



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 02:30 PM EDT

PDB ID : 7ACN / pdb_00007acn
Title : CRYSTAL STRUCTURES OF ACONITASE WITH ISOCITRATE AND NI-TROISOCITRATE BOUND
Authors : Lauble, H.; Kennedy, M.C.; Beinert, H.; Stout, C.D.
Deposited on : 1991-05-15
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)	:	2.50

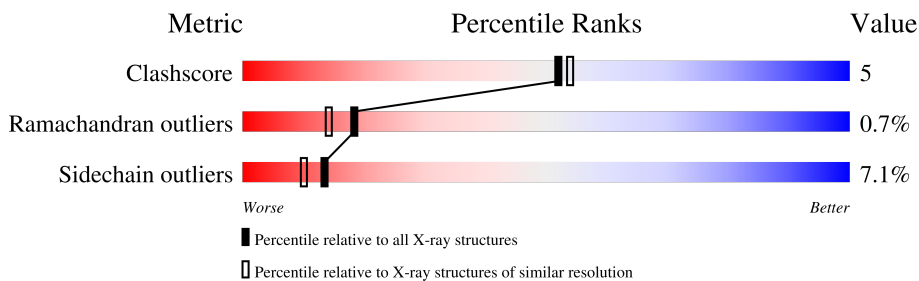
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6174 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.

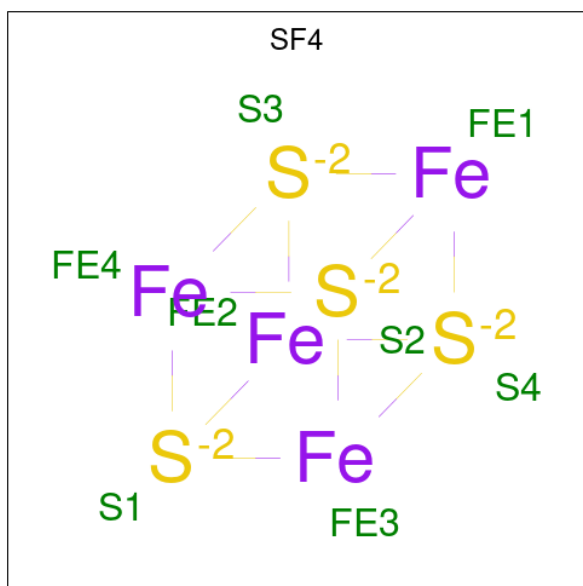
- Molecule 1 is a protein called ACONITASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	753	5815	3666	1034	1093	22	0	0	0

There is a discrepancy between the modelled and reference sequences:

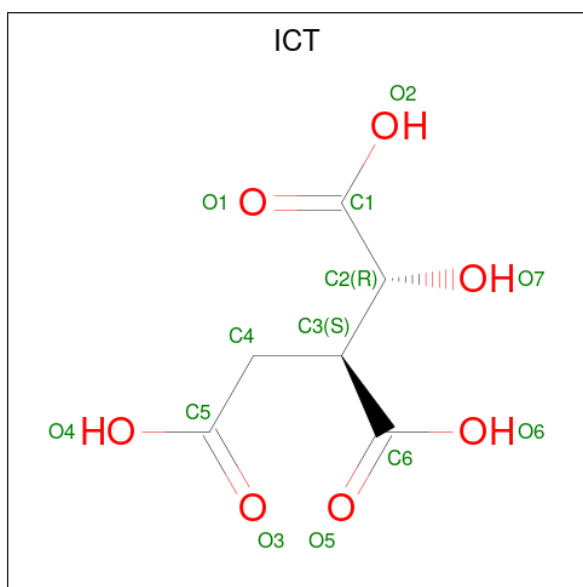
Chain	Residue	Modelled	Actual	Comment	Reference
A	647	SER	ARG	conflict	UNP P16276

- 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.

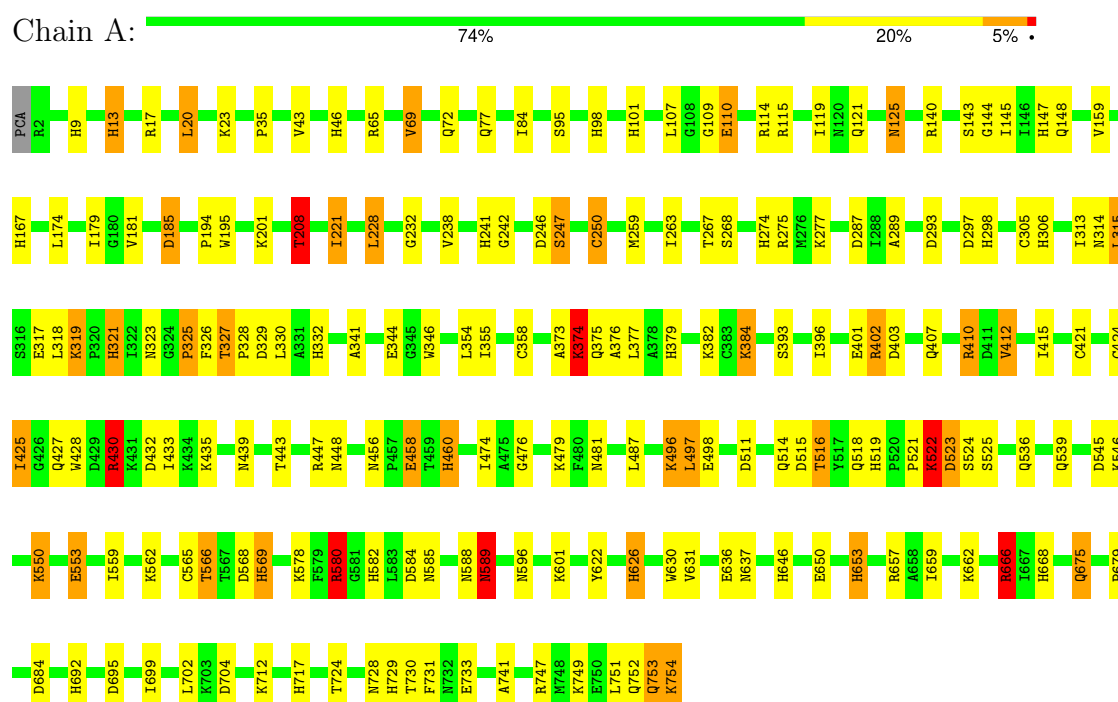
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	338	Total	O	0	0
			338	338		

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	185.50Å 72.00Å 73.00Å 90.00° 90.00° 77.70°	Depositor
Resolution (Å)	(Not available) – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.179 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6174	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, 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	1.09	32/5942 (0.5%)	1.78	120/8050 (1.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	HIS	CD2-NE2	-7.80	1.29	1.37
1	A	321	HIS	CD2-NE2	-7.24	1.29	1.37
1	A	692	HIS	CD2-NE2	-7.15	1.29	1.37
1	A	626	HIS	CD2-NE2	-7.09	1.30	1.37
1	A	167	HIS	CD2-NE2	-7.08	1.30	1.37
1	A	653	HIS	CD2-NE2	-6.98	1.30	1.37
1	A	46	HIS	CD2-NE2	-6.76	1.30	1.37
1	A	13	HIS	CD2-NE2	-6.74	1.30	1.37
1	A	559	ILE	CA-CB	6.72	1.62	1.55
1	A	569	HIS	CD2-NE2	-6.67	1.30	1.37
1	A	582	HIS	CD2-NE2	-6.59	1.30	1.37
1	A	147	HIS	CD2-NE2	-6.47	1.30	1.37
1	A	379	HIS	CD2-NE2	-6.35	1.30	1.37
1	A	332	HIS	CD2-NE2	-6.28	1.30	1.37
1	A	9	HIS	CD2-NE2	-6.22	1.31	1.37
1	A	646	HIS	CD2-NE2	-6.22	1.31	1.37
1	A	717	HIS	CD2-NE2	-6.15	1.31	1.37
1	A	668	HIS	CD2-NE2	-5.97	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	298	HIS	CD2-NE2	-5.93	1.31	1.37
1	A	519	HIS	CD2-NE2	-5.92	1.31	1.37
1	A	159	VAL	CA-CB	5.91	1.62	1.54
1	A	396	ILE	CA-CB	5.80	1.61	1.54
1	A	306	HIS	CD2-NE2	-5.75	1.31	1.37
1	A	415	ILE	CA-CB	5.69	1.61	1.54
1	A	460	HIS	CD2-NE2	-5.61	1.31	1.37
1	A	241	HIS	CD2-NE2	-5.61	1.31	1.37
1	A	221	ILE	CA-CB	5.50	1.61	1.54
1	A	580	ARG	CD-NE	-5.38	1.38	1.46
1	A	98	HIS	CD2-NE2	-5.17	1.32	1.37
1	A	729	HIS	CD2-NE2	-5.09	1.32	1.37
1	A	43	VAL	CA-CB	5.08	1.60	1.54
1	A	274	HIS	CD2-NE2	-5.04	1.32	1.37

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	580	ARG	NE-CZ-NH1	12.39	133.89	121.50
1	A	580	ARG	NE-CZ-NH2	-11.30	109.03	119.20
1	A	402	ARG	NE-CZ-NH2	-9.21	110.91	119.20
1	A	430	ARG	NE-CZ-NH2	-8.96	111.13	119.20
1	A	566	THR	N-CA-CB	-8.55	98.14	110.36
1	A	379	HIS	CA-CB-CG	-7.92	105.88	113.80
1	A	407	GLN	OE1-CD-NE2	-7.83	114.77	122.60
1	A	46	HIS	CB-CG-CD2	-7.53	121.41	131.20
1	A	481	ASN	OD1-CG-ND2	-7.53	115.07	122.60
1	A	274	HIS	CB-CG-CD2	-7.32	121.69	131.20
1	A	101	HIS	CB-CG-CD2	-7.26	121.77	131.20
1	A	167	HIS	CB-CG-ND1	7.21	133.51	122.70
1	A	753	GLN	N-CA-C	7.00	125.72	110.80
1	A	519	HIS	CB-CG-CD2	-6.97	122.14	131.20
1	A	208	THR	N-CA-CB	-6.96	99.44	111.55
1	A	675	GLN	OE1-CD-NE2	-6.91	115.69	122.60
1	A	329	ASP	CA-CB-CG	6.84	119.44	112.60
1	A	84	ILE	CA-C-O	-6.78	113.98	121.17
1	A	637	ASN	OD1-CG-ND2	-6.72	115.88	122.60
1	A	427	GLN	OE1-CD-NE2	-6.69	115.91	122.60
1	A	582	HIS	CB-CG-CD2	-6.68	122.52	131.20
1	A	147	HIS	CB-CG-CD2	-6.66	122.55	131.20
1	A	731	PHE	CA-CB-CG	6.66	120.46	113.80
1	A	167	HIS	CB-CG-CD2	-6.62	122.59	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	585	ASN	OD1-CG-ND2	-6.58	116.02	122.60
1	A	9	HIS	CA-CB-CG	-6.53	107.27	113.80
1	A	46	HIS	CB-CG-ND1	6.50	132.45	122.70
1	A	569	HIS	CB-CG-CD2	-6.45	122.82	131.20
1	A	447	ARG	NE-CZ-NH2	-6.40	113.44	119.20
1	A	519	HIS	CB-CG-ND1	6.31	132.17	122.70
1	A	684	ASP	CA-CB-CG	6.21	118.81	112.60
1	A	539	GLN	CG-CD-NE2	6.16	125.64	116.40
1	A	588	ASN	OD1-CG-ND2	-6.03	116.57	122.60
1	A	481	ASN	CA-C-N	6.03	125.91	119.28
1	A	481	ASN	C-N-CA	6.03	125.91	119.28
1	A	582	HIS	CB-CG-ND1	5.96	131.65	122.70
1	A	246	ASP	CA-CB-CG	-5.96	106.64	112.60
1	A	384	LYS	N-CA-C	-5.95	104.18	112.45
1	A	699	ILE	N-CA-C	-5.94	99.87	108.36
1	A	545	ASP	CA-CB-CG	5.92	118.52	112.60
1	A	298	HIS	CB-CG-CD2	-5.88	123.56	131.20
1	A	430	ARG	NE-CZ-NH1	5.87	127.37	121.50
1	A	695	ASP	CA-CB-CG	5.84	118.44	112.60
1	A	596	ASN	CA-CB-CG	5.84	118.44	112.60
1	A	13	HIS	CB-CG-CD2	-5.84	123.61	131.20
1	A	460	HIS	CB-CG-CD2	-5.83	123.62	131.20
1	A	9	HIS	CB-CG-CD2	-5.83	123.63	131.20
1	A	536	GLN	OE1-CD-NE2	-5.82	116.78	122.60
1	A	733	GLU	CB-CG-CD	5.76	122.39	112.60
1	A	728	ASN	OD1-CG-ND2	-5.76	116.84	122.60
1	A	267	THR	CA-CB-CG2	5.75	120.28	110.50
1	A	250	CYS	O-C-N	-5.75	116.03	122.12
1	A	374	LYS	CA-CB-CG	5.74	125.57	114.10
1	A	323	ASN	OD1-CG-ND2	-5.73	116.87	122.60
1	A	569	HIS	CB-CG-ND1	5.73	131.29	122.70
1	A	325	PRO	N-CA-C	5.70	126.92	112.10
1	A	522	LYS	CG-CD-CE	5.68	124.36	111.30
1	A	247	SER	CA-CB-OG	5.65	122.40	111.10
1	A	287	ASP	CA-CB-CG	5.62	118.22	112.60
1	A	511	ASP	CA-C-O	5.62	123.48	119.32
1	A	692	HIS	CA-CB-CG	-5.61	108.19	113.80
1	A	717	HIS	CA-C-N	5.60	125.27	119.05
1	A	717	HIS	C-N-CA	5.60	125.27	119.05
1	A	749	LYS	CA-C-O	-5.59	113.54	119.97
1	A	274	HIS	CB-CG-ND1	5.58	131.07	122.70
1	A	523	ASP	N-CA-C	-5.55	98.97	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	424	CYS	CA-C-O	-5.52	114.70	120.55
1	A	646	HIS	CB-CG-CD2	-5.51	124.04	131.20
1	A	326	PHE	CA-C-O	5.50	125.34	119.34
1	A	98	HIS	CA-CB-CG	-5.50	108.30	113.80
1	A	69	VAL	O-C-N	-5.49	117.25	123.18
1	A	101	HIS	CB-CG-ND1	5.49	130.93	122.70
1	A	589	ASN	OD1-CG-ND2	-5.48	117.12	122.60
1	A	626	HIS	CA-CB-CG	-5.45	108.35	113.80
1	A	522	LYS	CA-C-O	5.44	128.28	120.51
1	A	263	ILE	N-CA-C	-5.43	107.01	112.17
1	A	448	ASN	OD1-CG-ND2	-5.42	117.18	122.60
1	A	321	HIS	CB-CG-CD2	-5.41	124.16	131.20
1	A	717	HIS	CB-CG-CD2	-5.41	124.16	131.20
1	A	565	CYS	CA-C-N	5.41	130.81	120.97
1	A	565	CYS	C-N-CA	5.41	130.81	120.97
1	A	666	ARG	NE-CZ-NH2	-5.40	114.34	119.20
1	A	185	ASP	CA-CB-CG	5.40	118.00	112.60
1	A	668	HIS	CA-CB-CG	-5.39	108.41	113.80
1	A	379	HIS	CB-CG-CD2	-5.37	124.22	131.20
1	A	730	THR	CA-CB-OG1	-5.36	101.55	109.60
1	A	679	PRO	CB-CA-C	5.36	116.28	111.40
1	A	77	GLN	OE1-CD-NE2	-5.36	117.25	122.60
1	A	521	PRO	N-CA-C	-5.33	102.31	110.95
1	A	626	HIS	CB-CG-CD2	-5.33	124.28	131.20
1	A	297	ASP	CB-CA-C	-5.32	101.96	110.79
1	A	293	ASP	CA-CB-CG	5.31	117.91	112.60
1	A	313	ILE	CA-C-O	5.31	125.99	120.36
1	A	659	ILE	N-CA-C	-5.31	99.91	107.77
1	A	318	LEU	CA-C-O	5.31	127.10	121.16
1	A	373	ALA	CA-C-O	-5.31	114.93	120.55
1	A	515	ASP	O-C-N	-5.29	116.71	123.06
1	A	332	HIS	CB-CG-CD2	-5.28	124.34	131.20
1	A	148	GLN	OE1-CD-NE2	-5.28	117.32	122.60
1	A	242	GLY	CA-C-N	5.25	124.92	119.56
1	A	242	GLY	C-N-CA	5.25	124.92	119.56
1	A	553	GLU	CA-CB-CG	5.25	124.60	114.10
1	A	267	THR	CA-CB-OG1	-5.22	101.77	109.60
1	A	692	HIS	CB-CG-CD2	-5.22	124.41	131.20
1	A	589	ASN	CB-CG-ND2	5.20	124.20	116.40
1	A	410	ARG	NE-CZ-NH2	-5.19	114.53	119.20
1	A	497	LEU	N-CA-C	5.19	117.69	109.96
1	A	666	ARG	N-CA-C	5.19	116.62	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	ILE	CA-C-N	5.17	125.92	120.43
1	A	179	ILE	C-N-CA	5.17	125.92	120.43
1	A	195	TRP	CG-CD1-NE1	-5.17	103.47	110.20
1	A	460	HIS	CB-CG-ND1	5.16	130.44	122.70
1	A	580	ARG	CB-CG-CD	5.16	123.18	111.30
1	A	195	TRP	CE2-CD2-CG	-5.16	101.01	107.20
1	A	306	HIS	CB-CG-CD2	-5.15	124.50	131.20
1	A	566	THR	CA-C-O	-5.11	115.95	121.87
1	A	662	LYS	CB-CG-CD	-5.09	99.58	111.30
1	A	630	TRP	CB-CG-CD1	-5.05	119.32	126.90
1	A	448	ASN	CA-C-O	5.04	124.71	119.97
1	A	522	LYS	O-C-N	5.03	129.28	122.59

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	580	ARG	Sidechain
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	5815	0	5804	59	0
2	A	8	0	0	0	0
3	A	13	0	4	2	0
4	A	338	0	0	1	0
All	All	6174	0	5808	59	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 (59) 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	1.31	0.77
1:A:430:ARG:HD2	1:A:432:ASP:OD1	1.88	0.73
1:A:566:THR:HG22	1:A:568:ASP:H	1.55	0.70
1:A:13:HIS:HB3	4:A:1202:HOH:O	1.95	0.65
1:A:622:TYR:O	1:A:626:HIS:HD2	1.83	0.62
1:A:221:ILE:HG12	1:A:259:MET:HB3	1.84	0.59
1:A:566:THR:HB	1:A:569:HIS:ND1	2.17	0.59
1:A:584:ASP:OD1	1:A:653:HIS:HE1	1.87	0.57
1:A:277:LYS:HG3	1:A:289:ALA:HB1	1.87	0.56
1:A:546:LYS:HD3	1:A:741:ALA:O	2.06	0.55
1:A:566:THR:HG22	1:A:568:ASP:N	2.22	0.55
1:A:430:ARG:HH22	1:A:439:ASN:ND2	2.01	0.54
1:A:712:LYS:HE2	1:A:724:THR:HG21	1.90	0.53
1:A:327:THR:HG22	1:A:328:PRO:HD2	1.90	0.52
1:A:402:ARG:HD2	1:A:403:ASP:OD1	2.09	0.52
1:A:580:ARG:HH22	3:A:755:ICT:C5	2.25	0.50
1:A:208:THR:O	1:A:315:LEU:HB2	2.12	0.50
1:A:17:ARG:HB3	1:A:20:LEU:HB2	1.94	0.50
1:A:208:THR:HG22	1:A:314:ASN:HA	1.93	0.50
1:A:319:LYS:O	1:A:321:HIS:HD2	1.96	0.48
1:A:341:ALA:HA	1:A:346:TRP:CE3	2.49	0.47
1:A:675:GLN:NE2	1:A:675:GLN:HA	2.28	0.47
1:A:522:LYS:HE3	1:A:522:LYS:HA	1.96	0.47
1:A:435:LYS:HD2	1:A:456:ASN:HA	1.97	0.47
1:A:143:SER:HB3	1:A:516:THR:HB	1.98	0.46
1:A:376:ALA:HB2	1:A:474:ILE:HD13	1.98	0.45
1:A:374:LYS:HD2	1:A:375:GLN:HG3	1.98	0.45
1:A:69:VAL:O	1:A:95:SER:HA	2.16	0.45
1:A:752:GLN:O	1:A:754:LYS:HG3	2.17	0.45
1:A:589:ASN:C	1:A:589:ASN:HD22	2.25	0.45
1:A:589:ASN:ND2	1:A:650:GLU:OE1	2.50	0.45
1:A:145:ILE:HG21	1:A:358:CYS:HB3	1.99	0.44
1:A:174:LEU:HD13	1:A:250:CYS:SG	2.56	0.44
1:A:13:HIS:CD2	1:A:13:HIS:H	2.34	0.44
1:A:35:PRO:HB2	1:A:305:CYS:HA	1.99	0.43
1:A:458:GLU:OE1	1:A:460:HIS:HE1	2.01	0.43
1:A:435:LYS:HD3	1:A:435:LYS:HA	1.73	0.43
1:A:181:VAL:HB	1:A:185:ASP:HB2	1.99	0.43
1:A:384:LYS:HD3	1:A:476:GLY:HA3	2.00	0.43
1:A:144:GLY:HA3	1:A:393:SER:HA	2.01	0.43
1:A:428:TRP:CZ2	1:A:430:ARG:HD3	2.54	0.43
1:A:479:LYS:HE3	1:A:479:LYS:HB3	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ARG:HA	1:A:275:ARG:HD2	1.92	0.42
1:A:550:LYS:HB2	1:A:550:LYS:NZ	2.34	0.42
1:A:110:GLU:O	1:A:114:ARG:HG3	2.19	0.42
1:A:140:ARG:HD3	1:A:518:GLN:OE1	2.20	0.42
1:A:72:GLN:NE2	3:A:755:ICT:H41	2.35	0.42
1:A:496:LYS:HE3	1:A:496:LYS:HB3	1.94	0.42
1:A:121:GLN:O	1:A:125:ASN:HB2	2.21	0.41
1:A:65:ARG:NH2	1:A:194:PRO:HG3	2.35	0.41
1:A:355:ILE:HD13	1:A:355:ILE:HG21	1.82	0.41
1:A:377:LEU:HG	1:A:412:VAL:HG13	2.02	0.41
1:A:421:CYS:HB2	1:A:425:ILE:HD11	2.01	0.41
1:A:115:ARG:HG2	1:A:119:ILE:HD12	2.03	0.40
1:A:228:LEU:O	1:A:232:GLY:HA3	2.20	0.40
1:A:238:VAL:O	1:A:268:SER:HA	2.21	0.40
1:A:354:LEU:HD13	1:A:443:THR:HG22	2.02	0.40
1:A:401:GLU:CD	1:A:410:ARG:HH22	2.30	0.40
1:A:751:LEU:HD23	1:A:751:LEU:HA	1.90	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	751/754 (100%)	717 (96%)	29 (4%)	5 (1%)	18 14

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	524	SER
1	A	753	GLN
1	A	109	GLY
1	A	523	ASP

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Mol	Chain	Res	Type
1	A	525	SER

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	622/622 (100%)	578 (93%)	44 (7%)	13	10

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	23	LYS
1	A	107	LEU
1	A	110	GLU
1	A	125	ASN
1	A	201	LYS
1	A	208	THR
1	A	228	LEU
1	A	247	SER
1	A	315	LEU
1	A	317	GLU
1	A	319	LYS
1	A	325	PRO
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	433	ILE
1	A	458	GLU
1	A	487	LEU
1	A	496	LYS

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Mol	Chain	Res	Type
1	A	497	LEU
1	A	498	GLU
1	A	514	GLN
1	A	516	THR
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	601	LYS
1	A	631	VAL
1	A	636	GLU
1	A	657	ARG
1	A	666	ARG
1	A	702	LEU
1	A	704	ASP
1	A	747	ARG
1	A	754	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	HIS
1	A	82	GLN
1	A	106	GLN
1	A	148	GLN
1	A	321	HIS
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	637	ASN
1	A	653	HIS
1	A	671	ASN
1	A	675	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 ⓘ

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	3,4,1	0,12,12	-	-	-		
3	ICT	A	755	2	12,12,12	1.50	3 (25%)	13,16,16	2.28	4 (30%)

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	3,4,1	-	-	0/6/5/5
3	ICT	A	755	2	-	6/16/16/16	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	755	ICT	O6-C6	-2.25	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	755	ICT	C2-C1	-2.16	1.49	1.52
3	A	755	ICT	O1-C1	2.15	1.28	1.22

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	755	ICT	O6-C6-C3	4.04	124.41	113.93
3	A	755	ICT	O6-C6-O5	-3.99	115.02	124.08
3	A	755	ICT	O3-C5-C4	-3.65	111.64	122.84
3	A	755	ICT	O4-C5-C4	3.55	125.02	114.00

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	755	ICT	C1-C2-C3-C4
3	A	755	ICT	O7-C2-C3-C4
3	A	755	ICT	C4-C3-C6-O6
3	A	755	ICT	C4-C3-C6-O5
3	A	755	ICT	C2-C3-C6-O5
3	A	755	ICT	C2-C3-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	755	ICT	2	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.