Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:55 PM GMT

PDB ID	:	1HTT
Title	:	HISTIDYL-TRNA SYNTHETASE
Authors	:	Arnez, J.G.; Harris, D.C.; Mitschler, A.; Rees, B.; Francklyn, C.S.; Moras, D.
Deposited on	:	1996-03-09
Resolution	:	2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

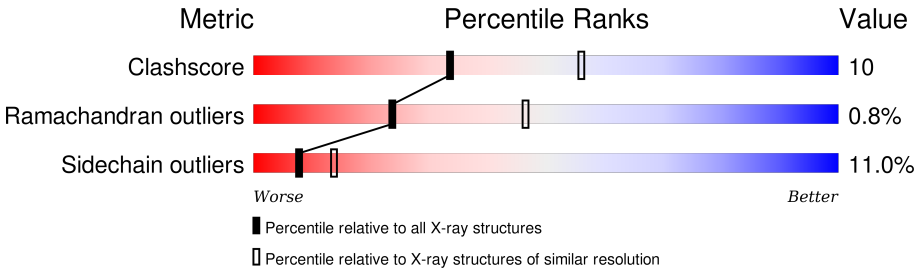
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	423	58% 24% • • 13%
1	B	423	53% 24% 5% • 16%
1	C	423	58% 23% • • 13%
1	D	423	60% 19% • • 16%

2 Entry composition

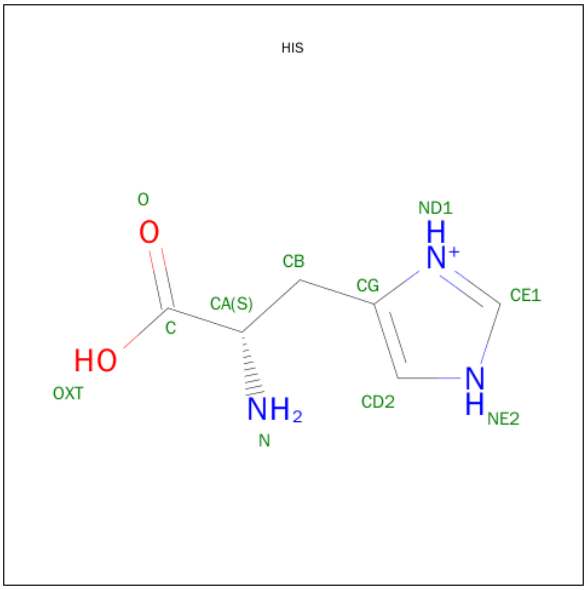
There are 4 unique types of molecules in this entry. The entry contains 11543 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HISTIDYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2848	1790	512	535	11			
1	B	357	Total	C	N	O	S	0	0	0
			2779	1748	499	521	11			
1	C	366	Total	C	N	O	S	0	0	0
			2848	1790	512	535	11			
1	D	357	Total	C	N	O	S	0	0	0
			2779	1748	499	521	11			

- Molecule 2 is HISTIDINE (three-letter code: HIS) (formula: $C_6H_{10}N_3O_2$).



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

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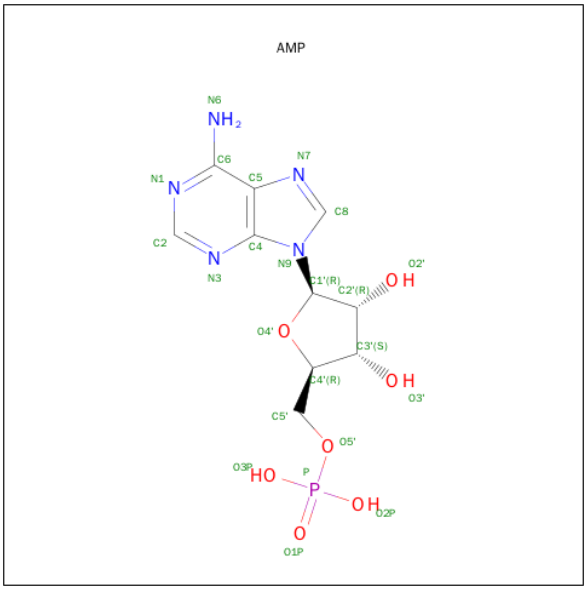
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C N O 10 6 3 1	0	0
2	D	1	Total C N O 10 6 3 1	0	0

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 23 10 5 7 1	0	0
3	B	1	Total C N O P 23 10 5 7 1	0	0
3	C	1	Total C N O P 23 10 5 7 1	0	0
3	D	1	Total C N O P 23 10 5 7 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	49	Total O 49 49	0	0
4	B	41	Total O 41 41	0	0
4	C	38	Total O 38 38	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	29	Total O 29 29	0	0

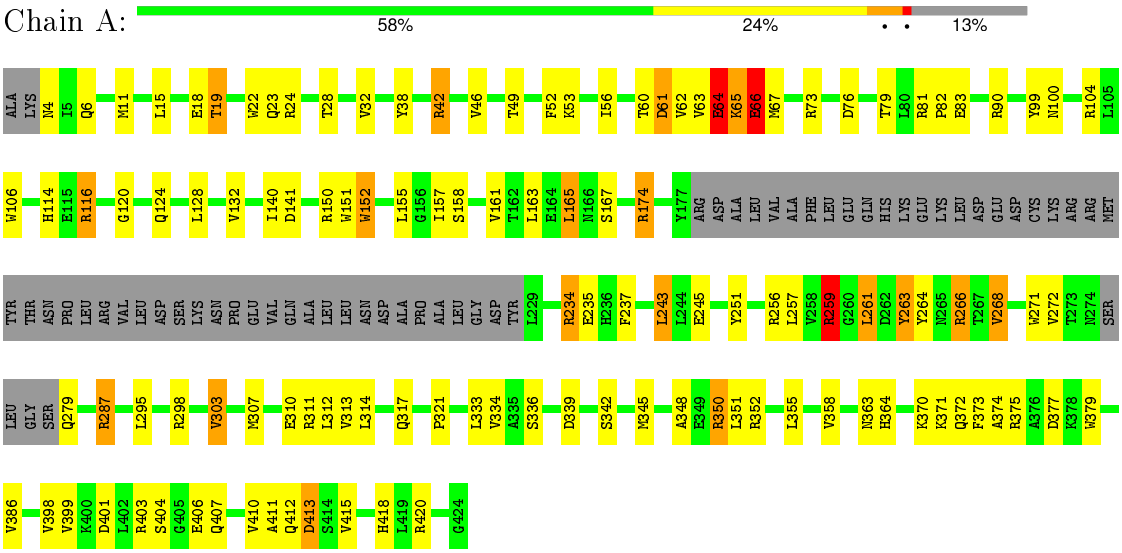
3 Residue-property plots (i)

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.

Note EDS was not executed.

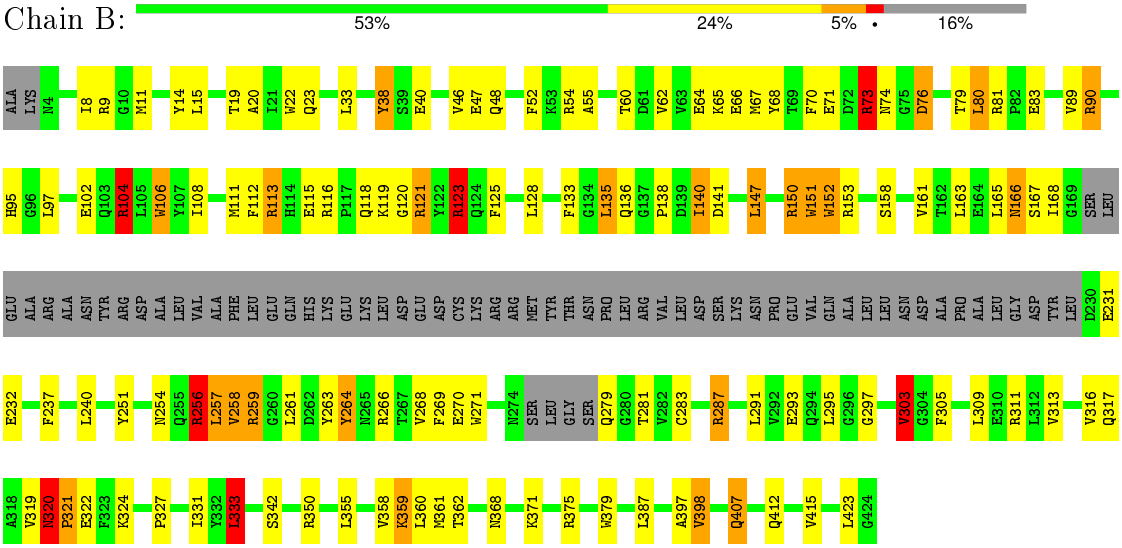
- Molecule 1: HISTIDYL-TRNA SYNTHETASE

Chain A:



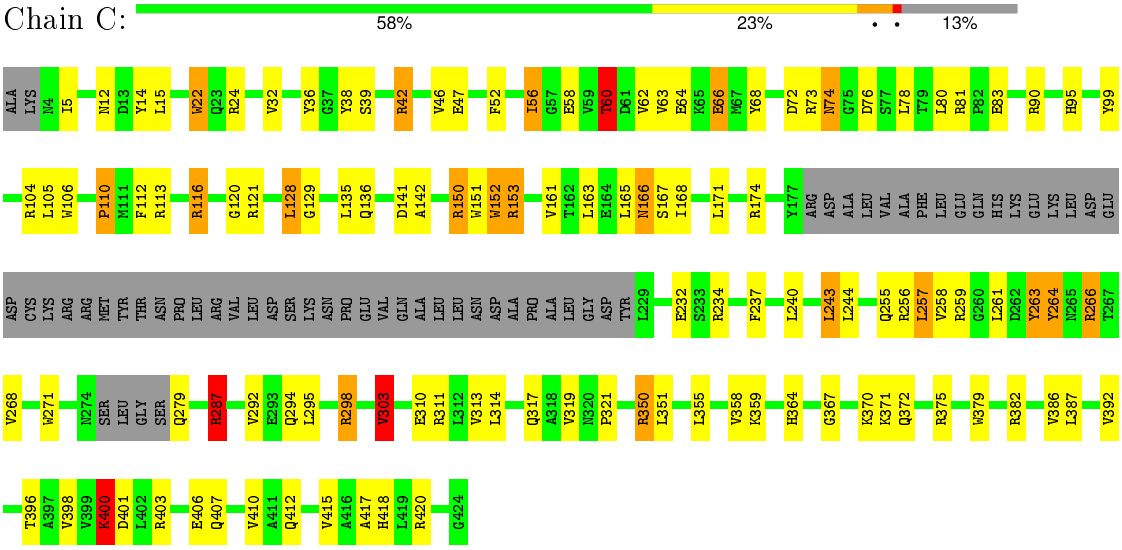
- Molecule 1: HISTIDYL-TRNA SYNTHETASE

Chain B:



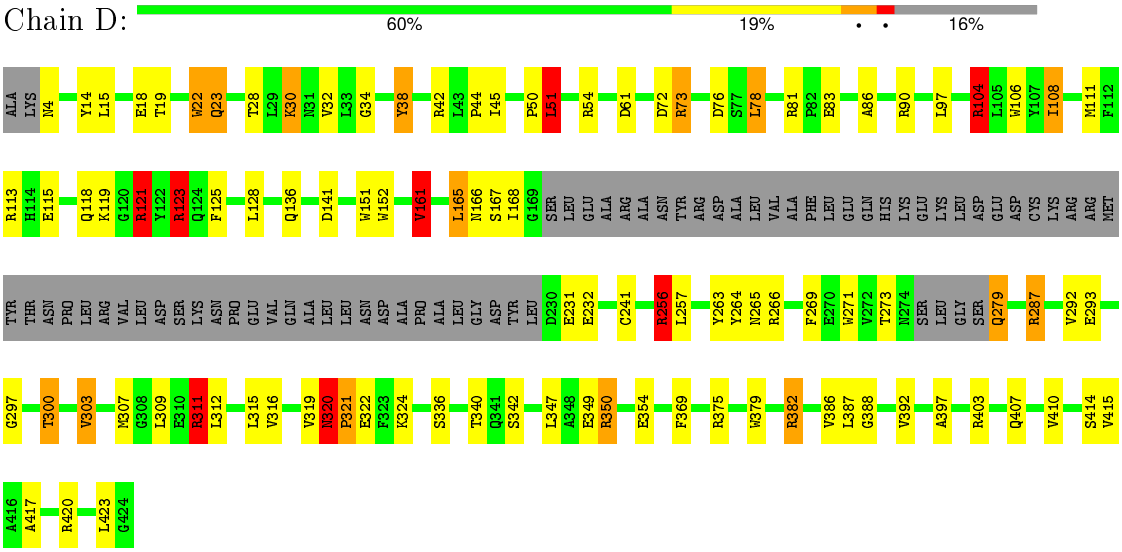
- Molecule 1: HISTIDYL-TRNA SYNTHETASE

Chain C:



- Molecule 1: HISTIDYL-TRNA SYNTHETASE

Chain D:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	61.40Å 110.70Å 108.70Å 115.00° 97.40° 90.00°	Depositor
Resolution (Å)	8.00 – 2.60	Depositor
% Data completeness (in resolution range)	69.9 (8.00-2.60)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.246 , 0.327	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11543	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.85	0/2899	1.57	54/3920 (1.4%)
1	B	0.86	1/2829 (0.0%)	1.57	65/3825 (1.7%)
1	C	0.87	1/2899 (0.0%)	1.58	59/3920 (1.5%)
1	D	0.85	1/2829 (0.0%)	1.53	50/3825 (1.3%)
All	All	0.86	3/11456 (0.0%)	1.56	228/15490 (1.5%)

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	C	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	379	TRP	CD1-NE1	-5.39	1.28	1.38
1	B	152	TRP	CD1-NE1	-5.05	1.29	1.38
1	D	152	TRP	CD1-NE1	-5.04	1.29	1.38

All (228) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	311	ARG	NE-CZ-NH1	11.50	126.05	120.30
1	C	311	ARG	NE-CZ-NH2	-11.42	114.59	120.30
1	D	104	ARG	NE-CZ-NH2	-11.08	114.76	120.30
1	B	90	ARG	NE-CZ-NH1	10.70	125.65	120.30
1	C	90	ARG	NE-CZ-NH2	-10.26	115.17	120.30
1	B	387	LEU	CA-CB-CG	10.09	138.51	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	90	ARG	NE-CZ-NH1	9.95	125.27	120.30
1	A	90	ARG	NE-CZ-NH1	9.86	125.23	120.30
1	C	379	TRP	CD1-CG-CD2	9.82	114.16	106.30
1	B	104	ARG	NE-CZ-NH2	-9.71	115.44	120.30
1	A	379	TRP	CD1-CG-CD2	9.53	113.92	106.30
1	D	311	ARG	NE-CZ-NH1	9.52	125.06	120.30
1	D	22	TRP	CD1-CG-CD2	9.43	113.84	106.30
1	B	152	TRP	CD1-CG-CD2	9.38	113.80	106.30
1	D	287	ARG	NE-CZ-NH1	9.32	124.96	120.30
1	A	116	ARG	NE-CZ-NH2	-9.20	115.70	120.30
1	D	152	TRP	CE2-CD2-CG	-9.17	99.97	107.30
1	B	152	TRP	CE2-CD2-CG	-9.05	100.06	107.30
1	D	152	TRP	CD1-CG-CD2	9.04	113.53	106.30
1	B	90	ARG	NE-CZ-NH2	-8.86	115.87	120.30
1	D	379	TRP	CD1-CG-CD2	8.85	113.38	106.30
1	D	375	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	C	379	TRP	CE2-CD2-CG	-8.58	100.44	107.30
1	B	104	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	D	81	ARG	NE-CZ-NH1	8.55	124.57	120.30
1	B	123	ARG	NE-CZ-NH1	8.43	124.51	120.30
1	B	153	ARG	NE-CZ-NH2	-8.38	116.11	120.30
1	A	152	TRP	CB-CG-CD1	-8.37	116.12	127.00
1	C	22	TRP	CD1-CG-CD2	8.36	112.98	106.30
1	C	152	TRP	CE2-CD2-CG	-8.32	100.64	107.30
1	B	150	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	A	152	TRP	CE2-CD2-CG	-8.29	100.67	107.30
1	D	152	TRP	CB-CG-CD1	-8.29	116.23	127.00
1	D	379	TRP	CE2-CD2-CG	-8.27	100.69	107.30
1	C	152	TRP	CB-CG-CD1	-8.27	116.25	127.00
1	B	73	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	B	121	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	B	22	TRP	CD1-CG-CD2	8.22	112.88	106.30
1	A	263	TYR	CB-CG-CD2	-8.22	116.07	121.00
1	C	266	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	C	271	TRP	CD1-CG-CD2	8.17	112.84	106.30
1	C	152	TRP	CG-CD2-CE3	8.16	141.24	133.90
1	B	379	TRP	CE2-CD2-CG	-8.14	100.78	107.30
1	A	271	TRP	CD1-CG-CD2	8.13	112.81	106.30
1	A	266	ARG	NE-CZ-NH2	-8.13	116.23	120.30
1	D	22	TRP	CE2-CD2-CG	-8.10	100.82	107.30
1	D	152	TRP	CG-CD2-CE3	8.10	141.19	133.90
1	A	403	ARG	NE-CZ-NH1	8.05	124.33	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	379	TRP	CD1-CG-CD2	8.02	112.72	106.30
1	A	379	TRP	CE2-CD2-CG	-8.02	100.89	107.30
1	C	152	TRP	CD1-CG-CD2	7.94	112.65	106.30
1	C	311	ARG	NE-CZ-NH1	7.91	124.26	120.30
1	B	81	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	C	298	ARG	NE-CZ-NH2	-7.89	116.35	120.30
1	A	106	TRP	CD1-CG-CD2	7.88	112.61	106.30
1	D	151	TRP	CD1-CG-CD2	7.82	112.56	106.30
1	C	22	TRP	CE2-CD2-CG	-7.81	101.06	107.30
1	A	271	TRP	CE2-CD2-CG	-7.79	101.07	107.30
1	A	152	TRP	CD1-CG-CD2	7.77	112.51	106.30
1	D	123	ARG	NE-CZ-NH1	7.77	124.18	120.30
1	B	22	TRP	CE2-CD2-CG	-7.71	101.13	107.30
1	C	106	TRP	CE2-CD2-CG	-7.68	101.16	107.30
1	D	106	TRP	CD1-CG-CD2	7.51	112.31	106.30
1	A	151	TRP	CD1-CG-CD2	7.48	112.28	106.30
1	C	271	TRP	CE2-CD2-CG	-7.45	101.34	107.30
1	C	116	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	A	106	TRP	CE2-CD2-CG	-7.40	101.38	107.30
1	C	153	ARG	NE-CZ-NH1	7.39	123.99	120.30
1	C	105	LEU	CA-CB-CG	7.39	132.29	115.30
1	A	152	TRP	CG-CD2-CE3	7.38	140.55	133.90
1	A	22	TRP	CE2-CD2-CG	-7.38	101.40	107.30
1	D	151	TRP	CE2-CD2-CG	-7.25	101.50	107.30
1	B	73	ARG	CA-CB-CG	7.25	129.35	113.40
1	D	121	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	B	333	LEU	CA-CB-CG	7.20	131.85	115.30
1	B	106	TRP	CD1-CG-CD2	7.19	112.05	106.30
1	B	259	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	C	153	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	B	379	TRP	CG-CD2-CE3	7.11	140.30	133.90
1	A	22	TRP	CD1-CG-CD2	7.11	111.98	106.30
1	B	38	TYR	CB-CG-CD2	-7.07	116.76	121.00
1	B	271	TRP	CE2-CD2-CG	-7.07	101.65	107.30
1	B	152	TRP	CB-CG-CD1	-7.07	117.81	127.00
1	A	174	ARG	NE-CZ-NH2	-7.05	116.77	120.30
1	B	152	TRP	CG-CD2-CE3	7.01	140.21	133.90
1	C	151	TRP	CD1-CG-CD2	6.99	111.89	106.30
1	A	420	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	B	271	TRP	CD1-CG-CD2	6.96	111.86	106.30
1	C	263	TYR	CB-CG-CD2	-6.93	116.84	121.00
1	C	136	GLN	CA-CB-CG	6.93	128.64	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	287	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	D	320	ASN	C-N-CD	-6.86	105.52	120.60
1	B	106	TRP	CE2-CD2-CG	-6.86	101.82	107.30
1	C	150	ARG	NE-CZ-NH1	6.85	123.73	120.30
1	D	271	TRP	CE2-CD2-CG	-6.84	101.83	107.30
1	A	287	ARG	NE-CZ-NH1	6.81	123.71	120.30
1	B	54	ARG	NE-CZ-NH1	6.81	123.71	120.30
1	D	54	ARG	NE-CZ-NH2	-6.81	116.89	120.30
1	C	106	TRP	CD1-CG-CD2	6.81	111.75	106.30
1	D	271	TRP	CD1-CG-CD2	6.81	111.75	106.30
1	A	261	LEU	CA-CB-CG	6.75	130.83	115.30
1	A	151	TRP	CE2-CD2-CG	-6.73	101.91	107.30
1	B	256	ARG	NE-CZ-NH2	-6.69	116.95	120.30
1	B	375	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	B	320	ASN	C-N-CD	-6.62	106.03	120.60
1	C	121	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	C	174	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	D	104	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	B	153	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	B	68	TYR	CB-CG-CD1	-6.53	117.08	121.00
1	A	243	LEU	CA-CB-CG	6.51	130.27	115.30
1	D	319	VAL	CA-CB-CG2	-6.50	101.15	110.90
1	C	298	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	A	314	LEU	CA-CB-CG	6.49	130.23	115.30
1	A	90	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	C	151	TRP	CE2-CD2-CG	-6.44	102.15	107.30
1	B	379	TRP	CB-CG-CD1	-6.44	118.63	127.00
1	D	106	TRP	CE2-CD2-CG	-6.43	102.16	107.30
1	D	303	VAL	CB-CA-C	-6.41	99.22	111.40
1	A	271	TRP	CG-CD2-CE3	6.36	139.62	133.90
1	A	104	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	A	350	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	B	151	TRP	CE2-CD2-CG	-6.25	102.30	107.30
1	B	287	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	A	24	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	D	256	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	B	264	TYR	CB-CG-CD2	-6.21	117.27	121.00
1	A	106	TRP	CG-CD2-CE3	6.19	139.47	133.90
1	D	287	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	C	264	TYR	CB-CG-CD2	-6.17	117.30	121.00
1	D	321	PRO	CA-N-CD	-6.15	102.89	111.50
1	A	81	ARG	NE-CZ-NH1	6.15	123.37	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	165	LEU	CA-CB-CG	6.14	129.42	115.30
1	C	42	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	C	232	GLU	CA-CB-CG	-6.09	100.00	113.40
1	A	298	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	B	256	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	B	360	LEU	CA-CB-CG	6.00	129.09	115.30
1	B	113	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	D	379	TRP	CG-CD2-CE3	5.91	139.22	133.90
1	A	106	TRP	CB-CG-CD1	-5.90	119.33	127.00
1	D	44	PRO	CA-N-CD	-5.89	103.25	111.50
1	D	287	ARG	CG-CD-NE	-5.86	99.50	111.80
1	D	73	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	C	174	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	B	361	MET	CG-SD-CE	-5.82	90.89	100.20
1	B	259	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	A	311	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	B	303	VAL	CB-CA-C	-5.78	100.41	111.40
1	D	38	TYR	CB-CG-CD2	-5.78	117.53	121.00
1	A	165	LEU	CA-CB-CG	5.78	128.58	115.30
1	A	22	TRP	CG-CD2-CE3	5.76	139.09	133.90
1	A	259	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	B	83	GLU	CA-CB-CG	5.74	126.03	113.40
1	B	106	TRP	CB-CG-CD1	-5.72	119.56	127.00
1	D	311	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	A	104	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	B	271	TRP	CG-CD2-CE3	5.68	139.01	133.90
1	C	110	PRO	CA-N-CD	-5.67	103.56	111.50
1	D	22	TRP	CG-CD1-NE1	-5.67	104.43	110.10
1	B	95	HIS	CA-CB-CG	-5.67	103.97	113.60
1	C	379	TRP	CG-CD2-CE3	5.66	138.99	133.90
1	C	36	TYR	CB-CG-CD2	-5.65	117.61	121.00
1	B	147	LEU	CA-CB-CG	5.64	128.28	115.30
1	A	259	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	C	121	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	C	319	VAL	CA-CB-CG2	-5.55	102.58	110.90
1	D	50	PRO	CA-N-CD	-5.54	103.75	111.50
1	A	403	ARG	CA-CB-CG	5.52	125.54	113.40
1	D	81	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	C	379	TRP	CG-CD1-NE1	-5.49	104.61	110.10
1	D	161	VAL	CG1-CB-CG2	-5.49	102.12	110.90
1	D	410	VAL	CG1-CB-CG2	-5.48	102.14	110.90
1	C	350	ARG	NE-CZ-NH2	-5.47	117.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	64	GLU	CA-CB-CG	5.46	125.42	113.40
1	B	321	PRO	CA-N-CD	-5.46	103.86	111.50
1	D	316	VAL	CG1-CB-CG2	-5.44	102.19	110.90
1	B	22	TRP	CG-CD2-CE3	5.42	138.78	133.90
1	A	38	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	A	234	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	123	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	B	116	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	C	298	ARG	CG-CD-NE	-5.39	100.48	111.80
1	A	379	TRP	CG-CD1-NE1	-5.38	104.72	110.10
1	C	81	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	D	152	TRP	CG-CD1-NE1	-5.36	104.74	110.10
1	A	150	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	D	106	TRP	CG-CD1-NE1	-5.33	104.77	110.10
1	A	266	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	106	TRP	CG-CD1-NE1	-5.31	104.79	110.10
1	C	136	GLN	N-CA-CB	-5.30	101.05	110.60
1	B	116	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	B	54	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	B	350	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	D	90	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	C	22	TRP	CG-CD2-CE3	5.24	138.62	133.90
1	B	151	TRP	CD1-CG-CD2	5.23	110.49	106.30
1	B	271	TRP	CB-CG-CD1	-5.21	120.22	127.00
1	B	287	ARG	CG-CD-NE	-5.20	100.87	111.80
1	B	319	VAL	CA-CB-CG2	-5.20	103.10	110.90
1	D	379	TRP	CB-CG-CD1	-5.20	120.24	127.00
1	C	400	LYS	CA-CB-CG	5.19	124.81	113.40
1	C	113	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	263	TYR	CB-CG-CD1	5.18	124.11	121.00
1	D	104	ARG	CG-CD-NE	-5.17	100.94	111.80
1	C	38	TYR	CB-CG-CD2	-5.17	117.90	121.00
1	A	99	TYR	CB-CG-CD2	-5.17	117.90	121.00
1	C	287	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	C	22	TRP	CG-CD1-NE1	-5.15	104.95	110.10
1	D	51	LEU	CA-CB-CG	5.15	127.14	115.30
1	C	95	HIS	CA-CB-CG	-5.13	104.88	113.60
1	C	60	THR	CA-CB-CG2	-5.13	105.22	112.40
1	C	379	TRP	CB-CG-CD1	-5.12	120.35	127.00
1	C	403	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	B	151	TRP	CG-CD2-CE3	5.10	138.49	133.90
1	C	303	VAL	CB-CA-C	-5.09	101.72	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	54	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	C	271	TRP	CG-CD1-NE1	-5.08	105.02	110.10
1	B	22	TRP	CB-CG-CD1	-5.07	120.41	127.00
1	C	104	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	A	42	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	B	398	VAL	CG1-CB-CG2	-5.05	102.82	110.90
1	B	106	TRP	CG-CD2-CE3	5.04	138.44	133.90
1	D	241	CYS	CA-CB-SG	-5.04	104.93	114.00
1	A	66	GLU	CA-CB-CG	-5.03	102.34	113.40
1	B	152	TRP	CG-CD1-NE1	-5.02	105.08	110.10
1	A	152	TRP	CG-CD1-NE1	-5.02	105.08	110.10
1	C	234	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	68	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	2848	0	2809	55	0
1	B	2779	0	2747	83	0
1	C	2848	0	2809	56	0
1	D	2779	0	2747	57	0
2	A	10	0	6	0	0
2	B	10	0	6	0	0
2	C	10	0	6	0	0
2	D	10	0	6	0	0
3	A	23	0	12	0	0
3	B	23	0	12	3	0
3	C	23	0	12	0	0
3	D	23	0	12	0	0
4	A	49	0	0	1	0
4	B	41	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	38	0	0	2	0
4	D	29	0	0	0	0
All	All	11543	0	11184	231	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 10.

All (231) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:GLU:HB3	1:A:65:LYS:HD3	1.61	0.82
1:B:20:ALA:HA	1:B:23:GLN:NE2	1.98	0.79
1:B:120:GLY:HA3	1:B:279:GLN:HG2	1.65	0.79
1:A:410:VAL:HG21	1:A:418:HIS:HD2	1.53	0.74
1:B:67:MET:SD	1:B:79:THR:HG21	2.26	0.74
1:A:46:VAL:HG22	1:B:11:MET:SD	2.28	0.73
1:A:19:THR:HG21	1:B:40:GLU:O	1.90	0.70
1:A:42:ARG:HB2	1:B:14:TYR:HB2	1.72	0.70
1:B:136:GLN:HA	1:B:287:ARG:NH2	2.07	0.69
1:C:168:ILE:HD11	1:C:258:VAL:HA	1.74	0.69
1:A:386:VAL:HB	1:A:398:VAL:HB	1.75	0.69
1:A:287:ARG:HG2	1:A:303:VAL:HG13	1.75	0.68
1:D:265:ASN:HD22	1:D:266:ARG:HG3	1.55	0.68
1:B:331:ILE:HD11	1:B:423:LEU:HD11	1.75	0.67
1:A:259:ARG:HG3	1:A:268:VAL:HG22	1.76	0.67
1:A:152:TRP:CD1	1:A:161:VAL:HG11	2.31	0.66
1:A:313:VAL:HG12	1:A:317:GLN:HE21	1.61	0.65
1:A:350:ARG:HH22	1:A:413:ASP:HA	1.61	0.65
1:A:307:MET:SD	1:A:312:LEU:HD22	2.36	0.65
1:D:136:GLN:HA	1:D:287:ARG:NH2	2.11	0.65
1:C:400:LYS:HD2	1:C:407:GLN:HB3	1.79	0.64
1:C:42:ARG:HB2	1:D:14:TYR:HB2	1.79	0.64
1:B:46:VAL:HG22	1:B:80:LEU:HD12	1.81	0.62
1:C:120:GLY:HA3	1:C:279:GLN:HB2	1.82	0.61
1:A:334:VAL:HG21	1:A:373:PHE:CE1	2.35	0.61
1:B:163:LEU:HD23	1:B:251:TYR:HB3	1.82	0.61
1:C:412:GLN:O	1:C:415:VAL:HG22	2.01	0.61
1:D:293:GLU:HA	1:D:297:GLY:O	2.00	0.61
1:D:369:PHE:HE2	1:D:386:VAL:HG13	1.66	0.60
1:D:292:VAL:HG21	1:D:300:THR:HG22	1.82	0.60
1:B:108:ILE:HD11	1:B:309:LEU:HD11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:30:LYS:HB2	1:D:30:LYS:NZ	2.17	0.59
1:D:266:ARG:HH21	1:D:287:ARG:HE	1.50	0.59
1:A:364:HIS:HD2	1:B:104:ARG:NH2	2.00	0.59
1:B:47:GLU:HB2	1:B:52:PHE:HE2	1.67	0.59
1:B:47:GLU:HB2	1:B:52:PHE:CE2	2.37	0.59
1:B:166:ASN:ND2	1:B:268:VAL:HG23	2.17	0.59
1:A:412:GLN:O	1:A:415:VAL:HG22	2.03	0.59
1:A:350:ARG:NH2	1:A:413:ASP:HA	2.17	0.59
1:D:165:LEU:HD23	1:D:269:PHE:HB3	1.85	0.58
1:C:58:GLU:HA	1:C:63:VAL:HG11	1.85	0.58
1:C:74:ASN:HD21	1:C:76:ASP:HB2	1.69	0.58
1:B:89:VAL:HG21	1:B:291:LEU:HD22	1.84	0.58
1:A:60:THR:O	1:A:64:GLU:HB2	2.03	0.58
1:B:20:ALA:HA	1:B:23:GLN:HE21	1.67	0.58
1:C:168:ILE:HD12	1:C:268:VAL:HG21	1.86	0.58
1:B:108:ILE:CD1	1:B:309:LEU:HD11	2.34	0.57
1:D:121:ARG:HH11	1:D:311:ARG:HH22	1.52	0.57
1:C:99:TYR:CD1	1:C:298:ARG:HG3	2.40	0.57
1:C:112:PHE:HZ	1:D:45:ILE:HD12	1.70	0.57
1:A:28:THR:O	1:A:32:VAL:HG23	2.04	0.57
1:C:401:ASP:HB3	1:C:406:GLU:HG2	1.86	0.56
1:C:359:LYS:HG2	1:D:34:GLY:O	2.06	0.56
1:B:412:GLN:O	1:B:415:VAL:HG22	2.06	0.56
1:D:38:TYR:CE1	1:D:104:ARG:HG2	2.41	0.56
1:C:310:GLU:HB2	4:C:627:HOH:O	2.05	0.55
1:B:254:ASN:HD21	1:B:256:ARG:NH2	2.04	0.55
1:B:266:ARG:HH21	1:B:287:ARG:HE	1.55	0.55
1:D:136:GLN:NE2	1:D:266:ARG:NH2	2.55	0.55
1:D:273:THR:HG21	1:D:315:LEU:HD22	1.88	0.55
1:B:166:ASN:HA	1:B:237:PHE:CZ	2.42	0.54
1:C:364:HIS:HD2	1:D:104:ARG:NH2	2.06	0.54
1:B:165:LEU:HD23	1:B:269:PHE:HB3	1.89	0.54
1:B:113:ARG:O	1:B:123:ARG:HA	2.08	0.53
1:C:14:TYR:HB2	1:D:42:ARG:HB2	1.89	0.53
1:B:136:GLN:HA	1:B:287:ARG:HH22	1.72	0.53
1:C:163:LEU:HG	1:C:165:LEU:HD12	1.89	0.53
1:D:30:LYS:HB2	1:D:30:LYS:HZ3	1.71	0.53
1:B:279:GLN:N	1:B:311:ARG:NE	2.57	0.53
1:A:313:VAL:O	1:A:317:GLN:HG3	2.09	0.53
1:B:254:ASN:OD1	1:B:256:ARG:HG3	2.09	0.52
1:C:367:GLY:HA3	1:C:375:ARG:HH12	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:TYR:HA	1:A:287:ARG:O	2.10	0.52
1:B:152:TRP:CD1	1:B:161:VAL:HG21	2.45	0.52
1:C:372:GLN:HA	1:C:375:ARG:HD3	1.92	0.52
1:A:350:ARG:HH12	1:A:412:GLN:HB3	1.74	0.51
1:B:70:PHE:HE1	1:B:80:LEU:HD13	1.74	0.51
1:B:283:CYS:SG	1:B:305:PHE:CD2	3.03	0.51
1:D:161:VAL:HG13	1:D:273:THR:HG22	1.91	0.51
1:A:49:THR:HG23	1:A:79:THR:OG1	2.10	0.51
1:B:333:LEU:HB3	1:B:362:THR:HA	1.91	0.51
1:B:259:ARG:NH1	1:B:264:TYR:OH	2.43	0.51
1:A:355:LEU:O	1:A:358:VAL:HG22	2.10	0.51
1:B:331:ILE:HD12	1:B:358:VAL:HG11	1.91	0.51
1:B:102:GLU:HA	1:B:133:PHE:O	2.11	0.50
1:D:51:LEU:HD22	1:D:86:ALA:HB1	1.94	0.50
1:A:120:GLY:HA3	1:A:279:GLN:HB2	1.93	0.50
1:D:311:ARG:HG2	1:D:311:ARG:HH11	1.76	0.50
1:B:397:ALA:HB3	1:B:415:VAL:HG11	1.93	0.50
1:A:401:ASP:HB3	1:A:406:GLU:HG2	1.94	0.50
1:B:60:THR:O	1:B:64:GLU:HB2	2.12	0.50
1:B:270:GLU:HG3	1:B:281:THR:HG23	1.93	0.50
1:C:56:ILE:HD11	1:C:62:VAL:HB	1.94	0.50
1:D:115:GLU:O	1:D:123:ARG:HD3	2.11	0.50
1:B:150:ARG:HD3	4:B:514:HOH:O	2.11	0.49
1:C:410:VAL:HG21	1:C:418:HIS:CD2	2.48	0.49
1:C:417:ALA:HA	1:C:420:ARG:NH1	2.28	0.49
1:D:256:ARG:NH1	1:D:257:LEU:HA	2.27	0.49
1:C:47:GLU:HB2	1:C:52:PHE:CE2	2.48	0.49
1:D:388:GLY:O	1:D:392:VAL:HG23	2.13	0.49
1:A:52:PHE:CE1	1:A:82:PRO:HD2	2.47	0.49
1:B:368:ASN:H	1:B:371:LYS:HZ2	1.60	0.49
1:B:111:MET:HB2	1:B:125:PHE:CE1	2.48	0.48
1:C:150:ARG:NH1	1:C:153:ARG:HH22	2.11	0.48
1:B:121:ARG:HD2	3:B:451:AMP:C6	2.47	0.48
1:D:264:TYR:HA	1:D:287:ARG:O	2.13	0.48
1:B:115:GLU:O	1:B:123:ARG:HD3	2.13	0.48
1:A:167:SER:HA	1:A:266:ARG:O	2.14	0.48
1:A:132:VAL:HG11	1:A:140:ILE:HG12	1.95	0.48
1:D:19:THR:O	1:D:23:GLN:HG2	2.14	0.48
1:C:310:GLU:O	1:C:314:LEU:HD23	2.13	0.48
1:B:167:SER:HA	1:B:266:ARG:O	2.14	0.48
1:B:279:GLN:N	1:B:311:ARG:HE	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:VAL:HA	1:C:66:GLU:HB2	1.96	0.47
1:A:61:ASP:HB3	1:A:65:LYS:HE3	1.96	0.47
1:A:62:VAL:HA	1:A:66:GLU:HB2	1.97	0.47
1:C:60:THR:O	1:C:64:GLU:HB2	2.14	0.47
1:B:398:VAL:HG13	1:B:407:GLN:HE21	1.79	0.47
1:A:371:LYS:HD3	1:A:375:ARG:HH21	1.78	0.47
1:B:254:ASN:HD21	1:B:256:ARG:HH21	1.62	0.47
1:D:111:MET:HB2	1:D:125:PHE:CZ	2.50	0.47
1:B:254:ASN:ND2	1:B:257:LEU:HB2	2.30	0.47
1:B:168:ILE:HG21	1:B:258:VAL:HG12	1.97	0.47
1:A:345:MET:SD	1:A:364:HIS:HE1	2.38	0.47
1:D:121:ARG:HH11	1:D:311:ARG:NH2	2.12	0.46
1:B:55:ALA:HB2	1:B:295:LEU:HD21	1.97	0.46
1:C:72:ASP:HB2	1:C:78:LEU:HD22	1.98	0.46
1:D:417:ALA:HA	1:D:420:ARG:HH11	1.80	0.46
1:D:136:GLN:NE2	1:D:266:ARG:HH22	2.14	0.46
1:D:397:ALA:HB3	1:D:415:VAL:HG21	1.97	0.46
1:B:320:ASN:O	1:B:322:GLU:N	2.48	0.46
1:B:293:GLU:HA	1:B:297:GLY:O	2.15	0.46
1:A:364:HIS:CD2	1:B:104:ARG:NH2	2.82	0.46
1:B:368:ASN:H	1:B:371:LYS:NZ	2.14	0.46
1:C:313:VAL:O	1:C:317:GLN:HG3	2.16	0.46
1:D:128:LEU:HB2	1:D:309:LEU:HD11	1.98	0.46
1:C:142:ALA:CB	1:C:243:LEU:HD22	2.45	0.46
1:C:264:TYR:HA	1:C:287:ARG:O	2.16	0.45
1:A:363:ASN:OD1	1:A:372:GLN:HG2	2.16	0.45
1:A:374:ALA:HA	1:A:377:ASP:OD2	2.15	0.45
1:B:283:CYS:SG	1:B:305:PHE:HD2	2.39	0.45
1:A:15:LEU:HD22	1:B:97:LEU:HD11	1.97	0.45
1:D:28:THR:O	1:D:32:VAL:HG23	2.16	0.45
1:C:387:LEU:HD23	1:C:392:VAL:HG12	1.99	0.45
1:C:46:VAL:HG22	1:C:80:LEU:HD12	1.99	0.45
1:D:340:THR:HG22	1:D:392:VAL:HG21	1.99	0.45
1:D:347:LEU:CD2	1:D:387:LEU:HD11	2.47	0.45
1:A:399:VAL:O	1:A:407:GLN:HA	2.17	0.45
1:D:265:ASN:ND2	1:D:266:ARG:HG3	2.28	0.45
1:B:138:PRO:HB3	1:B:240:LEU:HB2	1.98	0.45
1:D:266:ARG:HH21	1:D:287:ARG:NE	2.12	0.45
1:A:46:VAL:HG23	1:B:8:ILE:HG13	1.98	0.44
1:C:152:TRP:CD1	1:C:161:VAL:HG21	2.52	0.44
1:D:168:ILE:HA	1:D:168:ILE:HD13	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ILE:HG22	1:A:60:THR:HG21	1.98	0.44
1:B:135:LEU:HD23	1:B:140:ILE:HG12	1.98	0.44
1:C:355:LEU:O	1:C:358:VAL:HG22	2.17	0.44
1:D:18:GLU:O	1:D:22:TRP:HD1	2.00	0.44
1:B:237:PHE:O	1:B:240:LEU:HB3	2.18	0.44
1:C:386:VAL:HB	1:C:398:VAL:HB	1.99	0.44
1:D:72:ASP:HB2	1:D:78:LEU:HD22	2.00	0.44
1:C:15:LEU:HD22	1:D:97:LEU:HD11	1.99	0.44
1:B:264:TYR:HA	1:B:287:ARG:O	2.17	0.44
1:C:110:PRO:HG2	1:D:45:ILE:HD11	1.98	0.44
1:B:287:ARG:NH1	1:B:303:VAL:HG22	2.33	0.43
1:A:398:VAL:HG11	1:A:407:GLN:OE1	2.18	0.43
1:B:263:TYR:CG	1:B:291:LEU:HD12	2.53	0.43
1:B:151:TRP:HZ3	1:B:305:PHE:HE2	1.66	0.43
1:B:9:ARG:HA	1:B:9:ARG:HD2	1.75	0.43
1:B:263:TYR:CB	1:B:291:LEU:HD12	2.49	0.43
1:C:5:ILE:HD13	1:D:51:LEU:HA	1.99	0.43
1:A:333:LEU:CD1	1:A:348:ALA:HB2	2.47	0.43
1:C:150:ARG:NH2	1:D:349:GLU:OE1	2.51	0.43
1:B:311:ARG:HH12	3:B:451:AMP:H2'	1.83	0.43
1:A:410:VAL:HG21	1:A:418:HIS:CD2	2.42	0.43
1:C:371:LYS:HB3	1:C:375:ARG:HH11	1.83	0.43
1:D:113:ARG:O	1:D:123:ARG:HA	2.18	0.43
1:D:350:ARG:HD3	1:D:354:GLU:OE1	2.18	0.43
1:A:42:ARG:HD2	1:B:19:THR:HG22	2.00	0.43
1:D:167:SER:HA	1:D:266:ARG:O	2.18	0.43
1:B:355:LEU:HB3	1:B:358:VAL:HG21	2.01	0.43
1:D:279:GLN:N	1:D:311:ARG:HD2	2.34	0.42
1:A:62:VAL:O	1:A:67:MET:HG3	2.19	0.42
1:D:320:ASN:O	1:D:322:GLU:N	2.51	0.42
1:D:307:MET:SD	1:D:312:LEU:HD22	2.58	0.42
1:C:400:LYS:HZ2	1:C:400:LYS:HB3	1.84	0.42
1:B:38:TYR:CE1	1:B:104:ARG:HG2	2.53	0.42
1:C:255:GLN:O	1:C:255:GLN:NE2	2.52	0.42
1:A:114:HIS:CE1	1:B:73:ARG:HE	2.37	0.42
1:B:102:GLU:OE2	1:B:135:LEU:HD11	2.19	0.42
1:C:259:ARG:NH1	1:C:264:TYR:OH	2.53	0.42
1:A:351:LEU:O	1:A:355:LEU:HD12	2.19	0.42
1:C:56:ILE:HD13	1:C:261:LEU:HD22	2.01	0.42
1:A:53:LYS:HD3	1:A:63:VAL:CG1	2.50	0.42
1:A:46:VAL:CG2	1:B:11:MET:SD	3.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:VAL:O	1:B:317:GLN:HG3	2.20	0.42
1:C:128:LEU:HD13	1:C:129:GLY:N	2.34	0.42
1:B:74:ASN:HB3	1:B:76:ASP:OD1	2.20	0.42
1:C:237:PHE:O	1:C:240:LEU:HB3	2.19	0.42
1:D:369:PHE:HE2	1:D:386:VAL:CG1	2.31	0.41
1:D:136:GLN:HA	1:D:287:ARG:HH22	1.82	0.41
1:C:22:TRP:CE2	1:C:313:VAL:HG21	2.56	0.41
1:A:163:LEU:HD23	1:A:251:TYR:HB3	2.02	0.41
1:C:32:VAL:HG13	1:C:150:ARG:HD2	2.01	0.41
1:C:287:ARG:NH1	1:C:303:VAL:HG22	2.35	0.41
1:B:266:ARG:HH21	1:B:287:ARG:NE	2.18	0.41
1:B:33:LEU:HD13	1:B:106:TRP:CG	2.55	0.41
1:C:112:PHE:CZ	1:D:45:ILE:HD12	2.52	0.41
1:A:352:ARG:HD2	1:A:352:ARG:HH11	1.70	0.41
1:B:62:VAL:HA	1:B:66:GLU:HB2	2.03	0.41
1:D:382:ARG:NH2	1:D:423:LEU:HD22	2.36	0.41
1:A:410:VAL:HG12	1:A:411:ALA:O	2.21	0.41
1:C:72:ASP:HB3	1:C:74:ASN:ND2	2.36	0.41
1:D:279:GLN:N	1:D:311:ARG:NE	2.68	0.41
1:C:135:LEU:HD23	1:C:135:LEU:HA	1.89	0.41
1:A:11:MET:HG2	1:A:124:GLN:HB2	2.03	0.41
1:A:165:LEU:HG	1:A:237:PHE:CE1	2.56	0.41
1:B:327:PRO:O	1:B:359:LYS:NZ	2.54	0.41
1:B:128:LEU:HB2	1:B:309:LEU:HD21	2.02	0.41
1:D:336:SER:O	1:D:388:GLY:HA2	2.21	0.41
1:B:316:VAL:O	1:B:320:ASN:HB2	2.21	0.41
1:A:152:TRP:CE3	1:A:157:ILE:HD11	2.56	0.40
1:C:167:SER:HA	1:C:266:ARG:O	2.21	0.40
1:B:20:ALA:HA	1:B:23:GLN:HE22	1.80	0.40
1:A:310:GLU:HB2	4:A:594:HOH:O	2.21	0.40
1:C:166:ASN:ND2	1:C:257:LEU:O	2.53	0.40
1:B:259:ARG:NH2	3:B:451:AMP:O1P	2.54	0.40
1:D:108:ILE:HD13	1:D:309:LEU:HD21	2.02	0.40
1:C:351:LEU:O	1:C:355:LEU:HD12	2.21	0.40
1:B:112:PHE:HA	1:B:123:ARG:O	2.22	0.40
1:C:292:VAL:HG23	4:C:600:HOH:O	2.22	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	360/423 (85%)	344 (96%)	14 (4%)	2 (1%)	30	56
1	B	351/423 (83%)	334 (95%)	13 (4%)	4 (1%)	17	36
1	C	360/423 (85%)	341 (95%)	17 (5%)	2 (1%)	30	56
1	D	351/423 (83%)	327 (93%)	20 (6%)	4 (1%)	17	36
All	All	1422/1692 (84%)	1346 (95%)	64 (4%)	12 (1%)	24	46

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	321	PRO
1	B	321	PRO
1	C	321	PRO
1	D	321	PRO
1	A	73	ARG
1	C	73	ARG
1	D	73	ARG
1	B	73	ARG
1	B	119	LYS
1	D	119	LYS
1	B	320	ASN
1	D	320	ASN

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	291/341 (85%)	254 (87%)	37 (13%)	5 10
1	B	285/341 (84%)	255 (90%)	30 (10%)	8 16
1	C	291/341 (85%)	264 (91%)	27 (9%)	11 21
1	D	285/341 (84%)	252 (88%)	33 (12%)	7 12
All	All	1152/1364 (84%)	1025 (89%)	127 (11%)	8 14

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	6	GLN
1	A	18	GLU
1	A	19	THR
1	A	23	GLN
1	A	61	ASP
1	A	64	GLU
1	A	65	LYS
1	A	66	GLU
1	A	76	ASP
1	A	83	GLU
1	A	100	ASN
1	A	116	ARG
1	A	128	LEU
1	A	141	ASP
1	A	155	LEU
1	A	158	SER
1	A	174	ARG
1	A	234	ARG
1	A	235	GLU
1	A	243	LEU
1	A	245	GLU
1	A	256	ARG
1	A	257	LEU
1	A	259	ARG
1	A	261	LEU
1	A	263	TYR
1	A	268	VAL
1	A	272	VAL
1	A	295	LEU
1	A	303	VAL
1	A	336	SER
1	A	339	ASP

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Mol	Chain	Res	Type
1	A	342	SER
1	A	370	LYS
1	A	404	SER
1	A	413	ASP
1	B	15	LEU
1	B	48	GLN
1	B	65	LYS
1	B	71	GLU
1	B	73	ARG
1	B	76	ASP
1	B	80	LEU
1	B	90	ARG
1	B	104	ARG
1	B	118	GLN
1	B	123	ARG
1	B	135	LEU
1	B	140	ILE
1	B	141	ASP
1	B	147	LEU
1	B	158	SER
1	B	166	ASN
1	B	231	GLU
1	B	232	GLU
1	B	256	ARG
1	B	257	LEU
1	B	258	VAL
1	B	261	LEU
1	B	303	VAL
1	B	320	ASN
1	B	324	LYS
1	B	333	LEU
1	B	342	SER
1	B	359	LYS
1	B	407	GLN
1	C	12	ASN
1	C	24	ARG
1	C	39	SER
1	C	56	ILE
1	C	60	THR
1	C	66	GLU
1	C	74	ASN
1	C	83	GLU

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Mol	Chain	Res	Type
1	C	116	ARG
1	C	128	LEU
1	C	141	ASP
1	C	166	ASN
1	C	171	LEU
1	C	243	LEU
1	C	244	LEU
1	C	256	ARG
1	C	257	LEU
1	C	263	TYR
1	C	287	ARG
1	C	294	GLN
1	C	295	LEU
1	C	303	VAL
1	C	350	ARG
1	C	370	LYS
1	C	382	ARG
1	C	396	THR
1	C	400	LYS
1	D	4	ASN
1	D	15	LEU
1	D	23	GLN
1	D	30	LYS
1	D	51	LEU
1	D	61	ASP
1	D	76	ASP
1	D	78	LEU
1	D	83	GLU
1	D	104	ARG
1	D	108	ILE
1	D	118	GLN
1	D	121	ARG
1	D	123	ARG
1	D	141	ASP
1	D	161	VAL
1	D	166	ASN
1	D	231	GLU
1	D	232	GLU
1	D	256	ARG
1	D	263	TYR
1	D	279	GLN
1	D	300	THR

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Mol	Chain	Res	Type
1	D	303	VAL
1	D	311	ARG
1	D	320	ASN
1	D	324	LYS
1	D	342	SER
1	D	350	ARG
1	D	382	ARG
1	D	403	ARG
1	D	407	GLN
1	D	414	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	317	GLN
1	A	364	HIS
1	B	4	ASN
1	B	23	GLN
1	B	166	ASN
1	B	407	GLN
1	C	6	GLN
1	C	74	ASN
1	C	95	HIS
1	C	255	GLN
1	D	4	ASN
1	D	136	GLN
1	D	254	ASN
1	D	320	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HIS	A	450	3	5,10,11	1.07	0	3,12,14	3.89	3 (100%)
3	AMP	A	451	2	20,25,25	1.76	3 (15%)	22,38,38	1.19	2 (9%)
2	HIS	B	450	3	5,10,11	1.16	0	3,12,14	4.21	3 (100%)
3	AMP	B	451	2	20,25,25	1.59	2 (10%)	22,38,38	1.48	4 (18%)
2	HIS	C	450	3	5,10,11	1.21	0	3,12,14	4.22	3 (100%)
3	AMP	C	451	2	20,25,25	1.82	4 (20%)	22,38,38	1.41	2 (9%)
2	HIS	D	450	3	5,10,11	0.89	0	3,12,14	3.62	3 (100%)
3	AMP	D	451	2	20,25,25	1.51	1 (5%)	22,38,38	1.03	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HIS	A	450	3	-	0/4/6/8	0/1/1/1
3	AMP	A	451	2	-	0/6/26/26	0/3/3/3
2	HIS	B	450	3	-	0/4/6/8	0/1/1/1
3	AMP	B	451	2	-	0/6/26/26	0/3/3/3
2	HIS	C	450	3	-	0/4/6/8	0/1/1/1
3	AMP	C	451	2	-	0/6/26/26	0/3/3/3
2	HIS	D	450	3	-	0/4/6/8	0/1/1/1
3	AMP	D	451	2	-	0/6/26/26	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	451	AMP	C8-N7	-2.58	1.29	1.34
3	A	451	AMP	C8-N7	-2.47	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	451	AMP	P-O2P	-2.46	1.45	1.54
3	B	451	AMP	C8-N7	-2.37	1.30	1.34
3	C	451	AMP	P-O2P	-2.12	1.47	1.54
3	C	451	AMP	O4'-C1'	3.48	1.45	1.41
3	D	451	AMP	P-O3P	5.05	1.72	1.54
3	B	451	AMP	P-O3P	5.47	1.74	1.54
3	A	451	AMP	P-O3P	5.73	1.75	1.54
3	C	451	AMP	P-O3P	5.94	1.76	1.54

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	450	HIS	O-C-CA	-5.40	111.43	125.49
2	C	450	HIS	O-C-CA	-5.10	112.21	125.49
2	B	450	HIS	O-C-CA	-5.05	112.33	125.49
2	D	450	HIS	O-C-CA	-4.54	113.68	125.49
3	B	451	AMP	C2'-C1'-N9	-3.26	109.32	114.29
2	C	450	HIS	CG-CD2-NE2	-3.11	102.69	108.71
3	A	451	AMP	C2'-C1'-N9	-2.98	109.74	114.29
3	C	451	AMP	C2'-C1'-N9	-2.98	109.74	114.29
3	B	451	AMP	C4'-O4'-C1'	-2.93	106.50	109.72
2	B	450	HIS	CG-CD2-NE2	-2.92	103.06	108.71
3	B	451	AMP	C1'-N9-C4	-2.68	122.89	126.94
2	A	450	HIS	CG-CD2-NE2	-2.55	103.77	108.71
2	D	450	HIS	CG-CD2-NE2	-2.33	104.19	108.71
3	B	451	AMP	O2P-P-O1P	2.03	117.13	110.58
3	C	451	AMP	N3-C2-N1	2.83	131.06	128.89
3	A	451	AMP	N3-C2-N1	2.99	131.19	128.89
2	A	450	HIS	CD2-NE2-CE1	3.11	110.62	105.71
2	D	450	HIS	CD2-NE2-CE1	3.64	111.45	105.71
2	C	450	HIS	CD2-NE2-CE1	4.23	112.38	105.71
2	B	450	HIS	CD2-NE2-CE1	4.36	112.59	105.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	451	AMP	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.