55	GLN
1	C	78	HIS
1	C	98	GLN
1	C	159	GLN
1	C	216	HIS
1	C	218	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	233	HIS
1	C	286	ASN
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	233	HIS
1	D	286	ASN
1	D	414	ASN
1	D	438	GLN
1	D	444	HIS
1	D	489	GLN

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 carbohydrates 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	A	2002	-	27,34,34	2.66	4 (14%)	32,49,49	2.73	6 (18%)
3	KAA	B	2003	-	27,34,34	2.65	3 (11%)	32,49,49	2.67	6 (18%)
3	KAA	C	2004	-	27,34,34	2.61	4 (14%)	32,49,49	2.57	6 (18%)
3	KAA	D	2005	-	27,34,34	2.64	4 (14%)	32,49,49	2.54	5 (15%)

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	A	2002	-	-	0/18/40/40	0/3/3/3
3	KAA	B	2003	-	-	0/18/40/40	0/3/3/3
3	KAA	C	2004	-	-	0/18/40/40	0/3/3/3
3	KAA	D	2005	-	-	0/18/40/40	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2005	KAA	C-N8	-2.88	1.33	1.37
3	B	2003	KAA	C-N8	-2.85	1.33	1.37
3	C	2004	KAA	C-N8	-2.82	1.33	1.37
3	A	2002	KAA	C-N8	-2.79	1.33	1.37
3	D	2005	KAA	O4'-C1'	2.05	1.43	1.41
3	A	2002	KAA	O4'-C1'	2.51	1.44	1.41
3	C	2004	KAA	O4'-C1'	2.59	1.44	1.41
3	C	2004	KAA	O2S-S1	9.01	1.50	1.42
3	C	2004	KAA	O1S-S1	9.02	1.50	1.42
3	B	2003	KAA	O1S-S1	9.06	1.50	1.42
3	D	2005	KAA	O1S-S1	9.12	1.50	1.42
3	A	2002	KAA	O2S-S1	9.19	1.50	1.42
3	A	2002	KAA	O1S-S1	9.21	1.50	1.42
3	D	2005	KAA	O2S-S1	9.24	1.50	1.42
3	B	2003	KAA	O2S-S1	9.45	1.50	1.42

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2002	KAA	N3-C2-N1	-10.84	120.59	128.89
3	D	2005	KAA	N3-C2-N1	-10.35	120.97	128.89
3	B	2003	KAA	N3-C2-N1	-10.28	121.02	128.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2004	KAA	N3-C2-N1	-10.20	121.08	128.89
3	B	2003	KAA	O2S-S1-O1S	-8.57	110.50	120.77
3	A	2002	KAA	O2S-S1-O1S	-8.42	110.68	120.77
3	C	2004	KAA	O2S-S1-O1S	-7.88	111.33	120.77
3	D	2005	KAA	O2S-S1-O1S	-7.37	111.94	120.77
3	B	2003	KAA	C4-C5-N7	-2.67	107.02	109.48
3	B	2003	KAA	C1'-N9-C4	-2.53	123.12	126.94
3	A	2002	KAA	C4-C5-N7	-2.39	107.28	109.48
3	A	2002	KAA	C-N8-S1	-2.37	120.73	124.05
3	C	2004	KAA	C4-C5-N7	-2.26	107.40	109.48
3	C	2004	KAA	C-N8-S1	-2.12	121.08	124.05
3	D	2005	KAA	C4-C5-N7	-2.12	107.53	109.48
3	C	2004	KAA	O2S-S1-N8	2.08	111.27	108.50
3	A	2002	KAA	O2S-S1-N8	2.13	111.33	108.50
3	D	2005	KAA	O5'-S1-O2S	2.14	112.31	105.66
3	B	2003	KAA	O5'-S1-O2S	2.22	112.56	105.66
3	B	2003	KAA	O5'-C5'-C4'	3.03	113.74	107.90
3	C	2004	KAA	O5'-C5'-C4'	3.05	113.77	107.90
3	D	2005	KAA	O5'-C5'-C4'	3.55	114.72	107.90
3	A	2002	KAA	O5'-C5'-C4'	3.78	115.18	107.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	484/493 (98%)	-0.69	3 (0%) 90 92	12, 22, 45, 72	0
1	B	484/493 (98%)	-0.62	5 (1%) 84 87	14, 23, 52, 75	0
1	C	484/493 (98%)	-0.68	3 (0%) 90 92	12, 22, 45, 72	0
1	D	484/493 (98%)	-0.62	7 (1%) 78 82	13, 23, 51, 74	0
All	All	1936/1972 (98%)	-0.65	18 (0%) 85 88	12, 22, 49, 75	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	153	ILE	5.7
1	B	153	ILE	4.6
1	C	71	MET	3.9
1	A	71	MET	3.8
1	D	492	HIS	3.3
1	B	492	HIS	3.2
1	C	5	LEU	3.1
1	D	146	LYS	3.0
1	D	5	LEU	2.7
1	B	4	GLU	2.6
1	D	4	GLU	2.6
1	D	152	ASP	2.6
1	C	146	LYS	2.5
1	A	4	GLU	2.3
1	D	154	GLU	2.2
1	B	5	LEU	2.2
1	A	5	LEU	2.1
1	B	146	LYS	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	KAA	D	2005	32/32	0.98	0.09	0.85	10,18,22,25	0
3	KAA	B	2003	32/32	0.98	0.08	0.32	7,17,25,26	0
3	KAA	C	2004	32/32	0.98	0.08	0.24	10,15,20,24	0
3	KAA	A	2002	32/32	0.98	0.07	0.14	9,17,21,25	0
2	MG	C	2003	1/1	0.90	0.18	-	45,45,45,45	0
2	MG	A	2001	1/1	0.95	0.13	-	40,40,40,40	0
2	MG	D	2004	1/1	0.98	0.09	-	31,31,31,31	0
2	MG	B	2002	1/1	0.98	0.10	-	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.