



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:51 PM UTC

PDB ID : 1FO6 / pdb_00001fo6
Title : CRYSTAL STRUCTURE ANALYSIS OF N-CARBAMOYL-D-AMINO-ACID AMIDOHYDROLASE
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Deposited on : 2000-08-25
Resolution : 1.95 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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

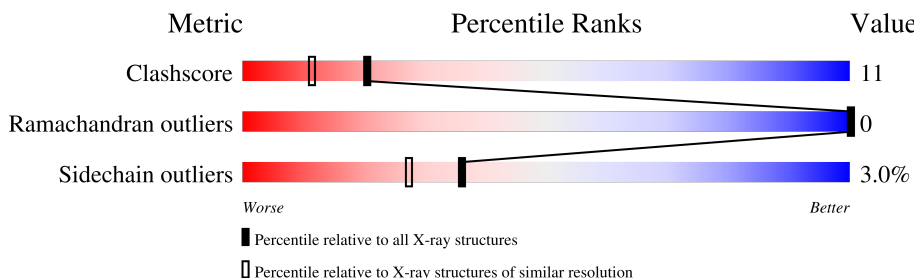
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	304	 65% 25% 8% ..
1	B	304	 64% 30% 5% .
1	C	304	 65% 30% . ..
1	D	304	 58% 32% 8% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10288 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 N-CARBAMoYL-D-AMINO-ACID AMIDOHYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	0	0	0
			2391	1527	419	431	14			
1	B	302	Total	C	N	O	S	0	0	0
			2391	1527	419	431	14			
1	C	302	Total	C	N	O	S	0	0	0
			2391	1527	419	431	14			
1	D	302	Total	C	N	O	S	0	0	0
			2391	1527	419	431	14			

- Molecule 2 is XENON (CCD ID: XE) (formula: Xe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Xe	0	0
			1	1		
2	C	1	Total	Xe	0	0
			1	1		

- Molecule 3 is water.

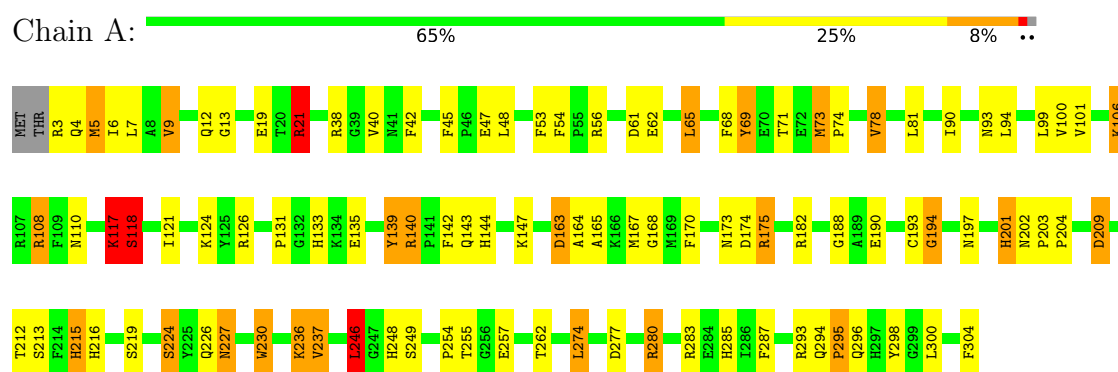
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	200	Total	O	0	0
			200	200		
3	B	202	Total	O	0	0
			202	202		
3	C	169	Total	O	0	0
			169	169		
3	D	151	Total	O	0	0
			151	151		

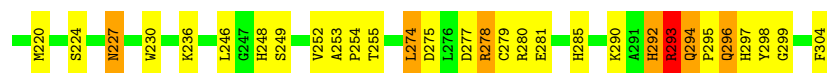
3 Residue-property plots

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. 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. 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.

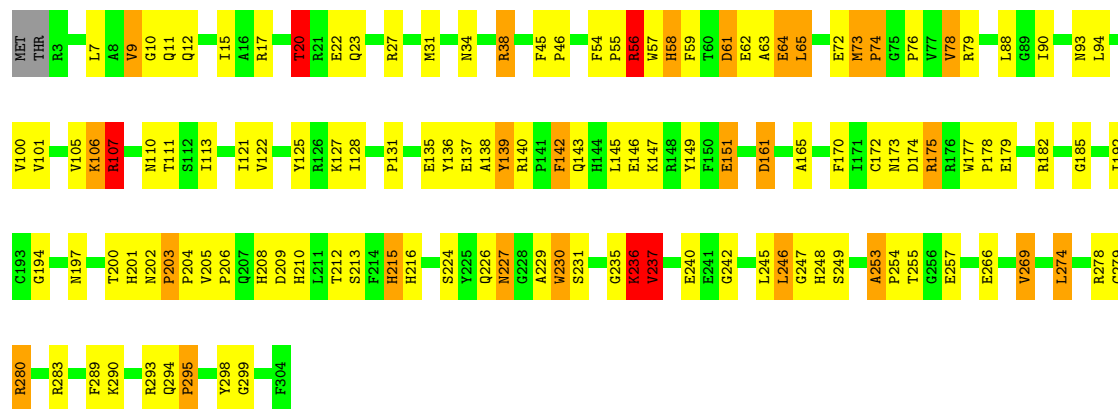
• Molecule 1: N-CARBAMoyL-D-AMINO-ACID AMIDOHYDROLASE





● Molecule 1: N-CARBAMOYL-D-AMINO-ACID AMIDOHYDROLASE

Chain D: 58% 32% 8% ..



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.23Å 67.53Å 137.48Å 90.00° 96.12° 90.00°	Depositor
Resolution (Å)	30.00 – 1.95	Depositor
% Data completeness (in resolution range)	94.9 (30.00-1.95)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.187 , 0.239	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10288	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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: XE

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	1.26	5/2455 (0.2%)	2.06	80/3327 (2.4%)
1	B	1.22	2/2455 (0.1%)	2.00	75/3327 (2.3%)
1	C	1.15	3/2455 (0.1%)	2.05	77/3327 (2.3%)
1	D	1.14	1/2455 (0.0%)	2.33	107/3327 (3.2%)
All	All	1.19	11/9820 (0.1%)	2.11	339/13308 (2.5%)

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	A	0	9
1	B	0	3
1	C	0	6
1	D	0	4
All	All	0	22

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	194	GLY	N-CA	6.50	1.52	1.45
1	B	194	GLY	N-CA	6.23	1.52	1.45
1	A	194	GLY	N-CA	5.98	1.52	1.45
1	A	108	ARG	CD-NE	5.93	1.54	1.46
1	A	215	HIS	CE1-NE2	5.70	1.38	1.32
1	C	195	GLY	N-CA	5.52	1.50	1.44
1	C	13	GLY	N-CA	5.39	1.52	1.44
1	A	194	GLY	C-N	-5.16	1.28	1.33
1	B	208	HIS	C-N	5.15	1.40	1.33
1	D	194	GLY	N-CA	5.10	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	93	ASN	N-CA	5.06	1.52	1.46

All (339) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	38	ARG	CD-NE-CZ	38.96	178.94	124.40
1	D	56	ARG	CD-NE-CZ	35.43	174.00	124.40
1	D	280	ARG	CD-NE-CZ	18.95	150.92	124.40
1	D	278	ARG	CD-NE-CZ	18.52	150.33	124.40
1	D	107	ARG	NE-CZ-NH2	16.49	134.04	119.20
1	C	38	ARG	NE-CZ-NH2	-14.48	106.17	119.20
1	A	280	ARG	CD-NE-CZ	14.06	144.09	124.40
1	C	280	ARG	CD-NE-CZ	13.32	143.05	124.40
1	D	38	ARG	NE-CZ-NH2	12.84	130.76	119.20
1	A	140	ARG	CD-NE-CZ	12.64	142.09	124.40
1	D	107	ARG	NE-CZ-NH1	-11.87	109.63	121.50
1	A	108	ARG	NE-CZ-NH1	-10.74	110.76	121.50
1	A	304	PHE	CA-CB-CG	9.84	123.64	113.80
1	A	108	ARG	NE-CZ-NH2	9.55	127.79	119.20
1	A	108	ARG	CD-NE-CZ	-9.39	111.25	124.40
1	B	227	ASN	OD1-CG-ND2	-9.17	113.43	122.60
1	D	227	ASN	CA-CB-CG	-9.12	103.48	112.60
1	D	20	THR	N-CA-CB	-9.06	97.13	110.17
1	B	227	ASN	CA-CB-CG	-8.96	103.64	112.60
1	B	79	ARG	CD-NE-CZ	8.95	136.92	124.40
1	C	297	HIS	CA-CB-CG	-8.63	105.17	113.80
1	A	110	ASN	OD1-CG-ND2	8.63	131.23	122.60
1	C	296	GLN	OE1-CD-NE2	-8.54	114.06	122.60
1	D	72	GLU	CA-CB-CG	8.40	130.90	114.10
1	C	285	HIS	CA-CB-CG	-8.34	105.46	113.80
1	C	34	ASN	CA-CB-CG	-8.15	104.45	112.60
1	B	294	GLN	OE1-CD-NE2	-8.10	114.50	122.60
1	C	38	ARG	NE-CZ-NH1	8.00	129.50	121.50
1	D	138	ALA	N-CA-C	7.99	119.99	111.28
1	A	227	ASN	CA-CB-CG	-7.93	104.67	112.60
1	D	34	ASN	CA-CB-CG	-7.84	104.76	112.60
1	B	280	ARG	CD-NE-CZ	7.78	135.29	124.40
1	D	299	GLY	O-C-N	-7.72	114.06	122.24
1	A	5	MET	CA-C-N	-7.67	113.15	123.12
1	A	5	MET	C-N-CA	-7.67	113.15	123.12
1	D	45	PHE	CA-C-N	7.63	127.54	120.21
1	D	45	PHE	C-N-CA	7.63	127.54	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	GLY	CA-C-O	-7.60	114.27	121.11
1	A	106	LYS	CA-C-O	-7.58	113.04	120.92
1	C	227	ASN	CA-CB-CG	-7.56	105.04	112.60
1	D	61	ASP	CA-CB-CG	7.56	120.16	112.60
1	A	174	ASP	CA-CB-CG	7.52	120.12	112.60
1	D	106	LYS	CA-C-O	-7.49	112.56	120.58
1	B	171	ILE	CA-C-O	7.46	127.81	120.27
1	A	287	PHE	CA-C-O	7.44	130.40	121.17
1	C	15	ILE	N-CA-CB	7.43	121.26	111.90
1	A	140	ARG	NE-CZ-NH2	-7.39	112.55	119.20
1	B	175	ARG	NE-CZ-NH1	-7.33	114.17	121.50
1	D	107	ARG	CG-CD-NE	7.33	128.12	112.00
1	A	202	ASN	OD1-CG-ND2	7.32	129.92	122.60
1	B	58	HIS	CA-CB-CG	-7.29	106.51	113.80
1	C	25	VAL	CA-C-N	7.28	128.06	119.98
1	C	25	VAL	C-N-CA	7.28	128.06	119.98
1	C	236	LYS	N-CA-C	-7.25	96.71	108.52
1	B	202	ASN	CA-CB-CG	-7.23	105.37	112.60
1	B	63	ALA	CA-C-O	7.18	128.16	120.55
1	D	179	GLU	CB-CG-CD	7.18	124.80	112.60
1	A	277	ASP	CA-CB-CG	-7.14	105.46	112.60
1	A	78	VAL	O-C-N	-7.14	113.84	122.12
1	A	13	GLY	N-CA-C	-7.12	103.61	112.23
1	D	88	LEU	CA-C-O	7.09	128.10	119.31
1	D	151	GLU	CA-C-O	-7.09	113.36	120.66
1	A	202	ASN	CA-CB-CG	-7.06	105.54	112.60
1	D	56	ARG	NH1-CZ-NH2	-7.05	110.14	119.30
1	C	278	ARG	NH1-CZ-NH2	7.04	128.45	119.30
1	A	140	ARG	NE-CZ-NH1	7.01	128.51	121.50
1	D	215	HIS	CA-CB-CG	6.93	120.73	113.80
1	A	274	LEU	CB-CA-C	-6.91	97.77	109.72
1	A	38	ARG	CD-NE-CZ	-6.86	114.80	124.40
1	D	161	ASP	O-C-N	-6.82	115.06	123.04
1	B	267	ASP	CA-C-O	-6.81	113.15	120.92
1	D	58	HIS	CA-CB-CG	-6.81	106.99	113.80
1	C	94	LEU	CA-C-O	-6.80	113.36	120.70
1	C	220	MET	O-C-N	6.78	129.06	122.07
1	A	295	PRO	CA-C-O	6.74	128.82	119.18
1	C	111	THR	N-CA-CB	-6.72	100.97	111.05
1	B	143	GLN	OE1-CD-NE2	-6.70	115.90	122.60
1	B	103	GLY	O-C-N	-6.65	114.06	122.70
1	A	73	MET	CG-SD-CE	6.62	115.46	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	151	GLU	O-C-N	6.59	126.95	121.35
1	C	17	ARG	NE-CZ-NH2	6.57	125.11	119.20
1	A	194	GLY	N-CA-C	-6.56	100.65	110.42
1	A	224	SER	O-C-N	6.55	129.17	122.09
1	C	25	VAL	CA-C-O	6.55	127.86	121.05
1	B	258	ILE	O-C-N	-6.54	115.51	122.83
1	B	93	ASN	OD1-CG-ND2	-6.53	116.07	122.60
1	B	182	ARG	NE-CZ-NH2	-6.53	113.32	119.20
1	B	233	ALA	CA-C-N	-6.50	113.96	123.05
1	B	233	ALA	C-N-CA	-6.50	113.96	123.05
1	C	35	ALA	CA-C-O	6.49	127.63	120.82
1	D	205	VAL	CA-C-N	6.49	126.18	119.82
1	D	205	VAL	C-N-CA	6.49	126.18	119.82
1	D	9	VAL	N-CA-CB	6.48	120.35	111.41
1	D	110	ASN	OD1-CG-ND2	6.48	129.08	122.60
1	B	261	LEU	CA-C-O	-6.47	112.58	120.54
1	C	278	ARG	NE-CZ-NH2	-6.46	113.39	119.20
1	D	236	LYS	N-CA-C	-6.45	98.00	108.52
1	D	140	ARG	NE-CZ-NH2	-6.45	113.40	119.20
1	A	106	LYS	CA-CB-CG	6.44	126.98	114.10
1	C	193	CYS	CA-C-N	-6.44	111.25	120.97
1	C	193	CYS	C-N-CA	-6.44	111.25	120.97
1	C	277	ASP	CA-CB-CG	-6.39	106.21	112.60
1	C	72	GLU	CA-C-O	-6.37	114.20	121.40
1	B	130	LEU	CA-C-O	6.37	123.43	119.29
1	A	71	THR	CA-C-O	6.35	126.39	119.15
1	A	219	SER	O-C-N	6.34	128.60	122.07
1	D	90	ILE	CA-C-N	6.32	128.60	120.64
1	D	90	ILE	C-N-CA	6.32	128.60	120.64
1	D	170	PHE	CA-CB-CG	-6.28	107.52	113.80
1	B	165	ALA	N-CA-C	6.26	120.13	110.42
1	D	72	GLU	CA-C-O	-6.26	113.78	121.11
1	D	289	PHE	CA-CB-CG	6.26	120.06	113.80
1	C	81	LEU	CA-C-O	6.25	127.14	120.70
1	B	236	LYS	N-CA-C	-6.25	98.34	108.52
1	C	165	ALA	N-CA-C	6.20	119.81	109.95
1	D	56	ARG	NE-CZ-NH2	6.19	124.77	119.20
1	A	9	VAL	N-CA-C	-6.16	99.26	108.12
1	B	283	ARG	NE-CZ-NH2	6.13	124.72	119.20
1	B	173	ASN	CA-CB-CG	6.12	118.72	112.60
1	B	175	ARG	CG-CD-NE	6.11	125.44	112.00
1	B	71	THR	N-CA-C	-6.11	105.78	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	142	PHE	CA-CB-CG	-6.11	107.69	113.80
1	B	116	ASP	CA-C-N	6.10	130.36	120.60
1	B	116	ASP	C-N-CA	6.10	130.36	120.60
1	D	202	ASN	CA-C-O	6.09	126.06	120.09
1	C	107	ARG	CA-C-O	-6.08	114.11	121.28
1	B	42	PHE	CA-C-N	-6.07	114.50	122.94
1	B	42	PHE	C-N-CA	-6.07	114.50	122.94
1	B	104	GLY	CA-C-O	-6.07	112.61	119.04
1	B	85	ALA	CA-C-O	-6.05	114.13	120.55
1	D	229	ALA	CA-C-O	-6.05	114.28	121.11
1	B	246	LEU	O-C-N	-6.04	115.60	122.97
1	A	224	SER	N-CA-C	-6.03	104.62	111.14
1	A	19	GLU	CA-C-O	-6.00	114.59	121.19
1	B	75	GLY	N-CA-C	-6.00	104.97	112.23
1	B	190	GLU	N-CA-C	-5.98	106.52	113.88
1	B	34	ASN	CA-CB-CG	-5.95	106.65	112.60
1	C	175	ARG	NE-CZ-NH2	5.95	124.55	119.20
1	D	137	GLU	CA-C-N	5.94	128.24	120.28
1	D	137	GLU	C-N-CA	5.94	128.24	120.28
1	C	173	ASN	CA-C-N	5.93	129.03	120.38
1	C	173	ASN	C-N-CA	5.93	129.03	120.38
1	C	252	VAL	O-C-N	5.92	129.62	123.05
1	A	175	ARG	CG-CD-NE	5.91	124.99	112.00
1	D	38	ARG	NH1-CZ-NH2	-5.90	111.62	119.30
1	C	17	ARG	CD-NE-CZ	5.90	132.66	124.40
1	C	19	GLU	N-CA-C	-5.90	101.55	110.28
1	D	299	GLY	CA-C-O	5.90	126.77	120.40
1	D	94	LEU	CA-C-O	-5.88	114.34	120.70
1	A	201	HIS	CA-CB-CG	-5.88	107.92	113.80
1	A	38	ARG	NE-CZ-NH1	5.87	127.36	121.50
1	C	175	ARG	NE-CZ-NH1	-5.86	115.64	121.50
1	D	280	ARG	NE-CZ-NH1	5.86	127.36	121.50
1	C	203	PRO	N-CA-C	5.85	117.84	110.70
1	B	261	LEU	O-C-N	5.83	130.23	123.41
1	B	180	THR	CA-C-O	5.82	127.47	121.07
1	C	299	GLY	O-C-N	-5.81	116.08	122.24
1	D	237	VAL	N-CA-C	5.81	117.28	108.80
1	D	280	ARG	N-CA-C	5.78	119.15	111.75
1	B	11	GLN	CA-C-O	-5.78	115.26	121.56
1	D	27	ARG	NE-CZ-NH2	5.77	124.39	119.20
1	B	236	LYS	N-CA-CB	5.76	119.60	110.55
1	C	54	PHE	CA-CB-CG	-5.76	108.04	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	GLN	OE1-CD-NE2	5.76	128.36	122.60
1	D	279	CYS	O-C-N	-5.75	116.02	122.12
1	A	164	ALA	N-CA-CB	-5.74	101.66	110.44
1	C	279	CYS	CA-C-N	5.74	129.78	120.60
1	C	279	CYS	C-N-CA	5.74	129.78	120.60
1	D	64	GLU	CA-CB-CG	5.73	125.56	114.10
1	B	237	VAL	N-CA-C	5.71	117.14	108.80
1	A	69	TYR	CA-C-O	-5.68	114.69	121.56
1	C	292	HIS	CA-CB-CG	-5.67	108.13	113.80
1	D	295	PRO	CA-C-O	5.67	127.29	119.18
1	A	45	PHE	CA-C-N	5.67	125.65	120.21
1	A	45	PHE	C-N-CA	5.67	125.65	120.21
1	C	220	MET	CA-C-O	-5.66	114.88	120.82
1	A	53	PHE	CA-CB-CG	-5.66	108.14	113.80
1	B	237	VAL	CA-C-O	-5.65	115.91	121.67
1	C	61	ASP	CA-CB-CG	5.63	118.23	112.60
1	D	175	ARG	CD-NE-CZ	5.63	132.28	124.40
1	A	163	ASP	CB-CG-OD1	5.62	131.33	118.40
1	A	165	ALA	N-CA-C	5.62	118.72	109.72
1	B	79	ARG	N-CA-C	5.62	121.19	113.77
1	A	193	CYS	N-CA-C	5.62	117.81	108.99
1	B	299	GLY	N-CA-C	5.61	119.67	112.83
1	D	63	ALA	CA-C-N	5.60	128.06	120.38
1	D	63	ALA	C-N-CA	5.60	128.06	120.38
1	B	175	ARG	NE-CZ-NH2	5.60	124.24	119.20
1	B	134	LYS	N-CA-CB	-5.59	101.86	110.42
1	D	246	LEU	CA-C-O	5.59	127.34	121.19
1	B	289	PHE	CA-CB-CG	5.58	119.39	113.80
1	A	94	LEU	CA-C-O	-5.58	114.67	120.70
1	A	293	ARG	CG-CD-NE	-5.58	99.72	112.00
1	B	135	GLU	CB-CA-C	-5.57	100.61	109.80
1	B	144	HIS	CA-CB-CG	-5.57	108.23	113.80
1	A	40	VAL	O-C-N	-5.56	116.62	122.57
1	D	178	PRO	O-C-N	5.56	129.70	122.24
1	D	235	GLY	CA-C-N	-5.56	115.27	123.05
1	D	235	GLY	C-N-CA	-5.56	115.27	123.05
1	C	154	ASP	CA-C-N	-5.55	113.82	122.37
1	C	154	ASP	C-N-CA	-5.55	113.82	122.37
1	A	68	PHE	CA-CB-CG	-5.54	108.26	113.80
1	A	21	ARG	NE-CZ-NH2	5.54	124.19	119.20
1	D	253	ALA	CA-C-N	5.54	125.21	119.56
1	D	253	ALA	C-N-CA	5.54	125.21	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	ILE	O-C-N	-5.54	116.64	122.68
1	D	237	VAL	CA-C-O	-5.54	116.02	121.67
1	D	266	GLU	CA-C-O	-5.53	115.07	121.49
1	A	304	PHE	CA-C-O	-5.53	111.41	120.80
1	D	161	ASP	CA-C-O	5.52	126.99	120.69
1	D	146	GLU	CA-C-O	-5.51	114.70	120.55
1	C	26	GLY	N-CA-C	-5.50	106.13	112.73
1	D	274	LEU	CB-CA-C	-5.50	98.87	109.37
1	A	61	ASP	CA-CB-CG	5.49	118.09	112.60
1	A	209	ASP	N-CA-C	5.49	117.26	111.28
1	B	166	LYS	CA-C-O	-5.49	114.49	120.36
1	A	6	ILE	CA-C-O	-5.48	114.67	120.53
1	A	12	GLN	CA-C-O	5.47	126.51	120.71
1	D	236	LYS	CA-C-O	-5.47	114.30	120.32
1	C	203	PRO	CB-CA-C	5.47	117.59	110.92
1	D	73	MET	CG-SD-CE	5.45	112.89	100.90
1	D	283	ARG	NE-CZ-NH2	5.45	124.10	119.20
1	C	279	CYS	O-C-N	-5.44	115.85	122.22
1	A	285	HIS	CA-CB-CG	-5.44	108.36	113.80
1	C	75	GLY	N-CA-C	-5.44	105.65	112.23
1	C	139	TYR	CA-C-O	-5.44	113.72	119.97
1	B	151	GLU	O-C-N	5.41	126.07	121.20
1	C	294	GLN	OE1-CD-NE2	-5.41	117.19	122.60
1	B	26	GLY	CA-C-O	-5.40	115.51	120.80
1	D	175	ARG	NE-CZ-NH1	-5.39	116.11	121.50
1	D	20	THR	N-CA-C	5.38	118.09	110.50
1	A	237	VAL	N-CA-C	5.38	116.66	108.80
1	C	279	CYS	CA-C-O	5.38	126.18	120.10
1	C	35	ALA	O-C-N	-5.38	116.53	122.07
1	B	269	VAL	CB-CA-C	-5.37	102.82	110.83
1	C	202	ASN	CA-CB-CG	-5.37	107.23	112.60
1	C	13	GLY	CA-C-N	5.37	125.31	119.78
1	C	13	GLY	C-N-CA	5.37	125.31	119.78
1	C	79	ARG	O-C-N	-5.36	115.53	120.51
1	B	182	ARG	NE-CZ-NH1	5.36	126.86	121.50
1	D	11	GLN	CA-C-N	-5.35	115.17	122.93
1	D	11	GLN	C-N-CA	-5.35	115.17	122.93
1	A	140	ARG	CA-C-N	5.34	124.85	119.19
1	A	140	ARG	C-N-CA	5.34	124.85	119.19
1	A	246	LEU	O-C-N	-5.34	116.45	122.97
1	C	143	GLN	O-C-N	5.34	128.82	122.20
1	C	285	HIS	CA-C-O	-5.34	116.73	119.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	300	LEU	N-CA-CB	5.33	118.43	110.22
1	A	230	TRP	N-CA-C	-5.33	103.50	110.53
1	A	3	ARG	NE-CZ-NH2	5.33	123.99	119.20
1	C	143	GLN	CA-C-O	-5.32	115.38	121.82
1	B	217	LEU	O-C-N	5.32	128.21	122.15
1	B	299	GLY	O-C-N	-5.32	117.01	122.17
1	B	212	THR	CA-CB-OG1	-5.32	101.63	109.60
1	B	293	ARG	NE-CZ-NH2	-5.32	114.42	119.20
1	B	61	ASP	CA-CB-CG	5.31	117.91	112.60
1	D	237	VAL	CB-CA-C	-5.30	102.97	110.82
1	C	71	THR	N-CA-C	-5.30	106.83	113.72
1	A	193	CYS	CA-C-N	-5.28	112.31	120.86
1	A	193	CYS	C-N-CA	-5.28	112.31	120.86
1	B	50	LEU	O-C-N	-5.28	115.74	122.34
1	D	230	TRP	CA-C-O	-5.28	115.81	121.56
1	A	173	ASN	OD1-CG-ND2	-5.27	117.33	122.60
1	D	46	PRO	O-C-N	5.27	129.40	122.86
1	D	174	ASP	CB-CA-C	-5.27	101.72	110.68
1	A	101	VAL	CA-C-O	-5.26	114.85	120.59
1	D	208	HIS	CA-C-O	-5.26	113.27	119.48
1	D	12	GLN	CA-C-N	-5.26	113.61	121.87
1	D	12	GLN	C-N-CA	-5.26	113.61	121.87
1	C	202	ASN	OD1-CG-ND2	5.26	127.86	122.60
1	D	165	ALA	N-CA-C	5.25	118.11	109.72
1	C	274	LEU	CB-CA-C	-5.24	99.35	109.37
1	A	262	THR	CA-C-N	-5.24	114.01	122.23
1	A	262	THR	C-N-CA	-5.24	114.01	122.23
1	B	11	GLN	O-C-N	5.24	129.04	122.86
1	B	111	THR	CA-C-O	-5.23	115.34	121.46
1	D	215	HIS	CB-CG-ND1	5.22	130.53	122.70
1	C	19	GLU	CA-C-O	-5.21	115.33	121.16
1	A	224	SER	CA-C-O	-5.21	115.34	120.70
1	B	122	VAL	CA-C-O	5.20	124.81	119.35
1	D	210	HIS	CA-C-N	5.20	130.97	122.65
1	D	210	HIS	C-N-CA	5.20	130.97	122.65
1	B	203	PRO	N-CA-C	5.19	117.04	110.70
1	C	167	MET	N-CA-C	5.19	117.53	108.76
1	C	192	ILE	CA-C-O	-5.18	115.00	120.39
1	C	11	GLN	CA-C-O	-5.17	115.92	121.56
1	C	141	PRO	O-C-N	-5.17	116.03	122.23
1	D	294	GLN	CA-C-N	5.17	124.83	119.56
1	D	294	GLN	C-N-CA	5.17	124.83	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	LEU	O-C-N	-5.16	116.75	122.07
1	D	113	ILE	N-CA-C	5.16	116.79	108.85
1	A	4	GLN	CA-CB-CG	-5.15	103.80	114.10
1	A	118	SER	CA-CB-OG	5.15	121.39	111.10
1	B	45	PHE	O-C-N	-5.15	116.57	121.20
1	A	165	ALA	N-CA-CB	-5.14	102.28	111.08
1	A	90	ILE	CA-C-O	-5.14	115.03	120.53
1	A	124	LYS	N-CA-CB	-5.14	102.61	111.55
1	C	104	GLY	CA-C-O	-5.14	114.11	119.20
1	C	293	ARG	N-CA-CB	-5.13	102.78	110.17
1	D	121	ILE	O-C-N	-5.13	116.89	122.64
1	D	106	LYS	CA-C-N	-5.13	114.96	122.19
1	D	106	LYS	C-N-CA	-5.13	114.96	122.19
1	D	101	VAL	CA-C-O	-5.12	114.66	120.65
1	C	275	ASP	CA-CB-CG	-5.12	107.48	112.60
1	C	211	LEU	O-C-N	-5.11	116.20	122.34
1	D	203	PRO	N-CA-C	5.11	116.94	110.70
1	D	293	ARG	CD-NE-CZ	5.11	131.55	124.40
1	C	156	GLY	O-C-N	5.11	128.07	122.60
1	C	21	ARG	CD-NE-CZ	5.11	131.55	124.40
1	C	26	GLY	O-C-N	5.11	127.09	122.19
1	B	71	THR	CA-C-O	5.10	124.66	119.05
1	A	118	SER	CB-CA-C	-5.10	99.34	109.99
1	D	146	GLU	N-CA-CB	5.10	117.61	110.12
1	B	232	ALA	CA-C-O	-5.09	114.42	120.43
1	C	33	THR	N-CA-CB	-5.09	102.62	110.01
1	C	174	ASP	CA-CB-CG	5.09	117.69	112.60
1	B	249	SER	CA-C-O	-5.09	116.01	121.56
1	D	125	TYR	O-C-N	-5.08	117.46	123.41
1	D	140	ARG	CA-C-N	5.08	124.74	119.56
1	D	140	ARG	C-N-CA	5.08	124.74	119.56
1	D	230	TRP	N-CA-C	-5.08	103.34	110.50
1	D	93	ASN	CA-CB-CG	5.07	117.67	112.60
1	B	32	LEU	CA-C-N	5.05	127.01	120.44
1	B	32	LEU	C-N-CA	5.05	127.01	120.44
1	C	138	ALA	N-CA-C	5.05	117.44	111.33
1	D	226	GLN	CB-CG-CD	-5.05	104.01	112.60
1	D	74	PRO	CB-CA-C	-5.04	99.39	112.00
1	B	111	THR	N-CA-CB	-5.04	103.03	111.20
1	D	294	GLN	O-C-N	-5.04	116.49	121.17
1	D	269	VAL	CB-CA-C	-5.03	104.00	110.84
1	B	43	ILE	CA-C-N	5.03	128.66	122.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	43	ILE	C-N-CA	5.03	128.66	122.37
1	B	4	GLN	CA-C-O	-5.03	115.23	121.11
1	D	105	VAL	CB-CA-C	-5.03	102.99	110.33
1	D	111	THR	N-CA-CB	-5.01	103.08	111.20
1	A	283	ARG	CA-C-N	-5.01	114.73	122.49
1	A	283	ARG	C-N-CA	-5.01	114.73	122.49
1	B	183	VAL	O-C-N	-5.01	117.00	121.91
1	D	197	ASN	N-CA-CB	5.01	119.03	110.87

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	LYS	Mainchain
1	A	118	SER	Mainchain
1	A	126	ARG	Mainchain
1	A	188	GLY	Mainchain
1	A	190	GLU	Mainchain
1	A	236	LYS	Mainchain
1	A	246	LEU	Mainchain
1	A	54	PHE	Mainchain
1	A	78	VAL	Mainchain
1	B	224	SER	Mainchain
1	B	256	GLY	Mainchain
1	B	87	GLU	Mainchain
1	C	101	VAL	Mainchain
1	C	139	TYR	Mainchain
1	C	184	MET	Mainchain
1	C	217	LEU	Mainchain
1	C	40	VAL	Mainchain
1	C	41	ASN	Mainchain
1	D	200	THR	Mainchain
1	D	236	LYS	Mainchain
1	D	242	GLY	Mainchain
1	D	78	VAL	Mainchain

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	2391	0	2335	48	0
1	B	2391	0	2335	57	0
1	C	2391	0	2335	42	0
1	D	2391	0	2335	78	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	200	0	0	2	0
3	B	202	0	0	2	0
3	C	169	0	0	4	0
3	D	151	0	0	8	0
All	All	10288	0	9340	212	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 11.

All (212) 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:C:7:LEU:HB2	1:C:274:LEU:HD11	1.37	1.05
1:D:20:THR:HG22	1:D:23:GLN:H	1.20	1.03
1:B:10:GLY:HA2	1:B:31:MET:HE1	1.43	0.97
1:D:10:GLY:HA2	1:D:31:MET:HE1	1.45	0.95
1:A:7:LEU:HB2	1:A:274:LEU:HD11	1.47	0.94
1:B:31:MET:HE3	1:B:269:VAL:HG22	1.47	0.94
1:A:21:ARG:HG2	1:A:21:ARG:HH11	1.33	0.92
1:B:175:ARG:HE	1:B:216:HIS:HD2	1.17	0.92
1:B:31:MET:HE3	1:B:269:VAL:CG2	2.03	0.88
1:D:175:ARG:HE	1:D:216:HIS:HD2	1.20	0.86
1:A:175:ARG:HE	1:A:216:HIS:HD2	1.27	0.80
1:D:107:ARG:HG2	1:D:107:ARG:HH11	1.47	0.80
1:B:31:MET:CE	1:B:269:VAL:HG22	2.12	0.79
1:C:7:LEU:CB	1:C:274:LEU:HD11	2.13	0.79
1:D:10:GLY:CA	1:D:31:MET:HE1	2.13	0.79
1:D:31:MET:SD	3:D:448:HOH:O	2.42	0.78
1:C:175:ARG:HE	1:C:216:HIS:HD2	1.30	0.76
1:D:31:MET:HE3	1:D:269:VAL:HG22	1.67	0.76
1:D:7:LEU:HB2	1:D:274:LEU:HD11	1.66	0.75
1:B:7:LEU:HB2	1:B:274:LEU:HD11	1.68	0.75
1:B:10:GLY:CA	1:B:31:MET:HE1	2.17	0.73
1:D:173:ASN:HD21	1:D:177:TRP:HE1	1.33	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:MET:HE3	1:D:269:VAL:CG2	2.18	0.73
1:B:31:MET:SD	3:B:1153:HOH:O	2.47	0.73
3:A:456:HOH:O	1:B:297:HIS:HD2	1.71	0.72
1:D:173:ASN:ND2	1:D:177:TRP:HE1	1.88	0.71
1:B:133:HIS:CE1	1:B:144:HIS:H	2.08	0.71
1:B:100:VAL:HG13	1:B:107:ARG:HB2	1.72	0.70
1:C:142:PHE:HB2	3:C:1169:HOH:O	1.91	0.70
1:B:278:ARG:HH11	1:B:278:ARG:HG3	1.54	0.70
1:D:107:ARG:NH1	1:D:151:GLU:OE2	2.23	0.70
1:B:7:LEU:HD22	1:B:274:LEU:HD11	1.74	0.69
1:D:203:PRO:HB2	1:D:204:PRO:HD3	1.74	0.69
1:C:278:ARG:HE	1:C:281:GLU:CD	2.00	0.69
1:A:69:TYR:CZ	1:A:108:ARG:HD3	2.28	0.68
1:B:201:HIS:HD2	1:B:209:ASP:OD2	1.76	0.68
1:A:7:LEU:CB	1:A:274:LEU:HD11	2.23	0.67
1:B:175:ARG:HE	1:B:216:HIS:CD2	2.08	0.67
1:A:21:ARG:HG2	1:A:21:ARG:NH1	2.05	0.66
1:D:20:THR:HG22	1:D:23:GLN:N	2.02	0.66
1:C:201:HIS:HD2	1:C:209:ASP:OD2	1.79	0.65
1:A:248:HIS:HE1	1:D:257:GLU:OE2	1.81	0.64
1:A:7:LEU:HB2	1:A:274:LEU:CD1	2.25	0.63
1:A:133:HIS:CE1	1:A:144:HIS:H	2.18	0.62
1:C:79:ARG:HG2	1:C:79:ARG:HH11	1.65	0.62
1:D:31:MET:CE	1:D:269:VAL:HG22	2.30	0.61
1:D:175:ARG:HE	1:D:216:HIS:CD2	2.11	0.61
1:A:62:GLU:OE2	1:A:106:LYS:NZ	2.32	0.61
1:C:7:LEU:HB2	1:C:274:LEU:CD1	2.23	0.61
1:B:7:LEU:HB2	1:B:274:LEU:CD1	2.30	0.61
1:A:99:LEU:HD11	1:A:106:LYS:HG3	1.82	0.60
1:D:56:ARG:NH1	1:D:240:GLU:OE1	2.35	0.60
1:D:65:LEU:C	1:D:65:LEU:HD23	2.27	0.60
1:C:182:ARG:HH11	1:C:227:ASN:ND2	2.00	0.59
1:D:10:GLY:HA2	1:D:31:MET:CE	2.27	0.59
1:C:79:ARG:NH1	1:C:83:GLU:OE2	2.35	0.59
1:C:215:HIS:HE1	1:D:255:THR:O	1.86	0.59
1:B:10:GLY:HA2	1:B:31:MET:CE	2.26	0.59
1:B:7:LEU:CB	1:B:274:LEU:HD11	2.33	0.58
1:D:172:CYS:SG	3:D:453:HOH:O	2.21	0.58
1:D:7:LEU:HD22	1:D:274:LEU:HD11	1.86	0.58
1:C:175:ARG:HE	1:C:216:HIS:CD2	2.19	0.57
1:B:201:HIS:HE1	3:B:1182:HOH:O	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:VAL:HA	1:B:245:LEU:HB2	1.87	0.57
1:B:278:ARG:HG3	1:B:278:ARG:NH1	2.20	0.57
1:B:295:PRO:HA	1:B:298:TYR:CD2	2.40	0.57
1:A:201:HIS:HD2	1:A:209:ASP:OD2	1.88	0.56
1:B:7:LEU:CD2	1:B:274:LEU:HD11	2.36	0.56
1:D:15:ILE:HD12	1:D:236:LYS:HE2	1.87	0.56
1:B:100:VAL:CG1	1:B:107:ARG:HB2	2.36	0.56
1:A:5:MET:HG3	1:A:274:LEU:HD12	1.89	0.55
1:C:201:HIS:HE1	3:C:1103:HOH:O	1.88	0.55
1:D:7:LEU:CB	1:D:274:LEU:HD11	2.35	0.55
1:B:175:ARG:NE	1:B:216:HIS:HD2	1.96	0.55
1:C:295:PRO:HA	1:C:298:TYR:CD1	2.43	0.54
1:B:31:MET:HE3	1:B:269:VAL:HG23	1.89	0.54
1:C:25:VAL:O	1:C:29:LEU:HG	2.08	0.54
1:D:182:ARG:HH11	1:D:227:ASN:ND2	2.06	0.54
1:A:147:LYS:NZ	1:B:292:HIS:HD2	2.06	0.53
1:D:100:VAL:CG1	1:D:107:ARG:HB2	2.39	0.53
1:A:133:HIS:HE1	1:A:144:HIS:H	1.55	0.53
1:A:257:GLU:OE2	1:D:248:HIS:HE1	1.92	0.53
1:D:61:ASP:O	1:D:64:GLU:HB3	2.09	0.53
1:C:166:LYS:HE3	1:C:188:GLY:O	2.09	0.53
1:D:56:ARG:HD3	1:D:142:PHE:CD2	2.44	0.52
1:A:255:THR:O	1:B:215:HIS:HE1	1.92	0.52
1:A:215:HIS:HE1	1:B:255:THR:O	1.92	0.52
1:A:216:HIS:HE1	1:A:248:HIS:O	1.93	0.52
1:C:293:ARG:HG3	1:D:177:TRP:CZ3	2.45	0.52
1:D:230:TRP:CD2	1:D:254:PRO:HD3	2.45	0.52
1:C:117:LYS:HE3	3:C:1102:HOH:O	2.09	0.51
1:A:294:GLN:OE1	1:A:296:GLN:NE2	2.44	0.51
1:B:175:ARG:HH21	1:B:216:HIS:CD2	2.29	0.51
1:A:65:LEU:HD22	1:A:69:TYR:HE1	1.74	0.51
1:A:295:PRO:HA	1:A:298:TYR:CD2	2.45	0.51
1:B:9:VAL:HG13	1:B:234:ALA:HB2	1.93	0.51
1:D:20:THR:HG23	1:D:22:GLU:H	1.75	0.51
1:A:47:GLU:HG2	1:A:48:LEU:HG	1.91	0.51
1:D:7:LEU:HB2	1:D:274:LEU:CD1	2.39	0.51
1:D:215:HIS:HD2	3:D:334:HOH:O	1.94	0.51
1:D:295:PRO:HA	1:D:298:TYR:CD2	2.46	0.51
1:D:213:SER:OG	1:D:248:HIS:HD2	1.94	0.50
1:C:5:MET:HG3	1:C:274:LEU:HD12	1.93	0.50
1:B:25:VAL:O	1:B:29:LEU:HG	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:VAL:HG11	1:B:247:GLY:HA2	1.94	0.50
1:C:216:HIS:HE1	1:C:248:HIS:O	1.95	0.50
1:A:69:TYR:CE2	1:A:108:ARG:HD3	2.47	0.49
1:B:133:HIS:HE1	1:B:144:HIS:H	1.59	0.49
1:D:58:HIS:HB2	1:D:136:TYR:HD1	1.77	0.49
1:D:38:ARG:NE	3:D:419:HOH:O	2.45	0.49
1:C:100:VAL:HG12	1:C:107:ARG:HB2	1.93	0.49
1:D:122:VAL:HG11	1:D:161:ASP:O	2.11	0.49
1:C:131:PRO:HG2	1:C:144:HIS:NE2	2.28	0.49
1:A:56:ARG:HA	1:A:143:GLN:O	2.12	0.49
1:B:278:ARG:HE	1:B:281:GLU:CD	2.20	0.49
1:D:20:THR:HB	1:D:23:GLN:OE1	2.11	0.49
1:D:38:ARG:NH1	3:D:423:HOH:O	2.44	0.49
1:D:212:THR:HG22	1:D:246:LEU:HD22	1.95	0.49
1:A:175:ARG:NE	1:A:216:HIS:HD2	2.05	0.49
1:A:213:SER:OG	1:A:248:HIS:HD2	1.96	0.49
1:C:253:ALA:HB1	1:C:254:PRO:HD2	1.94	0.49
1:C:292:HIS:CD2	1:D:147:LYS:NZ	2.80	0.49
1:A:133:HIS:HD2	1:A:135:GLU:O	1.95	0.49
1:D:203:PRO:O	1:D:206:PRO:HD3	2.12	0.49
1:C:100:VAL:CG1	1:C:107:ARG:HB2	2.43	0.48
1:B:133:HIS:HD2	1:B:135:GLU:O	1.97	0.48
1:D:56:ARG:HA	1:D:143:GLN:O	2.13	0.48
1:D:107:ARG:HH11	1:D:107:ARG:CG	2.15	0.48
1:D:76:PRO:HA	1:D:79:ARG:HH21	1.78	0.48
1:A:140:ARG:HG3	1:A:142:PHE:O	2.14	0.48
1:D:9:VAL:HG11	1:D:249:SER:HB3	1.96	0.48
1:A:117:LYS:HG2	1:A:163:ASP:OD1	2.14	0.47
1:D:175:ARG:HH21	1:D:216:HIS:CD2	2.33	0.47
1:A:212:THR:HG22	1:A:246:LEU:HD22	1.97	0.47
1:A:42:PHE:CE1	1:A:167:MET:HE1	2.49	0.47
1:A:298:TYR:CD2	1:B:179:GLU:HG2	2.49	0.47
1:B:61:ASP:HB3	1:B:64:GLU:HB3	1.97	0.47
1:C:9:VAL:HG11	1:C:249:SER:HB3	1.96	0.47
1:D:31:MET:HE3	1:D:269:VAL:HG23	1.96	0.47
1:D:127:LYS:NZ	1:D:172:CYS:HB3	2.30	0.47
1:B:10:GLY:CA	1:B:31:MET:CE	2.90	0.47
1:D:38:ARG:NH2	3:D:419:HOH:O	2.48	0.47
1:A:175:ARG:HE	1:A:216:HIS:CD2	2.19	0.47
1:C:255:THR:O	1:D:215:HIS:HE1	1.97	0.47
1:B:31:MET:HE2	1:B:31:MET:HB3	1.59	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:TRP:CE3	1:B:274:LEU:HD22	2.50	0.47
1:A:203:PRO:HB2	1:A:204:PRO:HD3	1.96	0.46
1:A:215:HIS:HD2	3:A:350:HOH:O	1.98	0.46
1:C:294:GLN:OE1	1:C:296:GLN:NE2	2.48	0.46
1:A:117:LYS:HB3	1:A:117:LYS:HE2	1.59	0.46
1:C:175:ARG:HH21	1:C:216:HIS:CD2	2.33	0.46
1:C:79:ARG:HG2	1:C:79:ARG:NH1	2.31	0.46
1:D:253:ALA:HB1	1:D:254:PRO:HD2	1.97	0.46
1:D:143:GLN:HB3	1:D:145:LEU:HG	1.98	0.46
1:D:192:ILE:O	1:D:231:SER:HA	2.16	0.45
1:A:182:ARG:HA	1:A:227:ASN:HD21	1.81	0.45
1:B:280:ARG:HD3	1:B:284:GLU:OE2	2.16	0.45
1:A:230:TRP:CD2	1:A:254:PRO:HD3	2.52	0.45
1:B:53:PHE:O	1:B:56:ARG:HG2	2.17	0.45
1:C:175:ARG:NE	1:C:216:HIS:HD2	2.08	0.45
1:B:73:MET:HA	1:B:74:PRO:HA	1.72	0.45
1:D:62:GLU:OE2	1:D:106:LYS:NZ	2.50	0.45
1:A:197:ASN:HD21	1:A:236:LYS:NZ	2.14	0.45
1:B:12:GLN:NE2	1:B:236:LYS:HD3	2.31	0.45
1:C:144:HIS:HE1	1:C:146:GLU:OE2	2.00	0.45
1:C:212:THR:HG22	1:C:246:LEU:HD22	1.99	0.44
1:A:139:TYR:C	1:A:139:TYR:CD1	2.94	0.44
1:B:294:GLN:OE1	1:B:296:GLN:NE2	2.51	0.44
1:C:203:PRO:O	1:C:206:PRO:HD3	2.18	0.44
1:D:7:LEU:CD2	1:D:274:LEU:HD11	2.48	0.44
1:C:230:TRP:CD2	1:C:254:PRO:HD3	2.53	0.43
1:D:100:VAL:HG12	1:D:107:ARG:HB2	1.99	0.43
1:B:109:PHE:CE1	1:B:151:GLU:HG3	2.53	0.43
1:B:9:VAL:HG13	1:B:234:ALA:CB	2.47	0.43
1:D:73:MET:HA	1:D:74:PRO:HA	1.65	0.43
1:D:185:GLY:HA2	3:D:387:HOH:O	2.19	0.43
1:A:182:ARG:HH11	1:A:227:ASN:ND2	2.15	0.43
1:B:182:ARG:HA	1:B:182:ARG:HD3	1.88	0.43
1:B:216:HIS:HE1	1:B:248:HIS:O	2.01	0.43
1:A:21:ARG:HH11	1:A:21:ARG:CG	2.07	0.43
1:D:17:ARG:HD2	1:D:57:TRP:CH2	2.54	0.43
1:D:38:ARG:CZ	3:D:419:HOH:O	2.67	0.43
1:D:139:TYR:CD1	1:D:139:TYR:C	2.97	0.43
1:D:237:VAL:HA	1:D:245:LEU:HB2	2.01	0.43
1:C:182:ARG:HH11	1:C:227:ASN:HD21	1.67	0.42
1:A:147:LYS:NZ	1:B:292:HIS:CD2	2.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:HIS:HE1	1:D:248:HIS:O	2.02	0.42
1:B:54:PHE:N	1:B:55:PRO:CD	2.81	0.42
1:C:304:PHE:HB3	1:D:295:PRO:HB2	2.00	0.42
1:D:54:PHE:CG	1:D:55:PRO:HD3	2.54	0.42
1:D:74:PRO:HB3	1:D:78:VAL:HG12	2.00	0.42
1:C:73:MET:HA	1:C:74:PRO:HA	1.70	0.42
1:A:9:VAL:HG11	1:A:249:SER:HB3	2.00	0.42
1:A:73:MET:HA	1:A:74:PRO:HA	1.71	0.42
1:C:210:HIS:HD2	3:C:1026:HOH:O	2.03	0.41
1:B:120:LYS:HD3	1:B:122:VAL:HG12	2.01	0.41
1:D:246:LEU:HG	1:D:247:GLY:O	2.20	0.41
1:D:182:ARG:HH11	1:D:227:ASN:HD21	1.65	0.41
1:D:10:GLY:CA	1:D:31:MET:CE	2.92	0.41
1:B:283:ARG:O	1:B:288:ASN:HA	2.21	0.41
1:D:31:MET:HB3	1:D:31:MET:HE2	1.64	0.41
1:A:170:PHE:O	1:A:194:GLY:HA3	2.20	0.40
1:B:139:TYR:C	1:B:139:TYR:CD1	2.99	0.40
1:B:246:LEU:HG	1:B:247:GLY:O	2.21	0.40
1:B:170:PHE:CD1	1:B:170:PHE:C	2.99	0.40
1:C:294:GLN:HG3	1:D:128:ILE:HG22	2.02	0.40
1:D:127:LYS:HE2	1:D:131:PRO:HD3	2.03	0.40
1:D:201:HIS:HA	1:D:209:ASP:CG	2.46	0.40
1:C:170:PHE:CD1	1:C:170:PHE:C	2.99	0.40
1:D:59:PHE:HD1	1:D:149:TYR:OH	2.05	0.40
1:A:5:MET:CG	1:A:274:LEU:HD12	2.52	0.40
1:C:5:MET:CG	1:C:274:LEU:HD12	2.51	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	300/304 (99%)	290 (97%)	10 (3%)	0	100	100
1	B	300/304 (99%)	291 (97%)	9 (3%)	0	100	100
1	C	300/304 (99%)	294 (98%)	6 (2%)	0	100	100
1	D	300/304 (99%)	288 (96%)	12 (4%)	0	100	100
All	All	1200/1216 (99%)	1163 (97%)	37 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	249/251 (99%)	239 (96%)	10 (4%)	28	17
1	B	249/251 (99%)	246 (99%)	3 (1%)	63	61
1	C	249/251 (99%)	242 (97%)	7 (3%)	38	30
1	D	249/251 (99%)	239 (96%)	10 (4%)	28	17
All	All	996/1004 (99%)	966 (97%)	30 (3%)	36	27

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	65	LEU
1	A	100	VAL
1	A	117	LYS
1	A	118	SER
1	A	131	PRO
1	A	139	TYR
1	A	224	SER
1	A	237	VAL
1	A	280	ARG
1	B	237	VAL
1	B	239	MET
1	B	278	ARG

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Mol	Chain	Res	Type
1	C	4	GLN
1	C	64	GLU
1	C	79	ARG
1	C	135	GLU
1	C	224	SER
1	C	290	LYS
1	C	293	ARG
1	D	20	THR
1	D	56	ARG
1	D	65	LEU
1	D	107	ARG
1	D	135	GLU
1	D	139	TYR
1	D	224	SER
1	D	237	VAL
1	D	280	ARG
1	D	290	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	133	HIS
1	A	197	ASN
1	A	201	HIS
1	A	215	HIS
1	A	216	HIS
1	A	227	ASN
1	A	248	HIS
1	A	292	HIS
1	A	294	GLN
1	A	296	GLN
1	B	12	GLN
1	B	133	HIS
1	B	201	HIS
1	B	215	HIS
1	B	216	HIS
1	B	226	GLN
1	B	292	HIS
1	C	11	GLN
1	C	144	HIS
1	C	201	HIS

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Mol	Chain	Res	Type
1	C	202	ASN
1	C	210	HIS
1	C	215	HIS
1	C	216	HIS
1	C	227	ASN
1	D	34	ASN
1	D	58	HIS
1	D	173	ASN
1	D	215	HIS
1	D	216	HIS
1	D	221	GLN
1	D	227	ASN
1	D	248	HIS
1	D	292	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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.