Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 12:15 AM EDT

PDB ID	:	1FO6
Title	:	CRYSTAL STRUCTURE ANALYSIS OF N-CARBAMoYL-D-AMINO-ACID AMIDOHYDROLASE
Authors	:	Wang, W.-C.; Hsu, W.-H.; Chien, F.-T.; Chen, C.-Y.
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 (i) 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 (i)) were used in the production of this report:

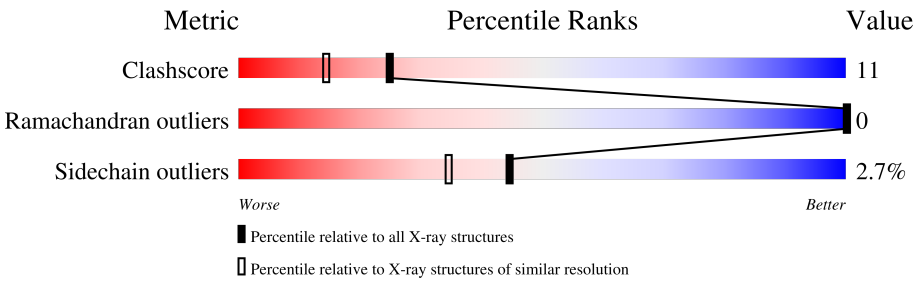
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 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	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	304	75% 18% 6% ••
1	B	304	75% 21% • •
1	C	304	73% 24% •••
1	D	304	67% 27% 5% ••

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	302	2391	1527	419	431	14	0	0	0
1	B	302	2391	1527	419	431	14	0	0	0
1	C	302	2391	1527	419	431	14	0	0	0
1	D	302	2391	1527	419	431	14	0	0	0

- Molecule 2 is XENON (three-letter code: XE) (formula: Xe).

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

- Molecule 3 is water.

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

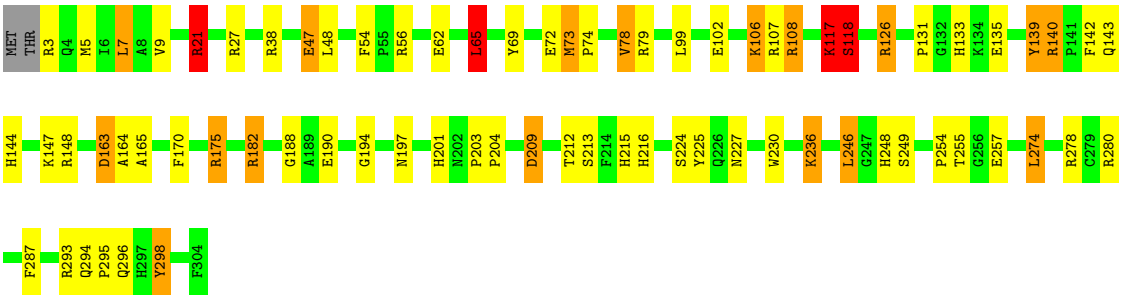
3 Residue-property plots (i)

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

Chain A:

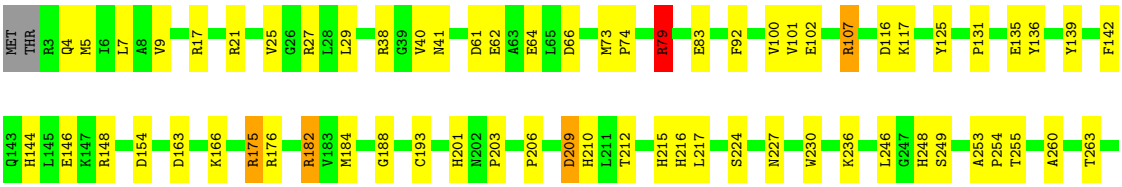


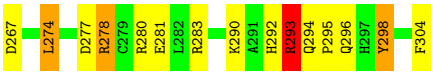
• Molecule 1: N-CARBAMoYL-D-AMINO-ACID AMIDOHYDROLASE

Chain B:

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

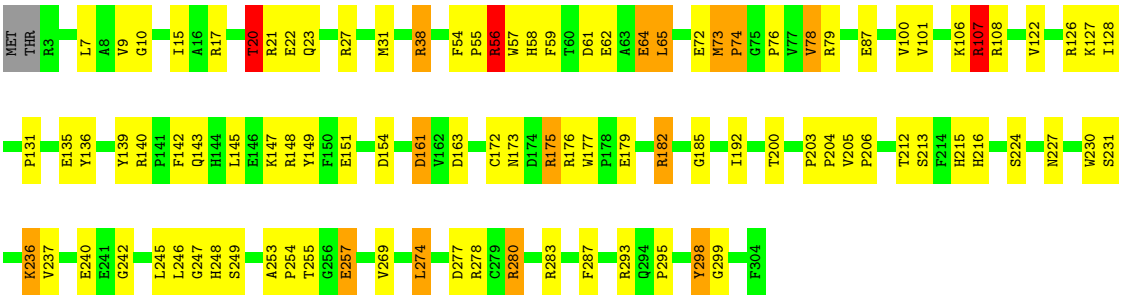
Chain C:





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

Chain D:



4 Data and refinement statistics (i)

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 (i)

5.1 Standard geometry (i)

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	0.98	0/2455	1.84	48/3327 (1.4%)
1	B	0.95	0/2455	1.71	33/3327 (1.0%)
1	C	0.87	0/2455	1.81	48/3327 (1.4%)
1	D	0.89	0/2455	2.15	54/3327 (1.6%)
All	All	0.92	0/9820	1.89	183/13308 (1.4%)

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

There are no bond length outliers.

All (183) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	38	ARG	CD-NE-CZ	39.53	178.94	123.60
1	D	56	ARG	CD-NE-CZ	36.00	174.00	123.60
1	C	38	ARG	NE-CZ-NH2	-28.27	106.17	120.30
1	D	107	ARG	NE-CZ-NH2	27.48	134.04	120.30
1	D	107	ARG	NE-CZ-NH1	-21.34	109.63	120.30
1	D	38	ARG	NE-CZ-NH2	20.91	130.76	120.30
1	D	280	ARG	CD-NE-CZ	19.52	150.92	123.60
1	D	278	ARG	CD-NE-CZ	19.09	150.33	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	108	ARG	NE-CZ-NH1	-19.09	110.76	120.30
1	C	38	ARG	NE-CZ-NH1	18.40	129.50	120.30
1	A	140	ARG	NE-CZ-NH1	16.42	128.51	120.30
1	A	140	ARG	NE-CZ-NH2	-15.51	112.55	120.30
1	A	108	ARG	NE-CZ-NH2	14.98	127.79	120.30
1	A	280	ARG	CD-NE-CZ	14.63	144.09	123.60
1	A	163	ASP	CB-CG-OD1	14.48	131.33	118.30
1	A	38	ARG	NE-CZ-NH1	14.13	127.36	120.30
1	D	280	ARG	NE-CZ-NH1	14.12	127.36	120.30
1	B	182	ARG	NE-CZ-NH2	-13.95	113.32	120.30
1	C	280	ARG	CD-NE-CZ	13.89	143.05	123.60
1	C	278	ARG	NE-CZ-NH2	-13.82	113.39	120.30
1	D	140	ARG	NE-CZ-NH2	-13.81	113.40	120.30
1	A	140	ARG	CD-NE-CZ	13.21	142.09	123.60
1	B	182	ARG	NE-CZ-NH1	13.11	126.86	120.30
1	B	175	ARG	NE-CZ-NH1	-12.25	114.17	120.30
1	B	293	ARG	NE-CZ-NH2	-11.77	114.42	120.30
1	B	56	ARG	NE-CZ-NH1	11.62	126.11	120.30
1	D	148	ARG	NE-CZ-NH1	11.42	126.01	120.30
1	C	267	ASP	CB-CG-OD1	11.08	128.27	118.30
1	A	293	ARG	NE-CZ-NH2	-10.95	114.83	120.30
1	B	163	ASP	CB-CG-OD1	10.83	128.05	118.30
1	A	280	ARG	NE-CZ-NH1	10.81	125.70	120.30
1	B	280	ARG	NE-CZ-NH1	10.52	125.56	120.30
1	A	107	ARG	NE-CZ-NH2	-10.43	115.08	120.30
1	D	163	ASP	CB-CG-OD2	10.20	127.48	118.30
1	A	27	ARG	NE-CZ-NH2	-10.10	115.25	120.30
1	A	27	ARG	NE-CZ-NH1	9.91	125.25	120.30
1	A	107	ARG	NE-CZ-NH1	9.85	125.23	120.30
1	D	161	ASP	CB-CG-OD1	9.82	127.14	118.30
1	C	163	ASP	CB-CG-OD2	9.76	127.09	118.30
1	C	17	ARG	NE-CZ-NH2	9.62	125.11	120.30
1	D	56	ARG	NE-CZ-NH1	9.58	125.09	120.30
1	A	73	MET	CG-SD-CE	9.54	115.46	100.20
1	B	79	ARG	CD-NE-CZ	9.52	136.92	123.60
1	C	21	ARG	NE-CZ-NH1	9.37	124.99	120.30
1	C	175	ARG	NE-CZ-NH1	-9.32	115.64	120.30
1	B	257	GLU	OE1-CD-OE2	-9.10	112.38	123.30
1	C	182	ARG	NE-CZ-NH2	-9.09	115.75	120.30
1	D	56	ARG	NE-CZ-NH2	8.94	124.77	120.30
1	B	283	ARG	NE-CZ-NH2	8.84	124.72	120.30
1	A	108	ARG	CD-NE-CZ	-8.82	111.25	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	277	ASP	CB-CG-OD2	8.80	126.22	118.30
1	D	278	ARG	NE-CZ-NH2	-8.58	116.01	120.30
1	C	175	ARG	NE-CZ-NH2	8.51	124.55	120.30
1	C	298	TYR	CB-CG-CD2	8.49	126.10	121.00
1	D	56	ARG	NH1-CZ-NH2	-8.42	110.14	119.40
1	D	175	ARG	NE-CZ-NH1	-8.38	116.11	120.30
1	B	280	ARG	CD-NE-CZ	8.35	135.29	123.60
1	A	38	ARG	NE-CZ-NH2	-8.30	116.15	120.30
1	C	278	ARG	NH1-CZ-NH2	8.23	128.45	119.40
1	C	148	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	D	27	ARG	NE-CZ-NH2	8.18	124.39	120.30
1	D	21	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	C	116	ASP	CB-CG-OD1	8.10	125.59	118.30
1	D	72	GLU	CA-CB-CG	7.95	130.90	113.40
1	C	107	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	D	73	MET	CG-SD-CE	7.93	112.89	100.20
1	B	175	ARG	NE-CZ-NH2	7.88	124.24	120.30
1	C	176	ARG	NE-CZ-NH2	-7.85	116.38	120.30
1	C	176	ARG	NE-CZ-NH1	7.85	124.22	120.30
1	D	148	ARG	NE-CZ-NH2	-7.83	116.39	120.30
1	C	102	GLU	OE1-CD-OE2	7.82	132.68	123.30
1	A	21	ARG	NE-CZ-NH2	7.77	124.19	120.30
1	D	107	ARG	CG-CD-NE	7.77	128.12	111.80
1	C	283	ARG	NE-CZ-NH2	-7.69	116.46	120.30
1	D	283	ARG	NE-CZ-NH2	7.61	124.10	120.30
1	D	140	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	A	163	ASP	CB-CG-OD2	-7.54	111.51	118.30
1	A	3	ARG	NE-CZ-NH2	7.38	123.99	120.30
1	D	277	ASP	CB-CG-OD1	7.35	124.91	118.30
1	A	182	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	C	298	TYR	CB-CG-CD1	-7.25	116.65	121.00
1	C	154	ASP	CB-CG-OD1	7.20	124.78	118.30
1	D	27	ARG	NE-CZ-NH1	-7.10	116.75	120.30
1	C	283	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	B	107	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	D	38	ARG	NH1-CZ-NH2	-7.07	111.62	119.40
1	C	21	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	D	20	THR	N-CA-CB	-6.93	97.13	110.30
1	D	182	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	C	209	ASP	CB-CG-OD1	6.84	124.45	118.30
1	B	160	TYR	CZ-CE2-CD2	-6.82	113.66	119.80
1	B	140	ARG	NE-CZ-NH1	-6.80	116.90	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	27	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	C	17	ARG	NE-CZ-NH1	-6.77	116.92	120.30
1	C	79	ARG	NE-CZ-NH2	6.69	123.65	120.30
1	D	280	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	A	47	GLU	OE1-CD-OE2	-6.65	115.32	123.30
1	D	126	ARG	NE-CZ-NH2	6.63	123.62	120.30
1	A	148	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	D	176	ARG	NE-CZ-NH1	-6.59	117.00	120.30
1	A	274	LEU	CB-CA-C	-6.54	97.77	110.20
1	B	38	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	B	175	ARG	CG-CD-NE	6.50	125.44	111.80
1	D	257	GLU	OE1-CD-OE2	-6.49	115.51	123.30
1	C	17	ARG	CD-NE-CZ	6.47	132.66	123.60
1	B	56	ARG	NE-CZ-NH2	-6.45	117.07	120.30
1	A	280	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	C	148	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	D	298	TYR	CB-CG-CD2	-6.31	117.22	121.00
1	A	38	ARG	CD-NE-CZ	-6.28	114.80	123.60
1	A	175	ARG	CG-CD-NE	6.28	124.99	111.80
1	C	277	ASP	CB-CG-OD1	-6.25	112.67	118.30
1	A	287	PHE	CB-CG-CD1	6.21	125.14	120.80
1	D	175	ARG	CD-NE-CZ	6.20	132.28	123.60
1	C	61	ASP	CB-CG-OD2	6.20	123.88	118.30
1	B	3	ARG	NE-CZ-NH1	-6.18	117.21	120.30
1	A	106	LYS	CA-CB-CG	6.17	126.98	113.40
1	B	293	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	C	293	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	B	18	ALA	CB-CA-C	6.04	119.16	110.10
1	A	164	ALA	N-CA-CB	-6.03	101.66	110.10
1	D	274	LEU	CB-CA-C	-5.96	98.87	110.20
1	B	209	ASP	CB-CG-OD1	5.88	123.59	118.30
1	C	136	TYR	CB-CG-CD1	-5.86	117.48	121.00
1	A	293	ARG	CG-CD-NE	-5.75	99.72	111.80
1	D	101	VAL	CA-CB-CG2	-5.72	102.31	110.90
1	C	92	PHE	CB-CG-CD2	-5.72	116.79	120.80
1	C	125	TYR	CB-CG-CD2	5.71	124.43	121.00
1	C	274	LEU	CB-CA-C	-5.71	99.35	110.20
1	C	263	THR	CA-CB-CG2	-5.71	104.41	112.40
1	D	293	ARG	CD-NE-CZ	5.68	131.55	123.60
1	C	21	ARG	CD-NE-CZ	5.68	131.55	123.60
1	A	118	SER	CB-CA-C	-5.67	99.34	110.10
1	C	260	ALA	N-CA-CB	5.66	118.03	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	102	GLU	OE1-CD-OE2	5.65	130.08	123.30
1	C	116	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	A	209	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	A	165	ALA	N-CA-CB	-5.58	102.28	110.10
1	A	126	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	79	ARG	CD-NE-CZ	5.54	131.35	123.60
1	A	78	VAL	O-C-N	-5.54	113.84	122.70
1	D	21	ARG	NH1-CZ-NH2	-5.53	113.31	119.40
1	D	64	GLU	CA-CB-CG	5.53	125.56	113.40
1	D	163	ASP	CB-CG-OD1	-5.48	113.36	118.30
1	D	154	ASP	CB-CG-OD1	5.46	123.22	118.30
1	D	161	ASP	OD1-CG-OD2	-5.45	112.95	123.30
1	A	126	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	D	38	ARG	NE-CZ-NH1	-5.41	117.59	120.30
1	C	293	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	D	299	GLY	O-C-N	-5.40	114.06	122.70
1	D	148	ARG	CD-NE-CZ	5.40	131.16	123.60
1	B	103	GLY	O-C-N	-5.38	114.06	123.20
1	B	280	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	C	66	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	65	LEU	CA-CB-CG	5.37	127.64	115.30
1	B	27	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	B	126	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	D	293	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	A	298	TYR	CB-CG-CD2	-5.32	117.81	121.00
1	C	280	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	C	236	LYS	N-CA-C	-5.29	96.71	111.00
1	B	61	ASP	CB-CG-OD1	5.28	123.05	118.30
1	C	193	CYS	C-N-CA	-5.26	111.25	122.30
1	D	205	VAL	CG1-CB-CG2	-5.24	102.52	110.90
1	D	179	GLU	OE1-CD-OE2	5.23	129.57	123.30
1	A	278	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	A	293	ARG	NH1-CZ-NH2	5.19	125.11	119.40
1	B	154	ASP	CB-CG-OD1	5.18	122.96	118.30
1	B	38	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	D	87	GLU	OE1-CD-OE2	-5.15	117.12	123.30
1	A	225	TYR	CB-CG-CD2	5.14	124.09	121.00
1	C	175	ARG	CG-CD-NE	5.14	122.59	111.80
1	A	72	GLU	OE1-CD-OE2	5.11	129.44	123.30
1	B	73	MET	CG-SD-CE	5.11	108.38	100.20
1	D	287	PHE	CB-CG-CD2	-5.11	117.22	120.80
1	B	109	PHE	CB-CG-CD2	-5.09	117.24	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	8	ALA	CB-CA-C	-5.05	102.52	110.10
1	D	108	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	D	74	PRO	CB-CA-C	-5.04	99.39	112.00
1	B	17	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	21	ARG	NE-CZ-NH1	-5.04	117.78	120.30
1	A	148	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	A	7	LEU	CB-CG-CD1	-5.01	102.48	111.00

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 (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	2391	0	2335	47	0
1	B	2391	0	2335	55	0
1	C	2391	0	2335	41	0
1	D	2391	0	2335	75	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	205	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 (205) 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:31:MET:HE3	1:B:269:VAL:HG22	1.43	0.98
1:A:7:LEU:HB2	1:A:274:LEU:HD11	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:D:31:MET:HE3	1:D:269:VAL:HG22	1.55	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:B:31:MET:HE3	1:B:269:VAL:CG2	2.11	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:31:MET:HE3	1:D:269:VAL:CG2	2.14	0.78
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: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:D:173:ASN:HD21	1:D:177:TRP:HE1	1.33	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:D:10:GLY:HA2	1:D:31:MET:HE1	1.71	0.71
1:B:133:HIS:CE1	1:B:144:HIS:H	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:10:GLY:HA2	1:B:31:MET:CE	2.26	0.66
1:C:201:HIS:HD2	1:C:209:ASP:OD2	1.79	0.65
1:D:10:GLY:HA2	1:D:31:MET:CE	2.27	0.65
1:C:278:ARG:HE	1:C:281:GLU:CD	2.00	0.64
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: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:C:182:ARG:HH11	1:C:227:ASN:ND2	2.00	0.59
1:B:10:GLY:HA2	1:B:31:MET:HE1	1.85	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:CA	1:B:31:MET:HE2	2.33	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:65:LEU:C	1:D:65:LEU:HD23	2.27	0.54
1:C:295:PRO:HA	1:C:298:TYR:CD1	2.43	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:B:10:GLY:HA2	1:B:31:MET:HE2	1.90	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:A:62:GLU:OE2	1:A:106:LYS:NZ	2.32	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:10:GLY:CA	1:B:31:MET:CE	2.90	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: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:127:LYS:NZ	1:D:172:CYS:HB3	2.30	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: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:D:10:GLY:CA	1:D:31:MET:CE	2.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:GLY:HA3	1:B:31:MET:HE2	1.97	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:B:278:ARG:HE	1:B:281:GLU:CD	2.20	0.44
1:C:212:THR:HG22	1:C:246:LEU:HD22	1.99	0.44
1:D:31:MET:HE3	1:D:269:VAL:HG23	1.99	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:MET:HA	1:C:74:PRO:HA	1.70	0.42
1:D:10:GLY:CA	1:D:31:MET:HE2	2.50	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:B:283:ARG:O	1:B:288:ASN:HA	2.21	0.41
1:A:170:PHE:O	1:A:194:GLY:HA3	2.20	0.40
1:A:139:TYR:C	1:A:139:TYR:CD1	2.94	0.40
1:B:246:LEU:HG	1:B:247:GLY:O	2.21	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: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 (i)

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%)	242 (97%)	7 (3%)	43	33
1	B	249/251 (99%)	245 (98%)	4 (2%)	62	58
1	C	249/251 (99%)	241 (97%)	8 (3%)	39	27
1	D	249/251 (99%)	241 (97%)	8 (3%)	39	27
All	All	996/1004 (99%)	969 (97%)	27 (3%)	44	34

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	65	LEU
1	A	117	LYS
1	A	118	SER
1	A	131	PRO
1	A	139	TYR
1	A	224	SER
1	B	134	LYS
1	B	139	TYR
1	B	239	MET
1	B	278	ARG
1	C	4	GLN
1	C	62	GLU
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

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Mol	Chain	Res	Type
1	D	139	TYR
1	D	224	SER
1	D	280	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) 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	B	12	GLN
1	B	133	HIS
1	B	201	HIS
1	B	215	HIS
1	B	216	HIS
1	B	292	HIS
1	C	11	GLN
1	C	201	HIS
1	C	202	ASN
1	C	210	HIS
1	C	215	HIS
1	C	216	HIS
1	C	227	ASN
1	D	173	ASN
1	D	215	HIS
1	D	216	HIS
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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.