



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2026 – 09:08 PM EDT

PDB ID : 1B0J / pdb_00001b0j
Title : CRYSTAL STRUCTURE OF ACONITASE WITH ISOCITRATE
Authors : Lloyd, S.J.; Lauble, H.; Prasad, G.S.; Stout, C.D.
Deposited on : 1998-11-10
Resolution : 2.50 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
Mogul	:	2022.3.0, CSD as543be (2022)
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)	:	2.50

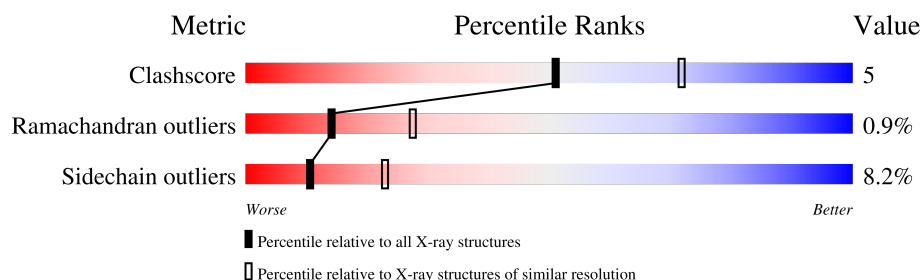
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	754	 66% 28% 5% •

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6153 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.

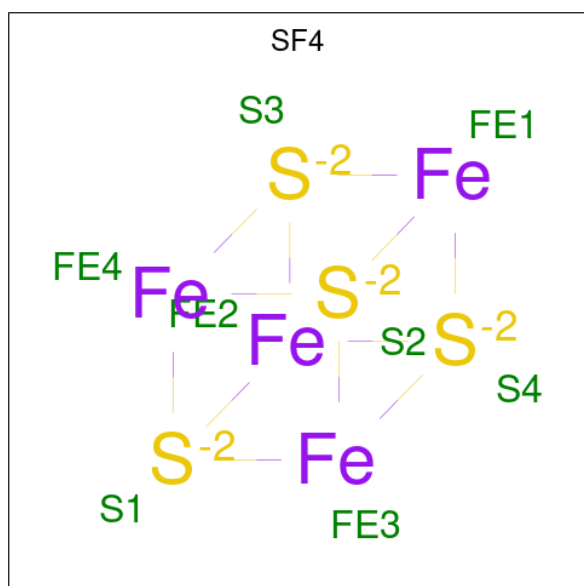
- Molecule 1 is a protein called ACONITATE HYDRATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	753	5814	3666	1034	1092	22	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

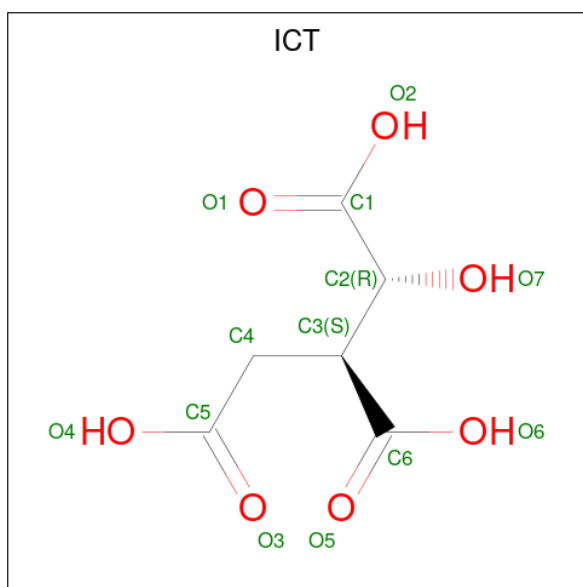
Chain	Residue	Modelled	Actual	Comment	Reference
A	642	ALA	SER	engineered mutation	UNP P16276
A	648	ALA	ARG	conflict	UNP P16276

- Molecule 2 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
2	A	1	8	4	4	0	0

- Molecule 3 is ISOCITRIC ACID (CCD ID: ICT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is water.

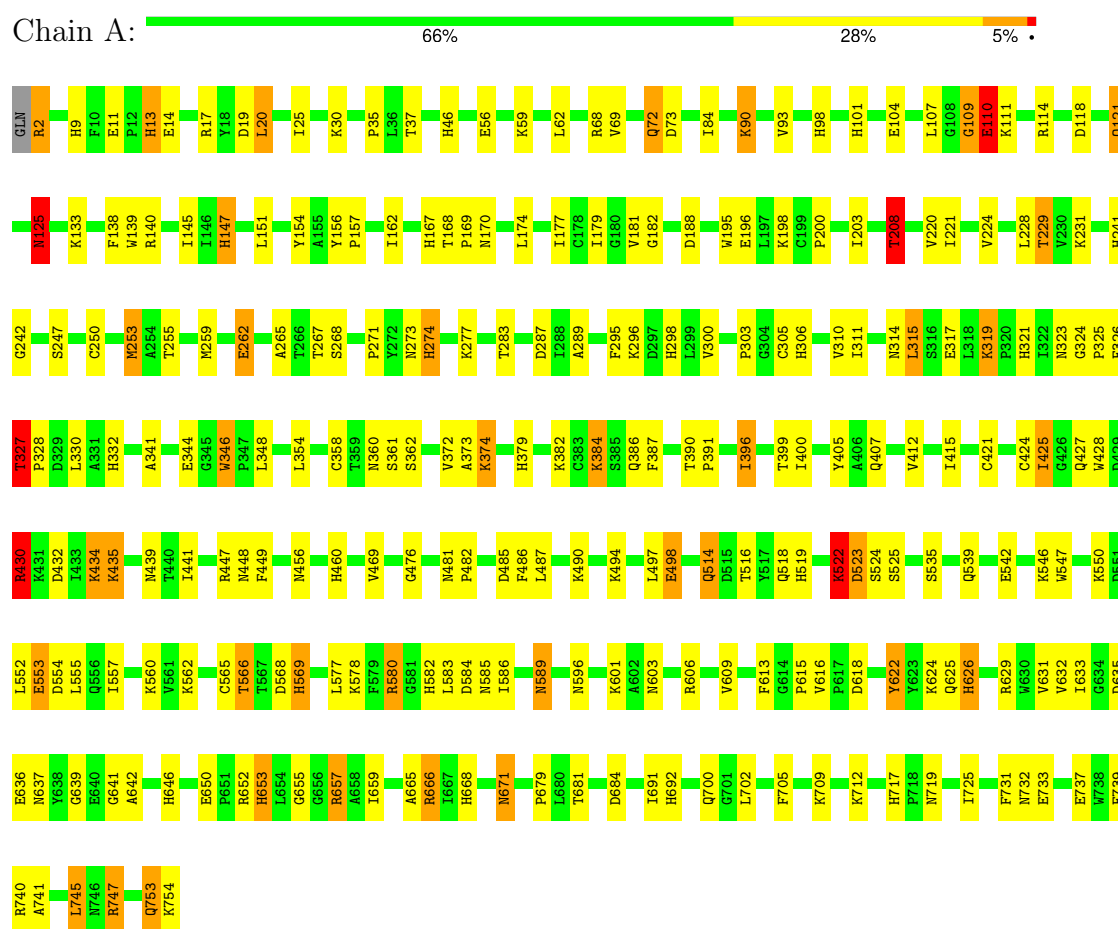
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	318	Total	O	0	0
			318	318		

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: ACONITATE HYDRATASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	B 1 1 2	Depositor
Cell constants a, b, c, α , β , γ	187.40Å 72.10Å 73.90Å 90.00° 90.00° 77.70°	Depositor
Resolution (Å)	20.00 – 2.50	Depositor
% Data completeness (in resolution range)	88.1 (20.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.162 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6153	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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: SF4, ICT

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	1.19	37/5941 (0.6%)	1.94	187/8049 (2.3%)

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	1

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	177	ILE	CA-CB	9.10	1.63	1.53
1	A	616	VAL	CA-CB	8.85	1.59	1.54
1	A	717	HIS	CD2-NE2	-7.98	1.29	1.37
1	A	167	HIS	CD2-NE2	-7.28	1.29	1.37
1	A	332	HIS	CD2-NE2	-7.18	1.29	1.37
1	A	415	ILE	CA-CB	6.91	1.62	1.54
1	A	519	HIS	CD2-NE2	-6.89	1.30	1.37
1	A	241	HIS	CD2-NE2	-6.77	1.30	1.37
1	A	653	HIS	CD2-NE2	-6.74	1.30	1.37
1	A	646	HIS	CD2-NE2	-6.66	1.30	1.37
1	A	46	HIS	CD2-NE2	-6.63	1.30	1.37
1	A	626	HIS	CD2-NE2	-6.62	1.30	1.37
1	A	569	HIS	CD2-NE2	-6.53	1.30	1.37
1	A	101	HIS	CD2-NE2	-6.44	1.30	1.37
1	A	98	HIS	CD2-NE2	-6.33	1.30	1.37
1	A	298	HIS	CD2-NE2	-6.17	1.31	1.37
1	A	379	HIS	CD2-NE2	-6.14	1.31	1.37
1	A	460	HIS	CD2-NE2	-6.05	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	692	HIS	CD2-NE2	-6.03	1.31	1.37
1	A	321	HIS	CD2-NE2	-6.03	1.31	1.37
1	A	668	HIS	CD2-NE2	-5.99	1.31	1.37
1	A	582	HIS	CD2-NE2	-5.97	1.31	1.37
1	A	668	HIS	CG-ND1	-5.95	1.31	1.38
1	A	147	HIS	CD2-NE2	-5.93	1.31	1.37
1	A	283	THR	CA-CB	5.75	1.60	1.53
1	A	13	HIS	CD2-NE2	-5.72	1.31	1.37
1	A	633	ILE	CA-CB	5.71	1.61	1.54
1	A	586	ILE	CA-CB	5.71	1.62	1.54
1	A	295	PHE	CA-CB	-5.69	1.44	1.53
1	A	9	HIS	CD2-NE2	-5.67	1.31	1.37
1	A	306	HIS	CD2-NE2	-5.67	1.31	1.37
1	A	717	HIS	CG-ND1	-5.56	1.32	1.38
1	A	332	HIS	CG-ND1	-5.49	1.32	1.38
1	A	229	THR	CA-CB	5.40	1.62	1.53
1	A	298	HIS	CG-ND1	-5.36	1.32	1.38
1	A	274	HIS	CD2-NE2	-5.32	1.32	1.37
1	A	271	PRO	CA-CB	-5.10	1.47	1.53

All (187) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	580	ARG	NE-CZ-NH1	9.98	131.48	121.50
1	A	430	ARG	NE-CZ-NH2	-9.43	110.71	119.20
1	A	372	VAL	N-CA-C	-8.77	102.31	110.82
1	A	274	HIS	CB-CG-CD2	-8.70	119.90	131.20
1	A	360	ASN	OD1-CG-ND2	-8.69	113.91	122.60
1	A	666	ARG	N-CA-C	8.40	120.06	111.07
1	A	327	THR	CB-CA-C	-7.73	98.24	109.45
1	A	188	ASP	CA-CB-CG	7.72	120.32	112.60
1	A	295	PHE	CA-CB-CG	-7.69	106.11	113.80
1	A	582	HIS	CB-CG-CD2	-7.62	121.30	131.20
1	A	407	GLN	OE1-CD-NE2	-7.54	115.06	122.60
1	A	641	GLY	N-CA-C	7.50	119.01	111.21
1	A	325	PRO	N-CA-C	7.46	131.50	112.10
1	A	522	LYS	O-C-N	7.46	132.51	122.59
1	A	753	GLN	N-CA-C	7.46	126.69	110.80
1	A	655	GLY	CA-C-N	7.46	127.08	119.92
1	A	655	GLY	C-N-CA	7.46	127.08	119.92
1	A	582	HIS	CB-CG-ND1	7.43	133.85	122.70
1	A	348	LEU	N-CA-C	7.43	122.44	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	TYR	O-C-N	-7.42	116.96	121.71
1	A	101	HIS	CB-CG-CD2	-7.21	121.82	131.20
1	A	273	ASN	CA-CB-CG	7.15	119.75	112.60
1	A	274	HIS	CB-CG-ND1	7.11	133.36	122.70
1	A	665	ALA	N-CA-C	-7.10	99.04	110.32
1	A	745	LEU	CA-C-O	-7.05	113.07	120.55
1	A	589	ASN	OD1-CG-ND2	-7.02	115.58	122.60
1	A	118	ASP	CA-CB-CG	7.01	119.61	112.60
1	A	569	HIS	CB-CG-CD2	-6.92	122.20	131.20
1	A	379	HIS	CA-CB-CG	-6.88	106.92	113.80
1	A	671	ASN	OD1-CG-ND2	-6.81	115.79	122.60
1	A	485	ASP	N-CA-C	6.80	120.59	110.52
1	A	133	LYS	N-CA-C	6.78	118.75	111.36
1	A	569	HIS	CB-CG-ND1	6.71	132.76	122.70
1	A	753	GLN	OE1-CD-NE2	-6.71	115.89	122.60
1	A	589	ASN	CB-CG-ND2	6.68	126.42	116.40
1	A	668	HIS	CA-CB-CG	-6.66	107.14	113.80
1	A	447	ARG	NE-CZ-NH2	-6.64	113.22	119.20
1	A	170	ASN	OD1-CG-ND2	-6.59	116.01	122.60
1	A	101	HIS	CB-CG-ND1	6.57	132.55	122.70
1	A	396	ILE	CA-C-O	-6.54	113.92	120.85
1	A	325	PRO	CA-C-O	-6.54	104.51	120.20
1	A	498	GLU	CA-CB-CG	6.45	127.00	114.10
1	A	311	ILE	CA-C-O	-6.45	114.45	121.28
1	A	717	HIS	CA-C-N	6.44	126.37	119.28
1	A	717	HIS	C-N-CA	6.44	126.37	119.28
1	A	542	GLU	N-CA-C	-6.43	100.42	110.14
1	A	646	HIS	CB-CG-CD2	-6.42	122.85	131.20
1	A	390	THR	CA-C-N	6.42	126.39	119.78
1	A	390	THR	C-N-CA	6.42	126.39	119.78
1	A	170	ASN	CA-CB-CG	6.32	118.92	112.60
1	A	441	ILE	O-C-N	-6.30	116.71	123.14
1	A	609	VAL	N-CA-C	6.30	117.31	111.45
1	A	650	GLU	CA-C-O	-6.29	113.10	119.08
1	A	138	PHE	CA-CB-CG	6.28	120.08	113.80
1	A	147	HIS	CB-CG-CD2	-6.28	123.03	131.20
1	A	255	THR	O-C-N	6.25	128.51	122.07
1	A	626	HIS	CB-CG-CD2	-6.23	123.10	131.20
1	A	580	ARG	NE-CZ-NH2	-6.21	113.61	119.20
1	A	731	PHE	CA-CB-CG	6.20	120.00	113.80
1	A	448	ASN	OD1-CG-ND2	-6.16	116.44	122.60
1	A	46	HIS	CB-CG-CD2	-6.14	123.22	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	522	LYS	CG-CD-CE	6.13	125.41	111.30
1	A	69	VAL	O-C-N	-6.12	116.65	123.26
1	A	326	PHE	CA-CB-CG	6.12	119.92	113.80
1	A	485	ASP	O-C-N	6.12	129.79	122.94
1	A	154	TYR	N-CA-C	6.10	122.17	114.31
1	A	539	GLN	CG-CD-NE2	6.06	125.50	116.40
1	A	93	VAL	O-C-N	-6.06	116.18	121.57
1	A	373	ALA	CA-C-O	-6.05	114.42	120.90
1	A	424	CYS	O-C-N	-6.04	115.26	122.15
1	A	298	HIS	CB-CG-CD2	-6.03	123.36	131.20
1	A	448	ASN	CA-CB-CG	6.00	118.60	112.60
1	A	519	HIS	CB-CG-ND1	5.99	131.69	122.70
1	A	671	ASN	CB-CG-ND2	5.99	125.39	116.40
1	A	523	ASP	N-CA-C	-5.99	98.05	110.80
1	A	522	LYS	CA-C-N	5.98	132.97	121.54
1	A	522	LYS	C-N-CA	5.98	132.97	121.54
1	A	719	ASN	OD1-CG-ND2	-5.97	116.63	122.60
1	A	179	ILE	N-CA-C	5.96	116.46	108.11
1	A	90	LYS	CA-CB-CG	5.93	125.96	114.10
1	A	13	HIS	CB-CG-CD2	-5.91	123.52	131.20
1	A	200	PRO	N-CA-C	5.90	121.53	111.68
1	A	319	LYS	CA-C-N	5.90	127.22	119.84
1	A	319	LYS	C-N-CA	5.90	127.22	119.84
1	A	596	ASN	CA-CB-CG	5.90	118.50	112.60
1	A	684	ASP	CA-CB-CG	5.90	118.50	112.60
1	A	59	LYS	N-CA-C	5.88	120.25	112.72
1	A	354	LEU	N-CA-C	5.87	118.29	108.02
1	A	539	GLN	OE1-CD-NE2	-5.83	116.77	122.60
1	A	391	PRO	N-CA-CB	5.82	108.42	103.35
1	A	332	HIS	CB-CG-CD2	-5.81	123.65	131.20
1	A	566	THR	CA-C-O	-5.78	115.51	121.87
1	A	262	GLU	N-CA-C	5.78	120.06	113.19
1	A	374	LYS	CA-CB-CG	5.77	125.63	114.10
1	A	73	ASP	N-CA-C	5.76	117.56	111.28
1	A	547	TRP	CG-CD2-CE3	5.75	139.65	133.90
1	A	519	HIS	CB-CG-CD2	-5.74	123.74	131.20
1	A	295	PHE	N-CA-C	5.74	120.99	113.30
1	A	59	LYS	CB-CG-CD	-5.73	98.12	111.30
1	A	569	HIS	N-CA-C	-5.72	105.40	112.90
1	A	705	PHE	CA-CB-CG	5.68	119.48	113.80
1	A	265	ALA	CA-C-O	-5.67	114.81	121.16
1	A	253	MET	N-CA-C	-5.67	105.18	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	THR	N-CA-CB	-5.65	101.86	111.69
1	A	535	SER	O-C-N	5.63	129.32	122.96
1	A	72	GLN	CA-C-O	-5.61	114.77	121.56
1	A	732	ASN	CA-CB-CG	5.59	118.19	112.60
1	A	554	ASP	N-CA-C	5.59	118.90	111.30
1	A	585	ASN	CA-C-O	-5.58	114.50	120.42
1	A	514	GLN	CA-CB-CG	5.58	125.26	114.10
1	A	522	LYS	CA-C-O	5.58	128.49	120.51
1	A	565	CYS	CA-C-N	5.56	130.26	120.87
1	A	565	CYS	C-N-CA	5.56	130.26	120.87
1	A	709	LYS	O-C-N	-5.54	116.21	121.20
1	A	203	ILE	N-CA-C	-5.53	99.78	107.80
1	A	486	PHE	N-CA-C	5.52	117.52	108.52
1	A	624	LYS	N-CA-C	5.52	116.98	111.07
1	A	2	ARG	N-CA-C	-5.51	95.58	111.00
1	A	9	HIS	CB-CG-CD2	-5.51	124.04	131.20
1	A	13	HIS	CB-CG-ND1	5.51	130.96	122.70
1	A	653	HIS	CB-CG-CD2	-5.50	124.05	131.20
1	A	424	CYS	N-CA-CB	-5.50	102.03	110.16
1	A	616	VAL	CA-C-N	5.50	124.95	119.24
1	A	616	VAL	C-N-CA	5.50	124.95	119.24
1	A	733	GLU	N-CA-C	5.49	119.08	112.38
1	A	241	HIS	CB-CG-CD2	-5.46	124.10	131.20
1	A	84	ILE	CA-C-O	-5.46	115.27	120.95
1	A	68	ARG	CA-CB-CG	5.45	125.00	114.10
1	A	603	ASN	N-CA-C	5.43	119.08	111.74
1	A	195	TRP	CE2-CD2-CG	-5.43	100.68	107.20
1	A	306	HIS	CB-CG-CD2	-5.41	124.17	131.20
1	A	195	TRP	CG-CD1-NE1	-5.38	103.20	110.20
1	A	679	PRO	CB-CA-C	5.38	116.30	111.40
1	A	635	ASP	CA-CB-CG	5.38	117.98	112.60
1	A	637	ASN	CB-CG-ND2	5.38	124.47	116.40
1	A	242	GLY	CA-C-N	5.37	125.70	119.47
1	A	242	GLY	C-N-CA	5.37	125.70	119.47
1	A	109	GLY	N-CA-C	5.34	125.83	113.18
1	A	231	LYS	CA-CB-CG	5.34	124.77	114.10
1	A	666	ARG	CA-CB-CG	5.33	124.76	114.10
1	A	700	GLN	N-CA-CB	-5.33	101.97	111.08
1	A	522	LYS	CB-CG-CD	5.32	123.53	111.30
1	A	447	ARG	CG-CD-NE	-5.31	100.33	112.00
1	A	168	THR	CA-C-N	5.30	126.47	119.84
1	A	168	THR	C-N-CA	5.30	126.47	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	469	VAL	CA-C-O	-5.26	115.80	121.27
1	A	625	GLN	OE1-CD-NE2	-5.26	117.34	122.60
1	A	482	PRO	O-C-N	5.26	128.54	122.23
1	A	434	LYS	O-C-N	-5.22	116.89	122.85
1	A	733	GLU	CA-C-N	5.21	127.22	120.44
1	A	733	GLU	C-N-CA	5.21	127.22	120.44
1	A	361	SER	N-CA-C	5.21	119.39	112.30
1	A	37	THR	CA-C-O	-5.21	116.00	121.88
1	A	324	GLY	O-C-N	-5.19	116.58	121.77
1	A	622	TYR	CA-C-O	-5.19	115.37	120.82
1	A	110	GLU	CB-CG-CD	5.19	121.42	112.60
1	A	310	VAL	O-C-N	-5.19	117.55	123.10
1	A	725	ILE	O-C-N	-5.18	117.43	122.97
1	A	125	ASN	CA-CB-CG	-5.18	107.42	112.60
1	A	469	VAL	N-CA-C	-5.17	104.93	110.36
1	A	481	ASN	CA-C-N	5.17	124.79	119.05
1	A	481	ASN	C-N-CA	5.17	124.79	119.05
1	A	460	HIS	CB-CG-CD2	-5.17	124.48	131.20
1	A	323	ASN	N-CA-C	5.16	117.98	109.72
1	A	747	ARG	CA-CB-CG	5.15	124.40	114.10
1	A	498	GLU	CB-CG-CD	5.15	121.35	112.60
1	A	346	TRP	CA-C-N	5.14	125.39	119.83
1	A	346	TRP	C-N-CA	5.14	125.39	119.83
1	A	139	TRP	CE2-CD2-CG	-5.13	101.04	107.20
1	A	732	ASN	OD1-CG-ND2	-5.13	117.47	122.60
1	A	300	VAL	O-C-N	-5.12	117.01	121.57
1	A	557	ILE	N-CA-CB	-5.12	105.45	111.39
1	A	626	HIS	CB-CG-ND1	5.12	130.38	122.70
1	A	386	GLN	N-CA-C	-5.09	102.75	110.28
1	A	387	PHE	N-CA-CB	-5.08	102.79	110.77
1	A	379	HIS	CB-CG-CD2	-5.07	124.61	131.20
1	A	639	GLY	N-CA-C	-5.06	108.25	115.64
1	A	700	GLN	CB-CG-CD	-5.06	104.00	112.60
1	A	553	GLU	CA-CB-CG	5.05	124.21	114.10
1	A	399	THR	CA-C-O	-5.05	115.06	120.42
1	A	25	ILE	N-CA-C	-5.04	105.48	110.62
1	A	547	TRP	CE2-CD2-CG	-5.04	101.16	107.20
1	A	566	THR	N-CA-CB	-5.01	103.10	110.26
1	A	167	HIS	CB-CG-CD2	-5.00	124.69	131.20
1	A	242	GLY	O-C-N	-5.00	116.77	121.77
1	A	583	LEU	N-CA-C	5.00	117.11	111.11

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	666	ARG	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5814	0	5804	60	0
2	A	8	0	0	1	0
3	A	13	0	5	2	0
4	A	318	0	0	6	0
All	All	6153	0	5809	60	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 5.

All (60) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:ARG:HH22	1:A:439:ASN:HD21	1.30	0.79
1:A:430:ARG:HD2	1:A:432:ASP:OD1	1.96	0.66
1:A:566:THR:HG22	1:A:568:ASP:H	1.61	0.64
1:A:629:ARG:HG2	1:A:657:ARG:HD3	1.80	0.64
1:A:449:PHE:CD2	1:A:566:THR:HG21	2.36	0.60
1:A:642:ALA:HB1	3:A:756:ICT:H3	1.83	0.60
1:A:13:HIS:HB3	4:A:884:HOH:O	2.03	0.58
1:A:182:GLY:HA3	1:A:671:ASN:HD21	1.69	0.56
1:A:384:LYS:HD3	1:A:476:GLY:HA3	1.89	0.54
1:A:552:LEU:HB3	1:A:555:LEU:HD21	1.90	0.52
1:A:435:LYS:HD2	1:A:456:ASN:HB2	1.91	0.52
1:A:121:GLN:O	1:A:125:ASN:HB2	2.11	0.51
1:A:652:ARG:HD2	4:A:813:HOH:O	2.09	0.50
1:A:632:VAL:HB	1:A:659:ILE:HG23	1.92	0.50
1:A:622:TYR:O	1:A:626:HIS:HD2	1.95	0.49
1:A:208:THR:O	1:A:315:LEU:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:GLU:HA	1:A:427:GLN:HB3	1.95	0.48
1:A:147:HIS:HD2	1:A:358:CYS:SG	2.36	0.48
1:A:580:ARG:HH22	3:A:756:ICT:C5	2.27	0.48
1:A:174:LEU:HD13	1:A:250:CYS:SG	2.54	0.48
1:A:566:THR:HB	1:A:569:HIS:ND1	2.30	0.47
1:A:400:ILE:HB	1:A:405:TYR:HB2	1.97	0.47
1:A:430:ARG:NH2	1:A:439:ASN:HD21	2.04	0.46
1:A:17:ARG:HB3	1:A:20:LEU:HB2	1.96	0.46
1:A:208:THR:HG22	1:A:314:ASN:HA	1.96	0.46
1:A:274:HIS:HB3	4:A:1014:HOH:O	2.15	0.46
1:A:384:LYS:O	1:A:384:LYS:HE2	2.15	0.46
1:A:739:PHE:HB2	4:A:853:HOH:O	2.15	0.46
1:A:277:LYS:HG3	1:A:289:ALA:HB1	1.98	0.45
1:A:162:ILE:HD12	1:A:181:VAL:HG21	1.97	0.45
1:A:327:THR:HG22	1:A:328:PRO:HD2	1.99	0.45
1:A:546:LYS:HD3	1:A:741:ALA:O	2.17	0.45
1:A:145:ILE:HG21	1:A:358:CYS:HB3	2.00	0.44
1:A:425:ILE:H	1:A:425:ILE:HG13	1.63	0.44
1:A:560:LYS:NZ	1:A:691:ILE:O	2.44	0.44
1:A:341:ALA:HA	1:A:346:TRP:CE3	2.53	0.44
1:A:62:LEU:O	1:A:196:GLU:HA	2.18	0.44
1:A:140:ARG:NH1	1:A:518:GLN:HB2	2.31	0.44
1:A:35:PRO:HB2	1:A:305:CYS:HA	2.00	0.43
1:A:250:CYS:HA	1:A:253:MET:HE3	2.01	0.43
1:A:425:ILE:HG12	2:A:755:SF4:S1	2.59	0.43
1:A:303:PRO:HD2	4:A:821:HOH:O	2.18	0.43
1:A:221:ILE:HG12	1:A:259:MET:HB3	2.01	0.43
1:A:362:SER:HA	1:A:396:ILE:HD13	2.01	0.42
1:A:2:ARG:HD3	1:A:19:ASP:HB3	2.02	0.42
1:A:107:LEU:HD23	1:A:111:LYS:HD3	2.01	0.42
1:A:428:TRP:CZ2	1:A:430:ARG:HD3	2.55	0.42
1:A:421:CYS:HB2	1:A:425:ILE:HD11	2.01	0.42
1:A:737:GLU:CD	1:A:740:ARG:HH21	2.27	0.42
1:A:220:VAL:O	1:A:224:VAL:HG23	2.20	0.42
1:A:615:PRO:HB2	1:A:618:ASP:OD1	2.20	0.41
1:A:110:GLU:O	1:A:114:ARG:HG3	2.20	0.41
1:A:745:LEU:HB2	4:A:1034:HOH:O	2.20	0.41
1:A:267:THR:OG1	1:A:268:SER:N	2.53	0.41
1:A:427:GLN:HE21	1:A:577:LEU:HD12	1.85	0.41
1:A:11:GLU:HB3	1:A:14:GLU:HG2	2.03	0.41
1:A:90:LYS:HE2	1:A:522:LYS:HD2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:ARG:HB2	1:A:613:PHE:CZ	2.56	0.41
1:A:584:ASP:OD1	1:A:653:HIS:HE1	2.04	0.41
1:A:427:GLN:NE2	1:A:577:LEU:HD12	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	751/754 (100%)	703 (94%)	41 (6%)	7 (1%)	14	27

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	524	SER
1	A	753	GLN
1	A	109	GLY
1	A	296	LYS
1	A	523	ASP
1	A	525	SER
1	A	157	PRO

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	621/622 (100%)	570 (92%)	51 (8%)	10	23

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

Mol	Chain	Res	Type
1	A	20	LEU
1	A	30	LYS
1	A	56	GLU
1	A	72	GLN
1	A	110	GLU
1	A	121	GLN
1	A	125	ASN
1	A	151	LEU
1	A	169	PRO
1	A	198	LYS
1	A	208	THR
1	A	228	LEU
1	A	229	THR
1	A	247	SER
1	A	262	GLU
1	A	315	LEU
1	A	317	GLU
1	A	319	LYS
1	A	327	THR
1	A	330	LEU
1	A	344	GLU
1	A	374	LYS
1	A	382	LYS
1	A	384	LYS
1	A	412	VAL
1	A	425	ILE
1	A	430	ARG
1	A	434	LYS
1	A	435	LYS
1	A	487	LEU
1	A	490	LYS
1	A	494	LYS
1	A	497	LEU
1	A	498	GLU
1	A	514	GLN
1	A	516	THR
1	A	522	LYS
1	A	550	LYS

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Mol	Chain	Res	Type
1	A	553	GLU
1	A	562	LYS
1	A	578	LYS
1	A	589	ASN
1	A	601	LYS
1	A	631	VAL
1	A	636	GLU
1	A	657	ARG
1	A	681	THR
1	A	702	LEU
1	A	712	LYS
1	A	747	ARG
1	A	754	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	13	HIS
1	A	53	GLN
1	A	241	HIS
1	A	273	ASN
1	A	306	HIS
1	A	321	HIS
1	A	419	ASN
1	A	427	GLN
1	A	439	ASN
1	A	519	HIS
1	A	536	GLN
1	A	582	HIS
1	A	585	ASN
1	A	589	ASN
1	A	637	ASN
1	A	646	HIS
1	A	653	HIS
1	A	671	ASN

5.3.3 RNA ⓘ

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](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ICT	A	756	2	12,12,12	1.24	0	13,16,16	1.15	2 (15%)
2	SF4	A	755	4,1,3	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ICT	A	756	2	-	9/16/16/16	-
2	SF4	A	755	4,1,3	-	-	0/6/5/5

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	756	ICT	C3-C4-C5	-2.48	109.30	113.95
3	A	756	ICT	O7-C2-C1	-2.30	105.77	110.69

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	756	ICT	C4-C3-C6-O5
3	A	756	ICT	C4-C3-C6-O6
3	A	756	ICT	C2-C3-C4-C5
3	A	756	ICT	O7-C2-C3-C4
3	A	756	ICT	C3-C4-C5-O3
3	A	756	ICT	C6-C3-C4-C5
3	A	756	ICT	C2-C3-C6-O5
3	A	756	ICT	C2-C3-C6-O6
3	A	756	ICT	C3-C4-C5-O4

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	756	ICT	2	0
2	A	755	SF4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.