



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 08:44 AM UTC

PDB ID : 1AMI / pdb_00001ami
Title : STERIC AND CONFORMATIONAL FEATURES OF THE ACONITASE
MECHANISM
Authors : Stout, C.D.
Deposited on : 1994-11-11
Resolution : 2.00 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)	:	2.49

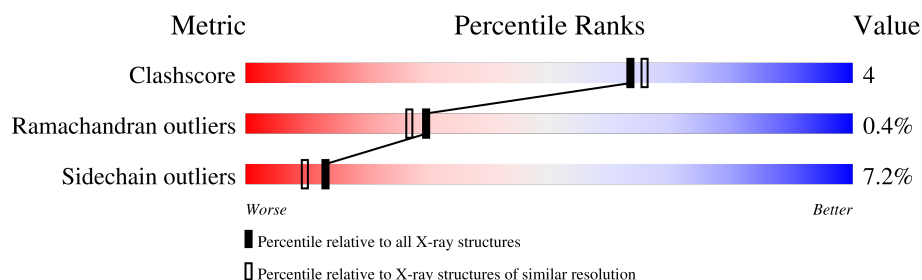
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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	 77% 18% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6095 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.

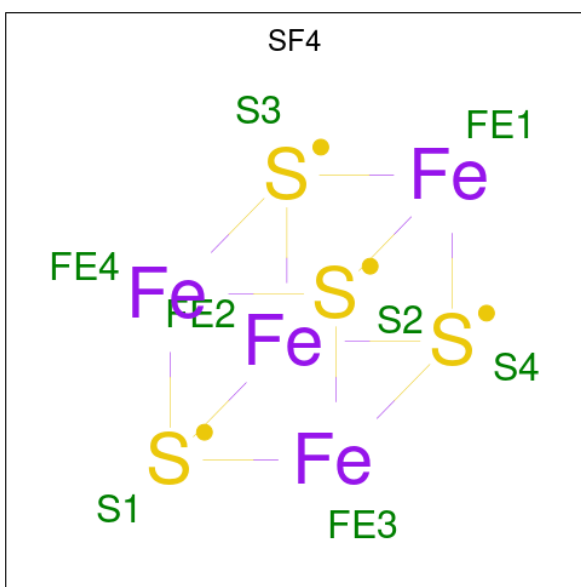
- Molecule 1 is a protein called ACONITASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	753	5812	3663	1031	1096	22	0	0	0

There are 15 discrepancies between the modelled and reference sequences:

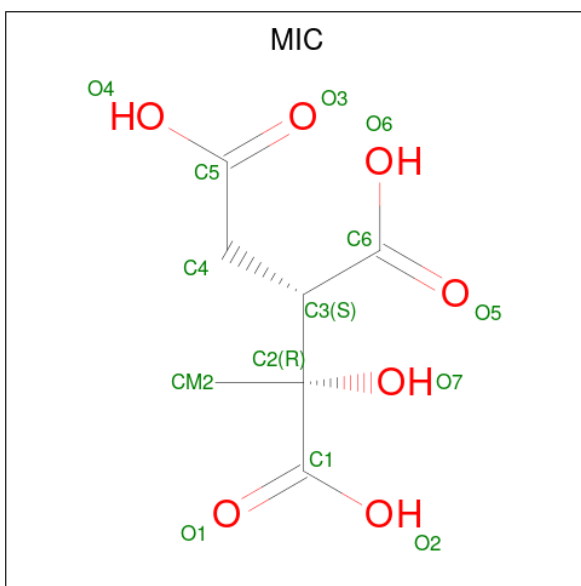
Chain	Residue	Modelled	Actual	Comment	Reference
A	13	HIS	ASN	conflict	UNP P20004
A	26	ASP	ASN	conflict	UNP P20004
A	72	GLN	ARG	conflict	UNP P20004
A	190	MET	THR	conflict	UNP P20004
A	382	LYS	GLN	conflict	UNP P20004
A	408	VAL	ILE	conflict	UNP P20004
A	528	ARG	GLN	conflict	UNP P20004
A	550	LYS	ARG	conflict	UNP P20004
A	597	SER	VAL	conflict	UNP P20004
A	600	ARG	GLY	conflict	UNP P20004
A	625	GLN	LYS	conflict	UNP P20004
A	647	SER	ALA	conflict	UNP P20004
A	653	PHE	HIS	conflict	UNP P20004
A	700	GLN	LYS	conflict	UNP P20004
A	752	GLN	-	insertion	UNP P20004

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



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

- Molecule 3 is ALPHA-METHYLISOCITRIC ACID (CCD ID: MIC) (formula: $C_7H_{10}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			14	7	7		

- Molecule 4 is water.

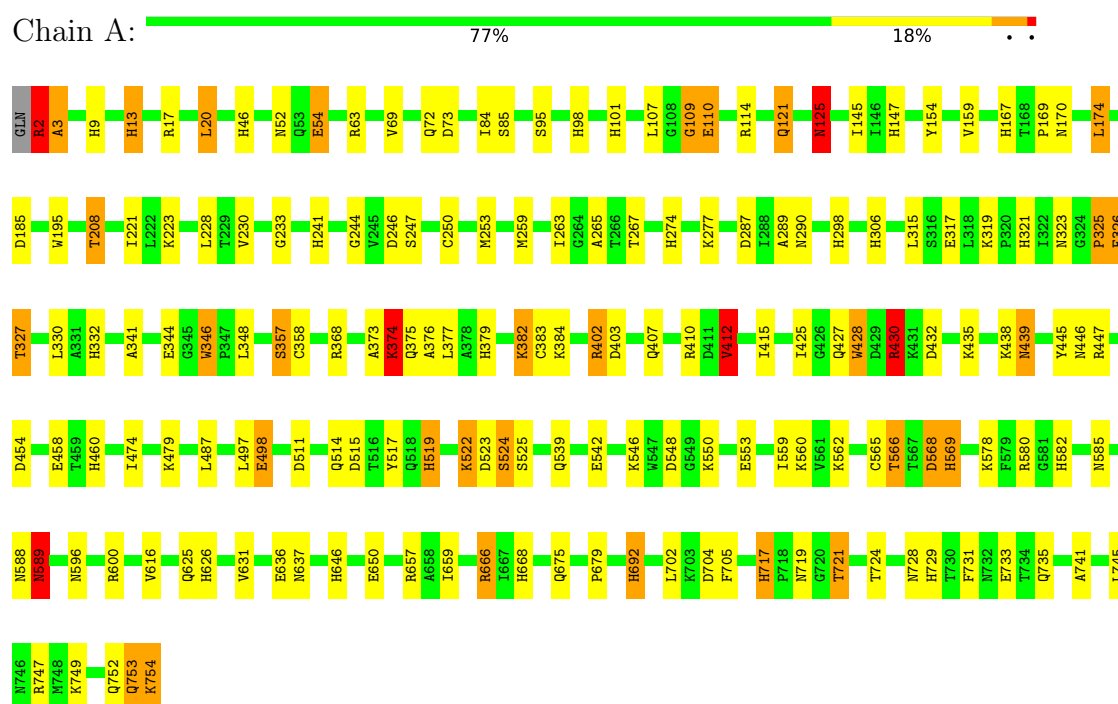
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	261	Total 261	O 261	0	0

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. 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: ACONITASE



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	185.90Å 71.80Å 73.20Å 90.00° 90.00° 77.70°	Depositor
Resolution (Å)	8.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.182 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6095	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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: SF4, MIC

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	1.05	30/5938 (0.5%)	1.77	126/8044 (1.6%)

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	1	0

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	325	PRO	C-N	-8.80	1.21	1.33
1	A	519	HIS	CD2-NE2	-7.57	1.29	1.37
1	A	13	HIS	CD2-NE2	-7.42	1.29	1.37
1	A	717	HIS	CD2-NE2	-7.26	1.29	1.37
1	A	321	HIS	CD2-NE2	-7.18	1.29	1.37
1	A	46	HIS	CD2-NE2	-6.83	1.30	1.37
1	A	569	HIS	CD2-NE2	-6.51	1.30	1.37
1	A	332	HIS	CD2-NE2	-6.47	1.30	1.37
1	A	559	ILE	CA-CB	6.44	1.62	1.55
1	A	626	HIS	CD2-NE2	-6.43	1.30	1.37
1	A	147	HIS	CD2-NE2	-6.38	1.30	1.37
1	A	298	HIS	CD2-NE2	-6.25	1.30	1.37
1	A	729	HIS	CD2-NE2	-6.11	1.31	1.37
1	A	582	HIS	CD2-NE2	-6.09	1.31	1.37
1	A	167	HIS	CD2-NE2	-6.06	1.31	1.37
1	A	646	HIS	CD2-NE2	-6.05	1.31	1.37
1	A	580	ARG	CD-NE	-5.97	1.37	1.46
1	A	101	HIS	CD2-NE2	-5.96	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	9	HIS	CD2-NE2	-5.92	1.31	1.37
1	A	460	HIS	CD2-NE2	-5.84	1.31	1.37
1	A	306	HIS	CD2-NE2	-5.68	1.31	1.37
1	A	98	HIS	CD2-NE2	-5.65	1.31	1.37
1	A	415	ILE	CA-CB	5.57	1.61	1.54
1	A	241	HIS	CD2-NE2	-5.54	1.31	1.37
1	A	616	VAL	CA-CB	5.51	1.57	1.54
1	A	379	HIS	CD2-NE2	-5.50	1.31	1.37
1	A	668	HIS	CD2-NE2	-5.36	1.31	1.37
1	A	692	HIS	CD2-NE2	-5.34	1.31	1.37
1	A	274	HIS	CD2-NE2	-5.24	1.32	1.37
1	A	159	VAL	CA-CB	5.17	1.60	1.54

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	580	ARG	NE-CZ-NH2	-13.49	107.06	119.20
1	A	580	ARG	NE-CZ-NH1	11.91	133.41	121.50
1	A	326	PHE	N-CA-C	11.69	135.70	110.80
1	A	566	THR	N-CA-CB	-9.68	96.52	110.36
1	A	402	ARG	NE-CZ-NH2	-9.47	110.68	119.20
1	A	447	ARG	NE-CZ-NH2	-8.84	111.25	119.20
1	A	539	GLN	CG-CD-NE2	8.14	128.61	116.40
1	A	498	GLU	CA-CB-CG	7.82	129.74	114.10
1	A	407	GLN	OE1-CD-NE2	-7.81	114.79	122.60
1	A	705	PHE	CA-CB-CG	7.63	121.43	113.80
1	A	666	ARG	NE-CZ-NH2	-7.63	112.34	119.20
1	A	46	HIS	CB-CG-CD2	-7.61	121.31	131.20
1	A	325	PRO	CA-C-O	-7.46	102.30	120.20
1	A	274	HIS	CB-CG-CD2	-7.43	121.53	131.20
1	A	539	GLN	OE1-CD-NE2	-7.37	115.23	122.60
1	A	332	HIS	CB-CG-CD2	-6.97	122.14	131.20
1	A	13	HIS	CA-CB-CG	-6.88	106.92	113.80
1	A	430	ARG	NE-CZ-NH2	-6.87	113.02	119.20
1	A	585	ASN	OD1-CG-ND2	-6.81	115.79	122.60
1	A	446	ASN	OD1-CG-ND2	-6.78	115.82	122.60
1	A	523	ASP	N-CA-C	-6.78	96.36	110.80
1	A	412	VAL	CB-CA-C	-6.75	100.22	111.29
1	A	589	ASN	OD1-CG-ND2	-6.71	115.89	122.60
1	A	519	HIS	CB-CG-ND1	6.67	132.71	122.70
1	A	323	ASN	OD1-CG-ND2	-6.58	116.02	122.60
1	A	321	HIS	CB-CG-CD2	-6.54	122.70	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	HIS	CB-CG-CD2	-6.50	122.75	131.20
1	A	410	ARG	NE-CZ-NH2	-6.49	113.36	119.20
1	A	46	HIS	CB-CG-ND1	6.47	132.40	122.70
1	A	569	HIS	CB-CG-CD2	-6.42	122.85	131.20
1	A	84	ILE	CA-C-O	-6.41	114.28	120.95
1	A	753	GLN	N-CA-C	6.41	120.41	112.47
1	A	511	ASP	N-CA-C	-6.38	100.37	109.24
1	A	589	ASN	CB-CG-ND2	6.38	125.96	116.40
1	A	379	HIS	CA-CB-CG	-6.37	107.43	113.80
1	A	522	LYS	O-C-N	6.36	130.08	122.26
1	A	626	HIS	CA-CB-CG	-6.34	107.46	113.80
1	A	208	THR	N-CA-CB	-6.33	100.55	111.55
1	A	569	HIS	CB-CG-ND1	6.32	132.18	122.70
1	A	410	ARG	NE-CZ-NH1	6.30	127.80	121.50
1	A	147	HIS	CB-CG-CD2	-6.29	123.02	131.20
1	A	524	SER	N-CA-C	6.29	124.20	110.80
1	A	519	HIS	CB-CG-CD2	-6.26	123.06	131.20
1	A	542	GLU	N-CA-C	-6.23	99.92	109.64
1	A	9	HIS	CA-CB-CG	-6.22	107.58	113.80
1	A	384	LYS	N-CA-C	-6.21	103.81	112.45
1	A	625	GLN	OE1-CD-NE2	-6.20	116.40	122.60
1	A	125	ASN	CA-CB-CG	-6.19	106.41	112.60
1	A	439	ASN	OD1-CG-ND2	-6.16	116.44	122.60
1	A	522	LYS	CA-C-O	6.15	127.21	119.95
1	A	582	HIS	CB-CG-CD2	-6.15	123.21	131.20
1	A	679	PRO	CB-CA-C	6.09	116.94	111.40
1	A	729	HIS	CB-CG-CD2	-6.08	123.29	131.20
1	A	101	HIS	CB-CG-CD2	-6.08	123.30	131.20
1	A	428	TRP	CG-CD2-CE3	6.06	139.96	133.90
1	A	637	ASN	OD1-CG-ND2	-6.01	116.59	122.60
1	A	522	LYS	CG-CD-CE	5.98	125.06	111.30
1	A	717	HIS	CA-C-N	5.97	125.68	119.05
1	A	717	HIS	C-N-CA	5.97	125.68	119.05
1	A	731	PHE	CA-CB-CG	5.97	119.77	113.80
1	A	274	HIS	CB-CG-ND1	5.97	131.65	122.70
1	A	306	HIS	CB-CG-CD2	-5.97	123.44	131.20
1	A	63	ARG	NE-CZ-NH2	-5.94	113.85	119.20
1	A	719	ASN	OD1-CG-ND2	-5.90	116.70	122.60
1	A	167	HIS	CB-CG-CD2	-5.88	123.56	131.20
1	A	3	ALA	N-CA-C	-5.87	101.80	110.48
1	A	675	GLN	OE1-CD-NE2	-5.86	116.74	122.60
1	A	290	ASN	OD1-CG-ND2	-5.82	116.78	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	735	GLN	OE1-CD-NE2	-5.82	116.78	122.60
1	A	515	ASP	CA-CB-CG	5.81	118.41	112.60
1	A	560	LYS	N-CA-C	-5.81	99.05	108.52
1	A	101	HIS	CB-CG-ND1	5.80	131.41	122.70
1	A	580	ARG	CG-CD-NE	-5.77	99.30	112.00
1	A	357	SER	CA-CB-OG	5.71	122.51	111.10
1	A	724	THR	CA-CB-OG1	-5.69	101.06	109.60
1	A	566	THR	CA-C-O	-5.61	115.37	121.87
1	A	287	ASP	CA-CB-CG	5.59	118.19	112.60
1	A	185	ASP	CA-CB-CG	5.59	118.19	112.60
1	A	412	VAL	N-CA-CB	5.57	120.42	111.23
1	A	447	ARG	CG-CD-NE	-5.54	99.82	112.00
1	A	154	TYR	N-CA-C	5.52	120.89	114.04
1	A	2	ARG	CB-CG-CD	5.51	123.97	111.30
1	A	327	THR	CB-CA-C	-5.49	100.97	109.20
1	A	374	LYS	CA-CB-CG	5.48	125.06	114.10
1	A	548	ASP	CA-CB-CG	5.45	118.05	112.60
1	A	666	ARG	CG-CD-NE	-5.42	100.07	112.00
1	A	568	ASP	CA-CB-CG	5.41	118.01	112.60
1	A	646	HIS	CB-CG-CD2	-5.40	124.18	131.20
1	A	73	ASP	CA-CB-CG	5.40	118.00	112.60
1	A	588	ASN	OD1-CG-ND2	-5.38	117.22	122.60
1	A	427	GLN	OE1-CD-NE2	-5.38	117.22	122.60
1	A	246	ASP	CA-CB-CG	-5.35	107.25	112.60
1	A	692	HIS	CB-CG-CD2	-5.35	124.25	131.20
1	A	267	THR	CA-CB-OG1	-5.34	101.58	109.60
1	A	98	HIS	CA-CB-CG	-5.33	108.47	113.80
1	A	460	HIS	CB-CG-CD2	-5.31	124.30	131.20
1	A	749	LYS	CA-C-O	-5.31	114.10	120.10
1	A	267	THR	CA-CB-CG2	5.28	119.48	110.50
1	A	717	HIS	CB-CG-CD2	-5.25	124.37	131.20
1	A	565	CYS	CA-C-N	5.25	130.53	120.97
1	A	565	CYS	C-N-CA	5.25	130.53	120.97
1	A	542	GLU	CA-C-N	5.24	125.16	119.76
1	A	542	GLU	C-N-CA	5.24	125.16	119.76
1	A	402	ARG	NE-CZ-NH1	5.24	126.74	121.50
1	A	298	HIS	CB-CG-CD2	-5.21	124.42	131.20
1	A	73	ASP	N-CA-C	5.21	118.89	112.54
1	A	733	GLU	CB-CG-CD	5.20	121.45	112.60
1	A	13	HIS	CB-CG-ND1	5.20	130.50	122.70
1	A	167	HIS	CB-CG-ND1	5.17	130.46	122.70
1	A	374	LYS	CB-CG-CD	5.14	123.11	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	626	HIS	CB-CG-CD2	-5.13	124.53	131.20
1	A	52	ASN	OD1-CG-ND2	-5.13	117.47	122.60
1	A	170	ASN	OD1-CG-ND2	-5.12	117.48	122.60
1	A	109	GLY	N-CA-C	5.12	125.31	113.18
1	A	368	ARG	CA-CB-CG	-5.11	103.88	114.10
1	A	728	ASN	OD1-CG-ND2	-5.11	117.49	122.60
1	A	659	ILE	N-CA-C	-5.10	100.22	107.77
1	A	379	HIS	CB-CG-CD2	-5.09	124.59	131.20
1	A	596	ASN	CA-CB-CG	5.08	117.68	112.60
1	A	346	TRP	CE2-CD2-CG	-5.08	101.11	107.20
1	A	410	ARG	CB-CG-CD	-5.08	99.62	111.30
1	A	428	TRP	CE2-CD2-CG	-5.07	101.11	107.20
1	A	98	HIS	CB-CG-CD2	-5.05	124.63	131.20
1	A	454	ASP	CA-CB-CG	5.03	117.63	112.60
1	A	373	ALA	CA-C-O	-5.01	115.24	120.55
1	A	195	TRP	CG-CD1-NE1	-5.01	103.69	110.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	326	PHE	CA

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	5812	0	5794	47	0
2	A	8	0	0	0	0
3	A	14	0	6	1	0
4	A	261	0	0	2	0
All	All	6095	0	5800	47	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 4.

All (47) 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	1.36	0.73
1:A:430:ARG:HH22	1:A:439:ASN:ND2	1.93	0.66
1:A:566:THR:HG22	1:A:568:ASP:H	1.60	0.64
1:A:517:TYR:OH	1:A:519:HIS:HD2	1.83	0.62
1:A:546:LYS:HD3	1:A:741:ALA:O	2.01	0.60
1:A:566:THR:HB	1:A:569:HIS:ND1	2.18	0.59
1:A:250:CYS:HA	1:A:253:MET:HE3	1.84	0.59
1:A:430:ARG:HD2	1:A:432:ASP:OD1	2.04	0.56
1:A:754:LYS:HZ2	1:A:754:LYS:C	2.15	0.55
1:A:357:SER:HB3	1:A:445:TYR:CD1	2.43	0.54
1:A:244:GLY:O	1:A:247:SER:HB3	2.07	0.54
1:A:517:TYR:OH	1:A:519:HIS:CD2	2.61	0.53
1:A:277:LYS:HG3	1:A:289:ALA:HB1	1.91	0.52
1:A:566:THR:HG22	1:A:568:ASP:N	2.26	0.51
1:A:402:ARG:HD2	1:A:403:ASP:OD1	2.10	0.51
1:A:348:LEU:HD12	1:A:479:LYS:HG3	1.94	0.49
1:A:174:LEU:HD13	1:A:250:CYS:SG	2.54	0.48
1:A:517:TYR:CE2	1:A:519:HIS:HD2	2.33	0.47
1:A:374:LYS:HD2	1:A:375:GLN:HG3	1.97	0.47
1:A:717:HIS:HD2	1:A:721:THR:HB	1.80	0.47
1:A:2:ARG:HE	1:A:3:ALA:N	2.14	0.46
1:A:85:SER:HB2	1:A:745:LEU:HD21	1.98	0.46
1:A:223:LYS:HD2	4:A:1221:HOH:O	2.16	0.46
1:A:221:ILE:HG12	1:A:259:MET:HB3	1.97	0.45
1:A:72:GLN:NE2	3:A:755:MIC:H41	2.32	0.45
1:A:17:ARG:HB3	1:A:20:LEU:HB2	1.98	0.45
1:A:110:GLU:O	1:A:114:ARG:HG3	2.16	0.45
1:A:752:GLN:O	1:A:753:GLN:HG2	2.17	0.45
1:A:233:GLY:O	1:A:265:ALA:HA	2.16	0.44
1:A:69:VAL:O	1:A:95:SER:HA	2.17	0.44
1:A:376:ALA:HB2	1:A:474:ILE:HD13	2.01	0.42
1:A:341:ALA:HA	1:A:346:TRP:CE3	2.54	0.42
1:A:377:LEU:HG	1:A:412:VAL:HG13	2.00	0.42
1:A:430:ARG:NH2	1:A:439:ASN:HD21	2.11	0.42
1:A:121:GLN:O	1:A:125:ASN:HB2	2.19	0.42
1:A:754:LYS:C	1:A:754:LYS:NZ	2.78	0.42
1:A:589:ASN:C	1:A:589:ASN:HD22	2.28	0.42
1:A:230:VAL:HA	1:A:263:ILE:HA	2.02	0.41
1:A:589:ASN:ND2	1:A:650:GLU:OE1	2.53	0.41
1:A:382:LYS:HE3	1:A:382:LYS:HB3	1.91	0.41
1:A:428:TRP:CZ2	1:A:430:ARG:HD3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ILE:HG21	1:A:358:CYS:HB3	2.03	0.41
1:A:383:CYS:HA	1:A:474:ILE:HA	2.03	0.41
1:A:13:HIS:CD2	1:A:13:HIS:H	2.38	0.40
1:A:692:HIS:ND1	4:A:1109:HOH:O	2.37	0.40
1:A:54:GLU:CD	1:A:54:GLU:H	2.29	0.40
1:A:438:LYS:HA	1:A:458:GLU:HB3	2.03	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%)	720 (96%)	28 (4%)	3 (0%)	30 27

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	524	SER
1	A	109	GLY
1	A	525	SER

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	622/623 (100%)	577 (93%)	45 (7%)	13	10

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	20	LEU
1	A	54	GLU
1	A	107	LEU
1	A	110	GLU
1	A	121	GLN
1	A	125	ASN
1	A	169	PRO
1	A	174	LEU
1	A	208	THR
1	A	228	LEU
1	A	315	LEU
1	A	317	GLU
1	A	319	LYS
1	A	325	PRO
1	A	326	PHE
1	A	327	THR
1	A	330	LEU
1	A	344	GLU
1	A	374	LYS
1	A	382	LYS
1	A	412	VAL
1	A	425	ILE
1	A	430	ARG
1	A	435	LYS
1	A	487	LEU
1	A	497	LEU
1	A	498	GLU
1	A	514	GLN
1	A	522	LYS
1	A	550	LYS
1	A	553	GLU
1	A	562	LYS
1	A	578	LYS
1	A	589	ASN
1	A	600	ARG
1	A	631	VAL
1	A	636	GLU

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Mol	Chain	Res	Type
1	A	657	ARG
1	A	666	ARG
1	A	702	LEU
1	A	704	ASP
1	A	721	THR
1	A	747	ARG
1	A	754	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	13	HIS
1	A	77	GLN
1	A	106	GLN
1	A	148	GLN
1	A	321	HIS
1	A	395	GLN
1	A	419	ASN
1	A	439	ASN
1	A	514	GLN
1	A	519	HIS
1	A	536	GLN
1	A	585	ASN
1	A	589	ASN
1	A	625	GLN
1	A	637	ASN
1	A	671	ASN
1	A	689	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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	$\# Z > 2$
2	SF4	A	999	1,3,4	0,12,12	-	-	-		
3	MIC	A	755	2	12,13,13	1.53	1 (8%)	14,19,19	1.79	3 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	A	999	1,3,4	-	-	0/6/5/5
3	MIC	A	755	2	-	4/20/20/20	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	755	MIC	C3-C6	2.21	1.57	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	755	MIC	O6-C6-C3	3.85	122.64	113.81
3	A	755	MIC	O6-C6-O5	-3.34	116.51	124.08
3	A	755	MIC	O7-C2-CM2	-2.80	102.45	108.80

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	755	MIC	C2-C3-C4-C5
3	A	755	MIC	C6-C3-C4-C5
3	A	755	MIC	C2-C3-C6-O5
3	A	755	MIC	C2-C3-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	755	MIC	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.