



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 04:33 PM UTC

PDB ID : 4G3H / pdb_00004g3h
Title : Crystal structure of helicobacter pylori arginase
Authors : Zhang, J.; Zhang, X.; Li, D.; Hu, Y.; Zou, Q.; Wang, D.
Deposited on : 2012-07-13
Resolution : 2.20 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

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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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

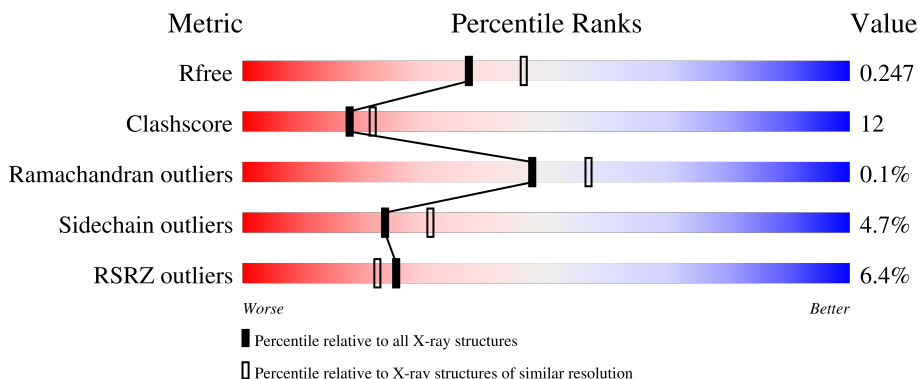
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	330	5% 62% 26% • 9%
1	B	330	6% 64% 25% • 8%
1	C	330	6% 67% 23% • 6%
1	D	330	6% 62% 27% • 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10439 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 Arginase (RocF).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	S	0	0	0
			2419	1539	411	454	15			
1	B	305	Total	C	N	O	S	0	0	0
			2447	1551	417	465	14			
1	C	310	Total	C	N	O	S	6	0	0
			2491	1581	424	471	15			
1	D	300	Total	C	N	O	S	0	0	0
			2399	1524	407	453	15			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	323	LEU	-	expression tag	UNP O25949
A	324	GLU	-	expression tag	UNP O25949
A	325	HIS	-	expression tag	UNP O25949
A	326	HIS	-	expression tag	UNP O25949
A	327	HIS	-	expression tag	UNP O25949
A	328	HIS	-	expression tag	UNP O25949
A	329	HIS	-	expression tag	UNP O25949
A	330	HIS	-	expression tag	UNP O25949
B	323	LEU	-	expression tag	UNP O25949
B	324	GLU	-	expression tag	UNP O25949
B	325	HIS	-	expression tag	UNP O25949
B	326	HIS	-	expression tag	UNP O25949
B	327	HIS	-	expression tag	UNP O25949
B	328	HIS	-	expression tag	UNP O25949
B	329	HIS	-	expression tag	UNP O25949
B	330	HIS	-	expression tag	UNP O25949
C	323	LEU	-	expression tag	UNP O25949
C	324	GLU	-	expression tag	UNP O25949
C	325	HIS	-	expression tag	UNP O25949
C	326	HIS	-	expression tag	UNP O25949
C	327	HIS	-	expression tag	UNP O25949

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Chain	Residue	Modelled	Actual	Comment	Reference
C	328	HIS	-	expression tag	UNP O25949
C	329	HIS	-	expression tag	UNP O25949
C	330	HIS	-	expression tag	UNP O25949
D	323	LEU	-	expression tag	UNP O25949
D	324	GLU	-	expression tag	UNP O25949
D	325	HIS	-	expression tag	UNP O25949
D	326	HIS	-	expression tag	UNP O25949
D	327	HIS	-	expression tag	UNP O25949
D	328	HIS	-	expression tag	UNP O25949
D	329	HIS	-	expression tag	UNP O25949
D	330	HIS	-	expression tag	UNP O25949

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

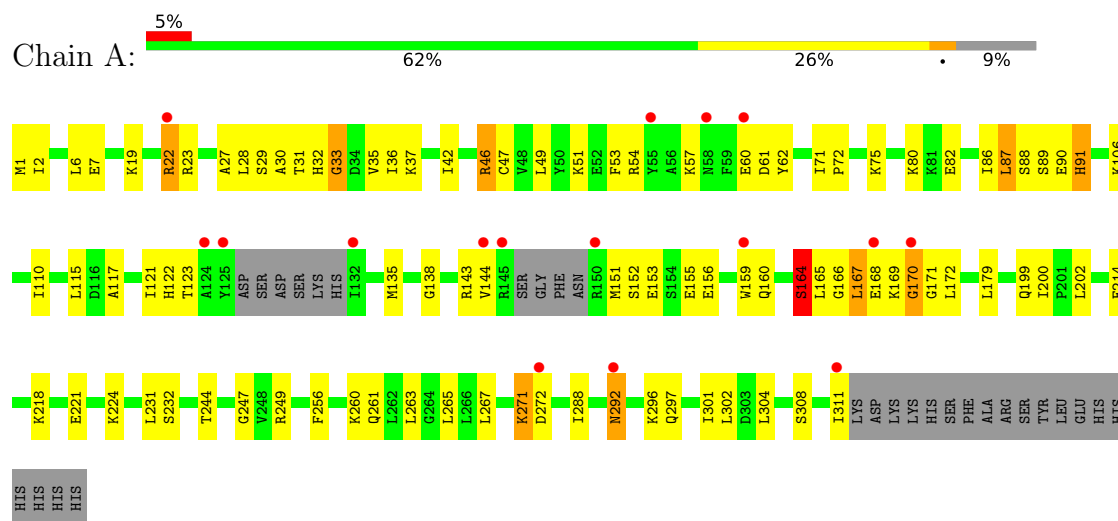
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	174	Total 174	O 174	0	0
3	B	153	Total 153	O 153	0	0
3	C	168	Total 168	O 168	0	0
3	D	180	Total 180	O 180	0	0

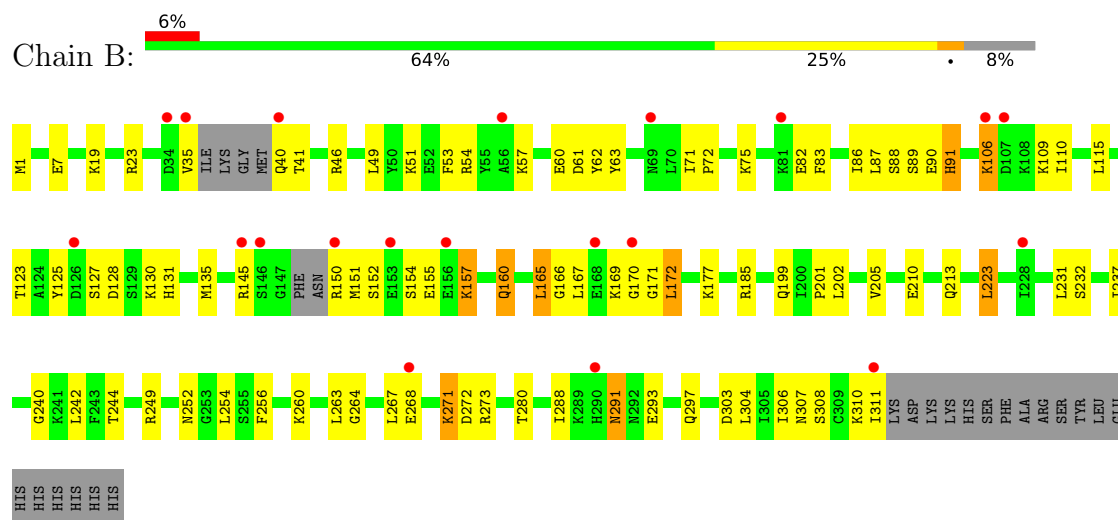
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Arginase (RocF)

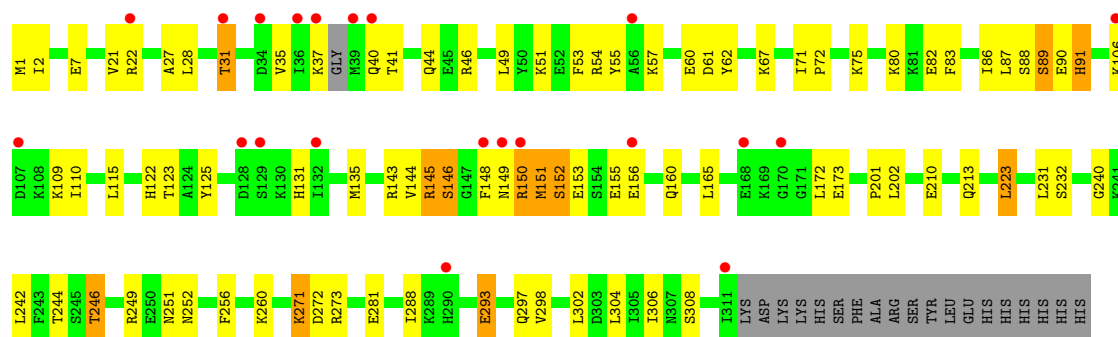


• Molecule 1: Arginase (RocF)

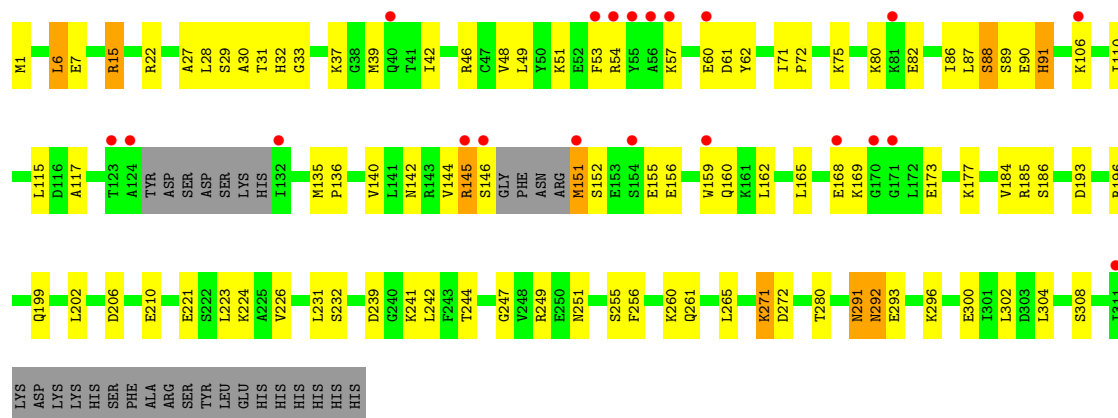


• Molecule 1: Arginase (RocF)





● Molecule 1: Arginase (RocF)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	94.69Å 102.24Å 148.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.90 – 2.20 34.90 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (34.90-2.20) 99.9 (34.90-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.62 (at 2.20Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.218 , 0.230 0.208 , 0.247	Depositor DCC
R_{free} test set	7448 reflections (10.10%)	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	1.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10439	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.93 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.5344e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.61	58/2453 (2.4%)	1.14	27/3289 (0.8%)
1	B	0.99	20/2482 (0.8%)	1.04	12/3329 (0.4%)
1	C	0.72	8/2528 (0.3%)	0.94	16/3391 (0.5%)
1	D	1.60	47/2432 (1.9%)	1.05	21/3261 (0.6%)
All	All	1.28	133/9895 (1.3%)	1.04	76/13270 (0.6%)

All (133) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	184	VAL	C-O	-25.22	0.99	1.24
1	D	89	SER	C-O	-23.32	0.94	1.24
1	A	89	SER	C-O	-23.05	0.94	1.24
1	D	88	SER	C-O	-20.77	0.97	1.24
1	D	185	ARG	C-O	-19.73	1.00	1.23
1	D	28	LEU	C-O	-18.51	1.02	1.24
1	A	29	SER	C-O	-18.27	1.02	1.24
1	D	30	ALA	C-O	-17.98	1.03	1.24
1	B	89	SER	C-O	-17.46	1.01	1.24
1	A	88	SER	C-O	-17.00	1.02	1.24
1	C	88	SER	C-O	-16.49	1.02	1.24
1	A	33	GLY	C-O	-15.96	1.03	1.23
1	B	165	LEU	C-O	-15.84	1.04	1.23
1	C	89	SER	C-O	-15.50	1.04	1.24
1	A	27	ALA	C-O	-15.32	1.06	1.24
1	B	88	SER	C-O	-15.07	1.04	1.24
1	A	30	ALA	C-O	-15.04	1.06	1.24
1	A	28	LEU	C-O	-14.73	1.06	1.24
1	A	171	GLY	C-O	-14.06	1.08	1.24
1	D	29	SER	C-O	-13.08	1.08	1.24
1	A	87	LEU	C-O	-12.72	1.06	1.23
1	D	27	ALA	C-O	-12.41	1.09	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	90	GLU	C-O	-11.83	1.08	1.24
1	A	172	LEU	C-O	-11.66	1.08	1.23
1	A	32	HIS	C-O	-11.44	1.10	1.24
1	A	165	LEU	C-O	-11.36	1.10	1.23
1	D	32	HIS	C-O	-11.31	1.09	1.24
1	D	87	LEU	C-O	-11.00	1.08	1.23
1	D	29	SER	N-CA	-10.94	1.33	1.46
1	D	89	SER	CB-OG	-10.79	1.20	1.42
1	A	166	GLY	C-O	-10.74	1.09	1.24
1	D	29	SER	CB-OG	-10.67	1.20	1.42
1	B	90	GLU	C-O	-10.58	1.11	1.24
1	B	167	LEU	C-O	-10.10	1.10	1.24
1	A	164	SER	C-O	-10.08	1.10	1.24
1	D	184	VAL	CB-CG2	-10.08	1.19	1.52
1	D	186	SER	N-CA	-10.08	1.34	1.46
1	B	89	SER	CB-OG	-10.06	1.22	1.42
1	A	31	THR	C-O	-9.57	1.11	1.24
1	A	29	SER	CB-OG	-9.56	1.23	1.42
1	C	89	SER	CB-OG	-9.52	1.23	1.42
1	C	90	GLU	C-O	-9.37	1.11	1.24
1	D	186	SER	C-O	-9.33	1.12	1.24
1	D	87	LEU	CG-CD1	-9.31	1.21	1.52
1	A	29	SER	N-CA	-9.15	1.35	1.46
1	B	166	GLY	C-O	-9.03	1.11	1.24
1	A	169	LYS	N-CA	-9.01	1.34	1.46
1	D	185	ARG	CZ-NH1	-8.89	1.20	1.32
1	B	169	LYS	C-O	-8.87	1.14	1.23
1	A	88	SER	CB-OG	-8.87	1.24	1.42
1	D	87	LEU	CG-CD2	-8.85	1.23	1.52
1	A	165	LEU	CG-CD1	-8.69	1.23	1.52
1	A	30	ALA	N-CA	-8.55	1.36	1.46
1	D	30	ALA	CA-CB	-8.46	1.40	1.53
1	D	186	SER	CB-OG	-8.37	1.25	1.42
1	A	172	LEU	C-N	-8.36	1.22	1.33
1	C	88	SER	CB-OG	-8.24	1.25	1.42
1	B	169	LYS	N-CA	-8.21	1.36	1.46
1	D	31	THR	CB-CG2	-8.17	1.25	1.52
1	A	167	LEU	CG-CD2	-8.16	1.25	1.52
1	A	87	LEU	CG-CD1	-8.12	1.25	1.52
1	D	28	LEU	CG-CD2	-8.01	1.26	1.52
1	D	88	SER	CB-OG	-7.95	1.26	1.42
1	D	90	GLU	C-O	-7.90	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	32	HIS	N-CA	-7.84	1.36	1.46
1	A	87	LEU	CG-CD2	-7.77	1.26	1.52
1	D	31	THR	C-O	-7.74	1.12	1.25
1	D	30	ALA	N-CA	-7.70	1.37	1.46
1	C	89	SER	N-CA	-7.66	1.36	1.46
1	A	171	GLY	CA-C	-7.64	1.43	1.51
1	A	27	ALA	N-CA	-7.58	1.37	1.46
1	D	185	ARG	CZ-NH2	-7.56	1.23	1.33
1	D	185	ARG	C-N	-7.43	1.23	1.33
1	A	31	THR	CB-CG2	-7.35	1.28	1.52
1	A	28	LEU	N-CA	-7.27	1.37	1.46
1	B	88	SER	CB-OG	-7.25	1.27	1.42
1	A	89	SER	CB-OG	-7.24	1.27	1.42
1	A	31	THR	N-CA	-7.20	1.36	1.46
1	A	165	LEU	CA-C	-7.14	1.43	1.52
1	C	87	LEU	C-N	-7.05	1.24	1.33
1	D	186	SER	CA-C	-6.95	1.44	1.52
1	A	167	LEU	C-O	-6.87	1.14	1.24
1	D	90	GLU	CA-C	-6.71	1.44	1.52
1	D	87	LEU	N-CA	-6.70	1.38	1.46
1	A	30	ALA	CA-CB	-6.69	1.42	1.53
1	D	185	ARG	CG-CD	-6.68	1.32	1.52
1	B	171	GLY	C-O	-6.65	1.14	1.23
1	D	28	LEU	N-CA	-6.63	1.38	1.46
1	A	89	SER	N-CA	-6.61	1.37	1.46
1	D	28	LEU	C-N	-6.57	1.25	1.33
1	A	32	HIS	CD2-NE2	-6.54	1.30	1.37
1	B	90	GLU	CB-CG	-6.54	1.32	1.52
1	A	27	ALA	CA-CB	-6.52	1.43	1.53
1	A	165	LEU	CB-CG	-6.52	1.40	1.53
1	A	172	LEU	CA-C	-6.52	1.44	1.53
1	A	86	ILE	C-N	-6.50	1.24	1.33
1	A	164	SER	N-CA	-6.50	1.37	1.46
1	B	87	LEU	C-N	-6.28	1.24	1.33
1	A	171	GLY	C-N	-6.24	1.24	1.33
1	D	29	SER	CA-CB	-6.23	1.43	1.53
1	B	165	LEU	CA-C	-6.21	1.44	1.52
1	A	32	HIS	CA-C	6.08	1.60	1.52
1	D	28	LEU	CG-CD1	-6.08	1.32	1.52
1	D	32	HIS	CD2-NE2	-6.07	1.31	1.37
1	A	165	LEU	C-N	-6.00	1.24	1.33
1	B	169	LYS	CA-C	-5.99	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	28	LEU	CG-CD2	-5.89	1.33	1.52
1	B	165	LEU	CG-CD1	-5.87	1.33	1.52
1	B	166	GLY	N-CA	-5.78	1.36	1.45
1	B	165	LEU	C-N	-5.77	1.25	1.33
1	D	90	GLU	CB-CG	-5.75	1.35	1.52
1	A	90	GLU	CD-OE2	-5.73	1.14	1.25
1	D	86	ILE	C-N	-5.72	1.25	1.33
1	B	89	SER	N-CA	-5.71	1.38	1.46
1	A	28	LEU	CG-CD1	-5.69	1.33	1.52
1	A	28	LEU	C-N	-5.69	1.26	1.33
1	A	164	SER	CB-OG	-5.67	1.30	1.42
1	A	87	LEU	N-CA	-5.51	1.39	1.46
1	B	165	LEU	CB-CG	-5.49	1.42	1.53
1	A	165	LEU	CG-CD2	-5.46	1.34	1.52
1	A	90	GLU	N-CA	-5.42	1.39	1.46
1	D	27	ALA	C-N	-5.41	1.26	1.33
1	D	27	ALA	CA-C	5.34	1.59	1.52
1	A	172	LEU	CG-CD2	-5.34	1.34	1.52
1	D	32	HIS	ND1-CE1	-5.31	1.27	1.32
1	D	89	SER	C-N	-5.25	1.26	1.33
1	A	32	HIS	CG-ND1	-5.23	1.32	1.38
1	A	89	SER	C-N	-5.22	1.25	1.33
1	D	87	LEU	C-N	-5.20	1.26	1.33
1	C	90	GLU	CD-OE2	-5.18	1.15	1.25
1	A	29	SER	CA-CB	-5.16	1.45	1.53
1	A	88	SER	N-CA	-5.04	1.39	1.46
1	D	88	SER	C-N	-5.00	1.26	1.33

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	171	GLY	N-CA-C	19.78	134.67	111.93
1	B	128	ASP	N-CA-C	-13.28	90.62	110.28
1	A	170	GLY	N-CA-C	10.58	126.01	112.68
1	C	149	ASN	N-CA-C	-10.28	93.97	110.20
1	A	169	LYS	N-CA-C	-9.93	101.11	113.02
1	B	170	GLY	N-CA-C	8.54	126.72	115.36
1	B	127	SER	N-CA-C	-8.36	101.41	111.69
1	A	168	GLU	N-CA-C	8.31	122.99	113.02
1	A	31	THR	CA-C-N	8.13	131.18	120.28
1	A	31	THR	C-N-CA	8.13	131.18	120.28
1	A	167	LEU	O-C-N	-7.76	113.02	122.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	SER	N-CA-C	7.68	121.90	112.54
1	A	164	SER	N-CA-C	7.57	122.54	113.16
1	A	168	GLU	N-CA-CB	7.54	121.40	110.47
1	D	89	SER	CA-C-N	7.44	133.48	122.99
1	D	89	SER	C-N-CA	7.44	133.48	122.99
1	B	169	LYS	CB-CA-C	-7.30	100.25	112.00
1	C	87	LEU	CA-C-N	6.84	132.15	120.72
1	C	87	LEU	C-N-CA	6.84	132.15	120.72
1	A	171	GLY	N-CA-C	-6.81	100.30	110.38
1	A	167	LEU	N-CA-C	6.67	121.12	112.92
1	D	31	THR	N-CA-C	6.59	119.35	108.48
1	B	86	ILE	N-CA-C	6.53	117.26	107.80
1	C	86	ILE	N-CA-C	6.47	117.19	107.80
1	A	86	ILE	N-CA-C	6.46	116.93	107.37
1	B	272	ASP	N-CA-C	6.43	118.29	111.28
1	D	86	ILE	N-CA-C	6.29	116.92	107.80
1	A	247	GLY	N-CA-C	6.22	120.20	112.73
1	C	153	GLU	N-CA-C	-6.18	105.00	112.54
1	D	88	SER	N-CA-C	6.18	120.08	112.54
1	D	247	GLY	N-CA-C	5.98	119.44	112.50
1	A	167	LEU	CA-C-N	-5.96	112.31	122.56
1	A	167	LEU	C-N-CA	-5.96	112.31	122.56
1	A	88	SER	CA-C-N	5.94	132.88	121.54
1	A	88	SER	C-N-CA	5.94	132.88	121.54
1	B	106	LYS	N-CA-C	5.93	118.53	111.71
1	A	27	ALA	CA-C-N	5.93	128.22	120.28
1	A	27	ALA	C-N-CA	5.93	128.22	120.28
1	D	272	ASP	N-CA-C	5.91	117.80	111.36
1	B	110	ILE	N-CA-C	5.91	116.44	108.17
1	A	46	ARG	CB-CG-CD	5.88	124.83	111.30
1	C	88	SER	CA-C-N	5.88	132.76	121.54
1	C	88	SER	C-N-CA	5.88	132.76	121.54
1	C	110	ILE	N-CA-C	5.84	116.35	108.17
1	A	165	LEU	CB-CA-C	-5.72	100.98	109.90
1	D	184	VAL	CA-C-N	5.72	131.87	121.41
1	D	184	VAL	C-N-CA	5.72	131.87	121.41
1	C	106	LYS	N-CA-C	5.66	118.22	111.71
1	D	110	ILE	N-CA-C	5.63	116.06	108.17
1	D	280	THR	N-CA-C	5.59	116.74	108.86
1	A	110	ILE	N-CA-C	5.56	115.95	108.17
1	D	106	LYS	N-CA-C	5.54	118.08	111.71
1	D	173	GLU	N-CA-C	-5.52	102.11	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	173	GLU	N-CA-C	-5.44	102.83	110.50
1	A	87	LEU	CA-C-N	5.42	129.76	120.72
1	A	87	LEU	C-N-CA	5.42	129.76	120.72
1	D	30	ALA	N-CA-C	5.33	117.09	111.28
1	A	272	ASP	N-CA-C	5.33	117.17	111.36
1	C	152	SER	N-CA-C	-5.31	103.48	110.33
1	C	89	SER	CA-CB-OG	5.28	121.66	111.10
1	A	106	LYS	N-CA-C	5.25	118.47	111.75
1	B	280	THR	N-CA-C	5.24	115.97	108.74
1	D	169	LYS	N-CA-C	-5.22	106.69	113.16
1	C	272	ASP	N-CA-C	5.21	117.86	111.82
1	B	89	SER	CA-C-N	5.19	130.31	122.99
1	B	89	SER	C-N-CA	5.19	130.31	122.99
1	C	144	VAL	N-CA-C	5.18	115.40	110.53
1	C	90	GLU	CB-CG-CD	5.17	121.39	112.60
1	C	88	SER	N-CA-C	5.11	118.77	112.54
1	D	31	THR	CA-C-N	5.09	127.61	120.28
1	D	31	THR	C-N-CA	5.09	127.61	120.28
1	A	117	ALA	N-CA-C	-5.08	106.59	112.89
1	D	87	LEU	CA-C-N	5.05	129.15	120.72
1	D	87	LEU	C-N-CA	5.05	129.15	120.72
1	D	89	SER	CA-CB-OG	5.03	121.15	111.10
1	D	117	ALA	N-CA-C	-5.02	106.66	112.89

There are no chirality outliers.

There are no planarity outliers.

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	2419	0	2472	62	0
1	B	2447	0	2482	66	0
1	C	2491	0	2531	65	0
1	D	2399	0	2446	59	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	174	0	0	4	0
3	B	153	0	0	7	0
3	C	168	0	0	8	0
3	D	180	0	0	4	0
All	All	10439	0	9931	244	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (244) 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:244:THR:HA	1:C:249:ARG:HD3	1.40	0.98
1:B:244:THR:HA	1:B:249:ARG:HD3	1.44	0.97
1:A:244:THR:HA	1:A:249:ARG:HD3	1.53	0.91
1:B:1:MET:HA	1:B:82:GLU:HG2	1.55	0.88
1:D:244:THR:HA	1:D:249:ARG:HD3	1.56	0.88
1:A:292:ASN:HB3	1:A:296:LYS:HZ3	1.38	0.86
1:C:1:MET:HA	1:C:82:GLU:HG2	1.62	0.81
1:D:151:MET:CE	1:D:156:GLU:HA	2.13	0.78
1:D:151:MET:HE3	1:D:156:GLU:HA	1.64	0.78
1:A:143:ARG:HD3	3:A:718:HOH:O	1.84	0.77
1:D:135:MET:HE1	1:D:144:VAL:HG13	1.67	0.76
1:A:311:ILE:HD12	1:A:311:ILE:H	1.50	0.76
1:C:151:MET:CB	1:C:155:GLU:HB2	2.18	0.74
1:D:156:GLU:O	1:D:160:GLN:HG2	1.90	0.72
1:A:22:ARG:HD3	1:A:23:ARG:N	2.06	0.70
1:B:106:LYS:HD3	3:B:695:HOH:O	1.93	0.68
1:B:1:MET:HB2	1:B:83:PHE:O	1.94	0.67
1:C:27:ALA:O	1:C:31:THR:HG23	1.95	0.66
1:C:1:MET:HB2	1:C:83:PHE:O	1.95	0.66
1:C:151:MET:HB2	1:C:155:GLU:HB2	1.77	0.66
1:C:151:MET:HB3	1:C:155:GLU:HB2	1.78	0.65
1:D:291:ASN:C	1:D:291:ASN:HD22	2.03	0.65
1:C:21:VAL:HG21	1:C:89:SER:HB2	1.79	0.65
1:A:123:THR:H	1:A:135:MET:CE	2.10	0.65
1:A:123:THR:H	1:A:135:MET:HE2	1.63	0.64
1:A:167:LEU:O	1:A:170:GLY:N	2.30	0.64
1:B:152:SER:OG	1:B:155:GLU:HG3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:LYS:HE2	3:D:755:HOH:O	1.98	0.63
1:D:145:ARG:O	1:D:146:SER:CB	2.47	0.62
1:B:154:SER:O	1:B:157:LYS:HG2	1.99	0.62
1:C:2:ILE:HD12	1:C:44:GLN:HB3	1.79	0.62
1:B:240:GLY:O	1:B:249:ARG:HD2	2.00	0.62
1:C:145:ARG:HB3	1:C:151:MET:HE2	1.82	0.61
1:B:271:LYS:HD3	3:B:720:HOH:O	1.99	0.61
1:D:54:ARG:HB2	1:D:57:LYS:HB2	1.81	0.61
1:A:297:GLN:O	1:A:301:ILE:HG12	2.01	0.60
1:B:157:LYS:NZ	1:B:157:LYS:HB3	2.17	0.60
1:B:154:SER:HA	1:B:157:LYS:HE2	1.84	0.60
1:D:53:PHE:HB2	1:D:62:TYR:CE1	2.37	0.60
1:A:311:ILE:HD12	1:A:311:ILE:N	2.18	0.59
1:B:256:PHE:CE2	1:B:260:LYS:HD2	2.37	0.59
1:C:246:THR:HG22	1:C:281:GLU:O	2.02	0.59
1:B:151:MET:HB3	1:B:155:GLU:HB2	1.85	0.59
1:B:123:THR:OG1	1:B:135:MET:HE2	2.03	0.58
1:C:223:LEU:O	1:C:273:ARG:NH2	2.36	0.58
1:C:256:PHE:CZ	1:C:260:LYS:HD2	2.38	0.58
1:A:53:PHE:HB2	1:A:62:TYR:CE1	2.39	0.58
1:A:271:LYS:HE3	1:A:308:SER:O	2.04	0.58
1:C:35:VAL:O	1:C:35:VAL:HG13	2.03	0.57
1:D:152:SER:HG	1:D:155:GLU:HG3	1.69	0.57
1:A:22:ARG:NH2	1:A:23:ARG:HG2	2.19	0.57
1:A:46:ARG:HG2	1:A:47:CYS:N	2.18	0.57
1:A:91:HIS:HE1	1:A:232:SER:OG	1.88	0.57
1:D:241:LYS:HE3	1:D:251:ASN:HD21	1.69	0.57
1:C:91:HIS:HE1	1:C:232:SER:OG	1.87	0.57
1:A:152:SER:HB2	1:A:155:GLU:HG3	1.87	0.56
1:B:145:ARG:NH1	1:B:160:GLN:HE22	2.03	0.56
1:A:256:PHE:CZ	1:A:260:LYS:HD2	2.41	0.56
1:D:292:ASN:H	1:D:292:ASN:HD22	1.53	0.56
1:C:151:MET:HB3	1:C:155:GLU:OE1	2.06	0.56
1:C:151:MET:HE3	1:C:156:GLU:OE2	2.06	0.55
1:D:292:ASN:HD22	1:D:292:ASN:N	2.03	0.55
1:D:293:GLU:HA	1:D:296:LYS:HZ3	1.70	0.55
1:B:271:LYS:HB2	1:B:271:LYS:NZ	2.21	0.55
1:A:22:ARG:HH21	1:A:23:ARG:HG2	1.72	0.55
1:B:256:PHE:CZ	1:B:260:LYS:HD2	2.41	0.55
1:D:33:GLY:HA2	1:D:42:ILE:HB	1.88	0.55
1:D:54:ARG:CB	1:D:57:LYS:HB2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:LEU:N	1:D:115:LEU:HD12	2.21	0.55
1:B:264:GLY:O	1:B:268:GLU:HG3	2.07	0.55
1:C:143:ARG:HG2	1:C:143:ARG:HH11	1.72	0.55
1:A:202:LEU:C	1:A:202:LEU:HD23	2.32	0.54
1:C:298:VAL:O	1:C:302:LEU:HD13	2.07	0.54
1:A:214:GLU:HG2	1:A:218:LYS:HE3	1.90	0.54
1:A:80:LYS:HE2	3:A:737:HOH:O	2.07	0.54
1:B:23:ARG:HH21	1:B:23:ARG:HG2	1.72	0.54
1:A:115:LEU:HD12	1:A:115:LEU:N	2.22	0.54
1:D:91:HIS:HE1	1:D:232:SER:OG	1.91	0.54
1:D:152:SER:OG	1:D:155:GLU:HG3	2.08	0.54
1:C:53:PHE:HB2	1:C:62:TYR:CE1	2.43	0.53
1:A:292:ASN:HB3	1:A:296:LYS:NZ	2.19	0.53
1:C:271:LYS:HE3	1:C:308:SER:O	2.09	0.53
1:B:1:MET:N	1:B:41:THR:O	2.41	0.53
1:B:53:PHE:HB2	1:B:62:TYR:CE1	2.43	0.53
1:B:291:ASN:HD22	1:B:291:ASN:H	1.56	0.53
1:A:54:ARG:HB2	1:A:57:LYS:HB2	1.91	0.53
1:A:153:GLU:O	1:A:156:GLU:HG2	2.09	0.53
1:D:145:ARG:O	1:D:145:ARG:HD3	2.09	0.53
1:A:160:GLN:O	1:A:164:SER:HB2	2.09	0.53
1:C:28:LEU:HD11	1:C:302:LEU:HD23	1.91	0.53
1:D:292:ASN:H	1:D:292:ASN:ND2	2.06	0.53
1:A:51:LYS:HE2	1:A:61:ASP:HB3	1.91	0.52
1:A:151:MET:HE3	1:A:156:GLU:HB3	1.91	0.52
1:D:6:LEU:HG	1:D:88:SER:HA	1.90	0.52
1:B:291:ASN:HD22	1:B:291:ASN:N	2.05	0.52
1:C:51:LYS:HE2	1:C:61:ASP:HB3	1.90	0.52
1:C:123:THR:OG1	1:C:135:MET:HE2	2.09	0.52
1:A:151:MET:HE3	1:A:156:GLU:CB	2.40	0.52
1:B:41:THR:HG21	1:B:306:ILE:CG2	2.40	0.52
1:C:145:ARG:HB3	1:C:151:MET:CE	2.39	0.51
1:A:221:GLU:O	1:A:224:LYS:HG2	2.11	0.51
1:B:51:LYS:HE2	1:B:61:ASP:HB3	1.91	0.51
1:C:271:LYS:HD3	3:C:760:HOH:O	2.09	0.51
1:B:19:LYS:NZ	3:B:724:HOH:O	2.43	0.51
1:B:54:ARG:CB	1:B:57:LYS:HB2	2.40	0.51
1:C:115:LEU:HD12	1:C:115:LEU:N	2.25	0.51
1:C:231:LEU:C	1:C:231:LEU:HD23	2.35	0.51
1:C:54:ARG:CB	1:C:57:LYS:HB2	2.40	0.51
1:D:145:ARG:O	1:D:146:SER:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:ARG:HB2	1:C:57:LYS:HB2	1.92	0.50
1:A:54:ARG:CB	1:A:57:LYS:HB2	2.42	0.50
1:B:223:LEU:O	1:B:273:ARG:NH2	2.45	0.50
1:C:240:GLY:O	1:C:249:ARG:HD2	2.12	0.50
1:B:54:ARG:HB2	1:B:57:LYS:HB2	1.92	0.50
1:D:51:LYS:HE2	1:D:61:ASP:HB3	1.93	0.50
1:B:115:LEU:N	1:B:115:LEU:HD12	2.26	0.50
1:C:54:ARG:HD3	3:C:637:HOH:O	2.12	0.50
1:B:213:GLN:CD	1:B:213:GLN:H	2.20	0.49
1:A:244:THR:HG22	1:A:249:ARG:NH1	2.27	0.49
1:C:80:LYS:HE2	3:C:745:HOH:O	2.12	0.49
1:B:202:LEU:HD23	1:B:202:LEU:C	2.37	0.49
1:D:15:ARG:HD2	3:D:648:HOH:O	2.13	0.49
1:C:210:GLU:HG3	3:C:750:HOH:O	2.13	0.49
1:A:261:GLN:HE21	1:D:261:GLN:HE21	1.61	0.49
1:B:150:ARG:HE	1:B:150:ARG:HA	1.78	0.49
1:C:213:GLN:CD	1:C:213:GLN:H	2.21	0.49
1:D:39:MET:HE2	3:D:728:HOH:O	2.12	0.49
1:C:67:LYS:HB2	1:C:165:LEU:HD22	1.96	0.48
1:D:1:MET:CA	1:D:82:GLU:HG2	2.42	0.48
1:A:19:LYS:HA	1:A:22:ARG:HG3	1.94	0.48
1:B:271:LYS:HE3	1:B:308:SER:O	2.13	0.48
1:B:291:ASN:N	1:B:291:ASN:ND2	2.61	0.48
1:C:35:VAL:HA	1:C:40:GLN:HB2	1.96	0.48
1:D:304:LEU:C	1:D:304:LEU:HD23	2.38	0.47
1:A:144:VAL:HG11	1:A:159:TRP:CD2	2.50	0.47
1:D:1:MET:HA	1:D:82:GLU:HG2	1.96	0.47
1:B:91:HIS:HE1	1:B:232:SER:OG	1.98	0.47
1:C:202:LEU:C	1:C:202:LEU:HD23	2.40	0.47
1:D:256:PHE:CZ	1:D:260:LYS:HD2	2.50	0.47
1:A:160:GLN:NE2	1:A:160:GLN:C	2.73	0.47
1:D:136:PRO:O	1:D:140:VAL:HG23	2.13	0.47
1:D:162:LEU:HD12	1:D:165:LEU:HD12	1.96	0.47
1:D:231:LEU:C	1:D:231:LEU:HD23	2.39	0.47
1:A:36:ILE:HD12	1:B:199:GLN:HE22	1.81	0.46
1:D:271:LYS:HE3	1:D:308:SER:O	2.15	0.46
1:B:293:GLU:O	1:B:297:GLN:HG3	2.15	0.46
1:B:63:TYR:CE1	1:B:165:LEU:HD21	2.51	0.46
1:B:109:LYS:HE2	3:B:706:HOH:O	2.14	0.46
1:B:231:LEU:C	1:B:231:LEU:HD23	2.41	0.46
1:B:242:LEU:HD23	3:B:701:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:GLU:HG2	3:B:718:HOH:O	2.16	0.46
1:B:125:TYR:CD1	1:B:131:HIS:HA	2.51	0.46
1:C:1:MET:HE3	1:C:306:ILE:HG23	1.98	0.46
1:C:293:GLU:O	1:C:297:GLN:HG3	2.16	0.46
1:B:35:VAL:HA	1:B:40:GLN:HB2	1.98	0.46
1:C:145:ARG:CB	1:C:151:MET:HE2	2.45	0.46
3:A:709:HOH:O	1:B:177:LYS:HB3	2.16	0.45
1:A:123:THR:OG1	1:A:135:MET:HE3	2.16	0.45
1:A:311:ILE:H	1:A:311:ILE:CD1	2.22	0.45
1:D:7:GLU:O	1:D:49:LEU:HA	2.16	0.45
1:C:125:TYR:CD1	1:C:131:HIS:HA	2.51	0.45
1:C:304:LEU:HD23	1:C:304:LEU:C	2.41	0.45
1:A:7:GLU:O	1:A:49:LEU:HA	2.16	0.45
1:B:71:ILE:HB	1:B:72:PRO:HD3	1.99	0.45
1:B:151:MET:HA	1:B:155:GLU:OE1	2.17	0.45
1:C:67:LYS:HB2	1:C:165:LEU:CD2	2.46	0.45
1:B:244:THR:HG21	1:B:288:ILE:HG12	1.99	0.45
1:D:292:ASN:N	1:D:292:ASN:ND2	2.65	0.45
1:A:1:MET:CA	1:A:82:GLU:HG2	2.46	0.45
1:B:310:LYS:O	1:B:311:ILE:HB	2.17	0.45
1:A:2:ILE:HG12	1:A:82:GLU:HB3	1.97	0.45
1:B:71:ILE:O	1:B:75:LYS:HG3	2.16	0.45
1:C:7:GLU:O	1:C:49:LEU:HA	2.17	0.45
1:D:71:ILE:HB	1:D:72:PRO:HD3	1.98	0.45
1:B:205:VAL:HG13	1:B:254:LEU:HD23	2.00	0.44
1:B:244:THR:HG22	1:B:249:ARG:NH1	2.32	0.44
1:D:223:LEU:O	1:D:226:VAL:HG22	2.17	0.44
1:D:145:ARG:HB3	1:D:151:MET:SD	2.58	0.44
1:B:304:LEU:C	1:B:304:LEU:HD23	2.43	0.44
1:A:261:GLN:HG3	1:D:261:GLN:CG	2.48	0.44
1:A:304:LEU:C	1:A:304:LEU:HD23	2.42	0.44
1:B:185:ARG:NH2	1:B:237:ILE:O	2.40	0.43
1:D:144:VAL:HG21	1:D:159:TRP:CE3	2.53	0.43
1:C:22:ARG:HG2	1:C:22:ARG:HH21	1.84	0.43
1:A:271:LYS:HB2	1:A:271:LYS:NZ	2.33	0.43
1:D:71:ILE:O	1:D:75:LYS:HG3	2.18	0.43
1:D:193:ASP:OD1	1:D:196:ARG:NH2	2.52	0.43
1:C:151:MET:HB3	1:C:155:GLU:CB	2.46	0.43
1:A:121:ILE:O	1:A:138:GLY:HA3	2.18	0.43
1:C:71:ILE:HB	1:C:72:PRO:HD3	2.00	0.43
1:C:246:THR:CG2	1:C:281:GLU:O	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:GLY:HA2	1:A:42:ILE:HB	1.99	0.43
1:A:71:ILE:HB	1:A:72:PRO:HD3	1.99	0.43
1:A:36:ILE:HD12	1:B:199:GLN:NE2	2.33	0.43
1:C:60:GLU:OE1	1:C:60:GLU:HA	2.19	0.43
1:C:244:THR:HG21	1:C:288:ILE:HG12	2.01	0.43
1:B:157:LYS:HB3	1:B:157:LYS:HZ2	1.83	0.43
1:C:256:PHE:CE2	1:C:260:LYS:HD2	2.54	0.43
1:D:144:VAL:HG11	1:D:159:TRP:CD2	2.54	0.43
1:A:263:LEU:O	1:A:267:LEU:HG	2.19	0.42
1:C:1:MET:N	1:C:41:THR:O	2.49	0.42
1:D:6:LEU:HD22	1:D:48:VAL:HB	2.01	0.42
1:C:122:HIS:CE1	1:C:146:SER:HB3	2.55	0.42
1:D:241:LYS:HG2	1:D:251:ASN:ND2	2.34	0.42
1:B:172:LEU:HD12	1:B:172:LEU:HA	1.87	0.42
1:A:122:HIS:HA	1:A:135:MET:HE2	2.01	0.42
1:D:242:LEU:HD23	1:D:255:SER:HA	2.01	0.42
1:C:1:MET:HE1	1:C:306:ILE:HA	2.00	0.42
1:D:199:GLN:NE2	3:D:661:HOH:O	2.51	0.42
1:A:71:ILE:O	1:A:75:LYS:HG3	2.19	0.42
1:D:296:LYS:O	1:D:300:GLU:HG3	2.20	0.42
1:A:244:THR:HG22	1:A:249:ARG:HH11	1.84	0.42
1:C:41:THR:HG21	1:C:306:ILE:CG2	2.50	0.42
1:A:231:LEU:C	1:A:231:LEU:HD23	2.44	0.42
1:B:23:ARG:HG2	1:B:23:ARG:NH2	2.33	0.42
1:B:60:GLU:OE1	1:B:60:GLU:HA	2.20	0.42
1:D:60:GLU:HA	1:D:60:GLU:OE1	2.20	0.42
1:C:251:ASN:ND2	3:C:685:HOH:O	2.53	0.41
1:C:71:ILE:O	1:C:75:LYS:HG3	2.20	0.41
1:C:304:LEU:HD23	1:C:304:LEU:O	2.19	0.41
1:A:160:GLN:NE2	3:A:747:HOH:O	2.52	0.41
1:B:7:GLU:O	1:B:49:LEU:HA	2.20	0.41
1:B:263:LEU:O	1:B:267:LEU:HG	2.20	0.41
1:C:242:LEU:HD23	3:C:666:HOH:O	2.19	0.41
1:D:291:ASN:C	1:D:291:ASN:ND2	2.75	0.41
1:B:307:ASN:O	1:B:310:LYS:HE2	2.21	0.41
1:C:201:PRO:HB3	1:D:37:LYS:HA	2.01	0.41
1:A:244:THR:HG21	1:A:288:ILE:HG12	2.01	0.41
1:B:145:ARG:CZ	1:B:160:GLN:HE22	2.33	0.41
1:D:202:LEU:C	1:D:202:LEU:HD23	2.46	0.41
1:B:210:GLU:HG3	3:B:702:HOH:O	2.21	0.41
1:D:206:ASP:O	1:D:210:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:LYS:HE2	3:C:668:HOH:O	2.20	0.41
1:D:239:ASP:HB3	1:D:242:LEU:HB2	2.01	0.41
1:A:22:ARG:HH21	1:A:23:ARG:CG	2.33	0.41
1:A:60:GLU:OE1	1:A:60:GLU:HA	2.21	0.41
1:A:179:LEU:HD23	1:A:200:ILE:HD13	2.02	0.40
1:D:221:GLU:O	1:D:224:LYS:HG2	2.21	0.40
1:A:1:MET:HA	1:A:82:GLU:HG2	2.02	0.40
1:B:252:ASN:HB2	1:D:199:GLN:HE22	1.87	0.40
1:A:199:GLN:HE22	1:C:252:ASN:HB2	1.87	0.40
1:C:55:TYR:HE2	1:C:135:MET:HE2	1.87	0.40
1:A:37:LYS:HA	1:B:201:PRO:HB3	2.02	0.40
1:C:273:ARG:HD3	3:C:732:HOH:O	2.21	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	295/330 (89%)	281 (95%)	14 (5%)	0	100	100
1	B	299/330 (91%)	287 (96%)	12 (4%)	0	100	100
1	C	306/330 (93%)	285 (93%)	20 (6%)	1 (0%)	36	42
1	D	294/330 (89%)	280 (95%)	14 (5%)	0	100	100
All	All	1194/1320 (90%)	1133 (95%)	60 (5%)	1 (0%)	48	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	150	ARG

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	269/296 (91%)	259 (96%)	10 (4%)	30	41
1	B	273/296 (92%)	263 (96%)	10 (4%)	30	41
1	C	278/296 (94%)	262 (94%)	16 (6%)	18	22
1	D	267/296 (90%)	252 (94%)	15 (6%)	19	24
All	All	1087/1184 (92%)	1036 (95%)	51 (5%)	23	31

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	22	ARG
1	A	35	VAL
1	A	87	LEU
1	A	91	HIS
1	A	164	SER
1	A	265	LEU
1	A	271	LYS
1	A	292	ASN
1	A	302	LEU
1	B	46	ARG
1	B	91	HIS
1	B	130	LYS
1	B	157	LYS
1	B	160	GLN
1	B	172	LEU
1	B	223	LEU
1	B	271	LYS
1	B	291	ASN
1	B	303	ASP
1	C	31	THR
1	C	37	LYS
1	C	46	ARG
1	C	91	HIS

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Mol	Chain	Res	Type
1	C	145	ARG
1	C	146	SER
1	C	148	PHE
1	C	150	ARG
1	C	151	MET
1	C	152	SER
1	C	160	GLN
1	C	172	LEU
1	C	223	LEU
1	C	246	THR
1	C	271	LYS
1	C	293	GLU
1	D	6	LEU
1	D	15	ARG
1	D	22	ARG
1	D	46	ARG
1	D	91	HIS
1	D	142	ASN
1	D	145	ARG
1	D	151	MET
1	D	168	GLU
1	D	177	LYS
1	D	265	LEU
1	D	271	LYS
1	D	291	ASN
1	D	292	ASN
1	D	302	LEU

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	40	GLN
1	A	44	GLN
1	A	69	ASN
1	A	91	HIS
1	A	160	GLN
1	A	199	GLN
1	A	217	GLN
1	A	251	ASN
1	A	261	GLN
1	A	292	ASN
1	B	40	GLN

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Mol	Chain	Res	Type
1	B	44	GLN
1	B	91	HIS
1	B	142	ASN
1	B	199	GLN
1	B	217	GLN
1	B	251	ASN
1	B	252	ASN
1	B	291	ASN
1	C	32	HIS
1	C	44	GLN
1	C	91	HIS
1	C	160	GLN
1	C	199	GLN
1	C	251	ASN
1	D	40	GLN
1	D	44	GLN
1	D	69	ASN
1	D	91	HIS
1	D	199	GLN
1	D	251	ASN
1	D	290	HIS
1	D	291	ASN
1	D	292	ASN
1	D	297	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 8 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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	301/330 (91%)	0.11	16 (5%) 32 29	15, 28, 69, 127	0
1	B	305/330 (92%)	0.29	20 (6%) 24 21	15, 31, 83, 118	1 (0%)
1	C	310/330 (93%)	0.12	21 (6%) 23 20	14, 28, 78, 130	1 (0%)
1	D	300/330 (90%)	0.07	21 (7%) 22 19	14, 27, 70, 117	0
All	All	1216/1320 (92%)	0.15	78 (6%) 25 22	14, 28, 77, 130	2 (0%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	148	PHE	7.3
1	D	55	TYR	5.4
1	B	311	ILE	5.4
1	B	35	VAL	4.8
1	A	125	TYR	4.7
1	D	124	ALA	4.5
1	B	290	HIS	4.2
1	C	290	HIS	4.1
1	A	55	TYR	4.0
1	D	146	SER	4.0
1	A	150	ARG	3.6
1	B	126	ASP	3.6
1	C	170	GLY	3.5
1	A	124	ALA	3.4
1	D	311	ILE	3.4
1	D	60	GLU	3.3
1	C	56	ALA	3.3
1	C	311	ILE	3.3
1	D	145	ARG	3.2
1	C	168	GLU	3.2
1	D	170	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	81	LYS	3.1
1	D	159	TRP	3.0
1	B	40	GLN	3.0
1	B	145	ARG	3.0
1	B	34	ASP	3.0
1	D	56	ALA	2.9
1	B	56	ALA	2.9
1	B	107	ASP	2.9
1	A	22	ARG	2.8
1	A	145	ARG	2.8
1	D	132	ILE	2.8
1	B	146	SER	2.8
1	D	40	GLN	2.8
1	C	129	SER	2.8
1	C	132	ILE	2.7
1	D	54	ARG	2.7
1	A	170	GLY	2.7
1	C	36	ILE	2.7
1	B	268	GLU	2.6
1	D	123	THR	2.6
1	C	150	ARG	2.6
1	C	128	ASP	2.6
1	A	292	ASN	2.5
1	C	149	ASN	2.5
1	D	57	LYS	2.5
1	C	22	ARG	2.5
1	A	311	ILE	2.4
1	C	40	GLN	2.4
1	B	150	ARG	2.4
1	D	168	GLU	2.4
1	D	154	SER	2.4
1	A	132	ILE	2.4
1	D	171	GLY	2.3
1	B	69	ASN	2.3
1	C	31	THR	2.3
1	A	272	ASP	2.3
1	A	159	TRP	2.3
1	C	34	ASP	2.2
1	C	107	ASP	2.2
1	B	168	GLU	2.2
1	B	106	LYS	2.2
1	D	106	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	58	ASN	2.2
1	B	153	GLU	2.2
1	B	81	LYS	2.2
1	D	53	PHE	2.2
1	B	156	GLU	2.2
1	C	39	MET	2.1
1	C	37	LYS	2.1
1	A	60	GLU	2.1
1	A	168	GLU	2.1
1	A	144	VAL	2.1
1	B	170	GLY	2.1
1	B	228	ILE	2.1
1	C	156	GLU	2.0
1	C	106	LYS	2.0
1	D	151	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MN	B	500	1/1	0.97	0.05	40,40,40,40	0
2	MN	A	500	1/1	0.98	0.05	32,32,32,32	0
2	MN	C	500	1/1	0.98	0.04	37,37,37,37	0
2	MN	D	500	1/1	0.98	0.04	34,34,34,34	0
2	MN	C	501	1/1	0.99	0.08	25,25,25,25	0
2	MN	B	501	1/1	0.99	0.09	26,26,26,26	0
2	MN	D	501	1/1	0.99	0.03	24,24,24,24	0
2	MN	A	501	1/1	1.00	0.05	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.