



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:21 AM UTC

PDB ID : 1B0K / pdb_00001b0k
Title : S642A:FLUOROCITRATE COMPLEX OF ACONITASE
Authors : Lloyd, S.J.; Lauble, H.; Prasad, G.S.; Stout, C.D.
Deposited on : 1998-11-11
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

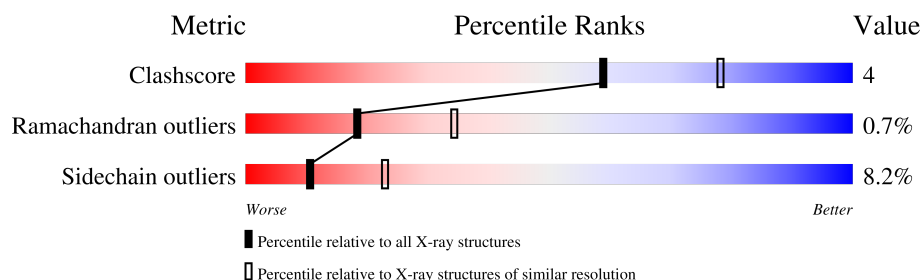
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	753	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FLC	A	756	-	X	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6139 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.

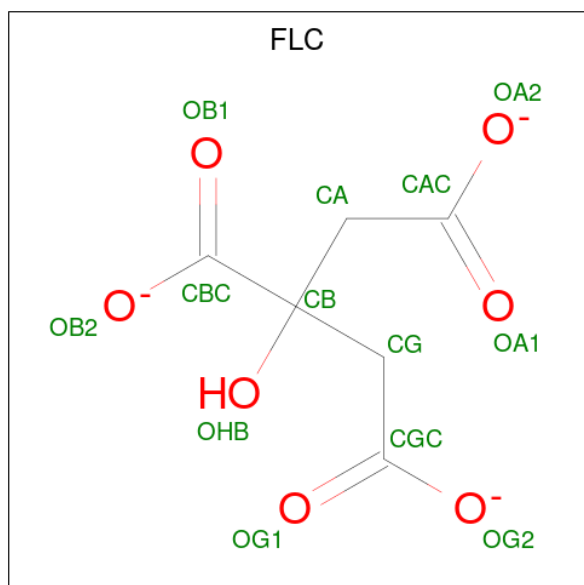
- Molecule 1 is a protein called PROTEIN (ACONITASE).

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	647	SER	ARG	conflict	UNP P16276

- Molecule 2 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7^-$).



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

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 4 is OXYGEN ATOM (CCD ID: O) (formula: O).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		

- Molecule 5 is water.

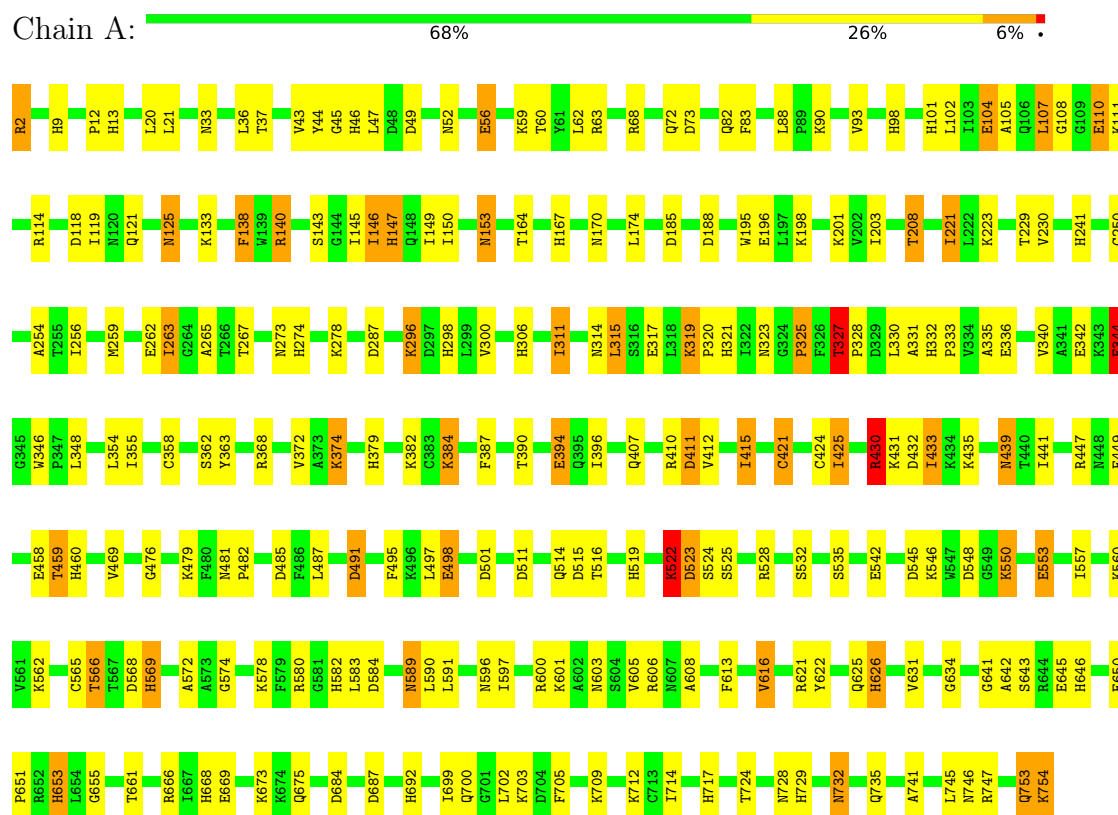
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	303	Total	O	0	0
			303	303		

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: PROTEIN (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	187.80Å 72.30Å 74.10Å 90.00° 90.00° 77.60°	Depositor
Resolution (Å)	20.00 – 2.50	Depositor
% Data completeness (in resolution range)	91.8 (20.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.172 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6139	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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, FLC, O

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	1.24	40/5941 (0.7%)	2.00	197/8049 (2.4%)

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

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

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	641	GLY	C-N	-12.09	1.17	1.33
1	A	643	SER	N-CA	-10.24	1.32	1.46
1	A	717	HIS	CD2-NE2	-7.15	1.29	1.37
1	A	646	HIS	CD2-NE2	-7.06	1.30	1.37
1	A	332	HIS	CD2-NE2	-7.01	1.30	1.37
1	A	221	ILE	CA-CB	6.96	1.63	1.54
1	A	241	HIS	CD2-NE2	-6.92	1.30	1.37
1	A	101	HIS	CD2-NE2	-6.74	1.30	1.37
1	A	167	HIS	CD2-NE2	-6.71	1.30	1.37
1	A	626	HIS	CD2-NE2	-6.60	1.30	1.37
1	A	582	HIS	CD2-NE2	-6.58	1.30	1.37
1	A	460	HIS	CD2-NE2	-6.57	1.30	1.37
1	A	46	HIS	CD2-NE2	-6.51	1.30	1.37
1	A	98	HIS	CD2-NE2	-6.48	1.30	1.37
1	A	519	HIS	CD2-NE2	-6.45	1.30	1.37
1	A	421	CYS	CA-CB	-6.43	1.43	1.53
1	A	441	ILE	CA-CB	6.33	1.62	1.54
1	A	298	HIS	CD2-NE2	-6.29	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	379	HIS	CD2-NE2	-6.26	1.30	1.37
1	A	729	HIS	CD2-NE2	-6.19	1.31	1.37
1	A	267	THR	CA-CB	6.17	1.63	1.53
1	A	569	HIS	CD2-NE2	-6.13	1.31	1.37
1	A	164	THR	CA-CB	6.13	1.60	1.52
1	A	146	ILE	CA-CB	6.10	1.62	1.54
1	A	321	HIS	CD2-NE2	-6.09	1.31	1.37
1	A	616	VAL	CA-CB	6.04	1.57	1.54
1	A	653	HIS	CD2-NE2	-5.95	1.31	1.37
1	A	692	HIS	CD2-NE2	-5.95	1.31	1.37
1	A	306	HIS	CD2-NE2	-5.92	1.31	1.37
1	A	13	HIS	CD2-NE2	-5.84	1.31	1.37
1	A	557	ILE	CA-CB	5.77	1.60	1.53
1	A	9	HIS	CD2-NE2	-5.61	1.31	1.37
1	A	98	HIS	CG-ND1	-5.60	1.32	1.38
1	A	332	HIS	CG-ND1	-5.52	1.32	1.38
1	A	668	HIS	CG-ND1	-5.40	1.32	1.38
1	A	43	VAL	CA-CB	5.39	1.60	1.54
1	A	415	ILE	CA-CB	5.36	1.61	1.54
1	A	668	HIS	CD2-NE2	-5.35	1.31	1.37
1	A	147	HIS	CD2-NE2	-5.32	1.32	1.37
1	A	333	PRO	CA-CB	-5.02	1.47	1.53

All (197) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	ASN	CA-CB-CG	10.71	123.31	112.60
1	A	170	ASN	OD1-CG-ND2	-9.62	112.98	122.60
1	A	582	HIS	CB-CG-CD2	-9.22	119.21	131.20
1	A	642	ALA	O-C-N	-9.20	111.04	122.82
1	A	101	HIS	CB-CG-CD2	-8.98	119.53	131.20
1	A	82	GLN	OE1-CD-NE2	-8.63	113.97	122.60
1	A	195	TRP	O-C-N	-8.55	113.47	123.22
1	A	746	ASN	CA-CB-CG	8.55	121.15	112.60
1	A	188	ASP	CA-CB-CG	8.44	121.04	112.60
1	A	596	ASN	CA-CB-CG	8.12	120.72	112.60
1	A	101	HIS	CB-CG-ND1	8.05	134.78	122.70
1	A	625	GLN	OE1-CD-NE2	-8.03	114.57	122.60
1	A	655	GLY	CA-C-N	7.86	127.57	120.10
1	A	655	GLY	C-N-CA	7.86	127.57	120.10
1	A	753	GLN	OE1-CD-NE2	-7.78	114.82	122.60
1	A	9	HIS	CB-CG-CD2	-7.75	121.12	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	HIS	CB-CG-CD2	-7.73	121.15	131.20
1	A	125	ASN	CA-CB-CG	-7.69	104.91	112.60
1	A	589	ASN	OD1-CG-ND2	-7.68	114.92	122.60
1	A	565	CYS	CA-C-N	7.62	133.75	120.87
1	A	565	CYS	C-N-CA	7.62	133.75	120.87
1	A	548	ASP	CA-CB-CG	7.62	120.22	112.60
1	A	642	ALA	CA-C-N	7.59	136.38	121.58
1	A	642	ALA	C-N-CA	7.59	136.38	121.58
1	A	298	HIS	CB-CG-CD2	-7.46	121.50	131.20
1	A	515	ASP	CA-CB-CG	7.44	120.04	112.60
1	A	485	ASP	N-CA-C	7.41	119.52	110.41
1	A	699	ILE	N-CA-C	-7.38	97.96	108.58
1	A	582	HIS	CB-CG-ND1	7.30	133.65	122.70
1	A	675	GLN	OE1-CD-NE2	-7.29	115.31	122.60
1	A	569	HIS	CB-CG-CD2	-7.27	121.74	131.20
1	A	325	PRO	N-CA-C	7.25	130.94	112.10
1	A	666	ARG	N-CA-C	7.23	119.79	111.11
1	A	729	HIS	CB-CG-CD2	-7.11	121.95	131.20
1	A	46	HIS	CB-CG-CD2	-7.04	122.05	131.20
1	A	616	VAL	CA-C-O	-6.89	114.07	118.69
1	A	646	HIS	CB-CG-CD2	-6.84	122.31	131.20
1	A	13	HIS	CB-CG-CD2	-6.83	122.32	131.20
1	A	705	PHE	CA-CB-CG	6.82	120.62	113.80
1	A	430	ARG	NE-CZ-NH2	-6.80	113.08	119.20
1	A	52	ASN	N-CA-C	6.75	121.68	113.38
1	A	273	ASN	CA-CB-CG	6.74	119.34	112.60
1	A	566	THR	N-CA-CB	-6.71	100.66	110.26
1	A	572	ALA	N-CA-C	6.70	119.21	110.43
1	A	265	ALA	CA-C-O	-6.62	113.90	121.19
1	A	133	LYS	N-CA-C	6.54	118.49	111.36
1	A	300	VAL	O-C-N	-6.49	117.18	121.72
1	A	441	ILE	O-C-N	-6.47	116.27	123.26
1	A	589	ASN	CB-CG-ND2	6.45	126.07	116.40
1	A	481	ASN	CA-C-N	6.44	126.37	119.28
1	A	481	ASN	C-N-CA	6.44	126.37	119.28
1	A	728	ASN	OD1-CG-ND2	-6.44	116.16	122.60
1	A	753	GLN	N-CA-C	6.43	124.50	110.80
1	A	411	ASP	CA-CB-CG	6.38	118.98	112.60
1	A	407	GLN	OE1-CD-NE2	-6.37	116.23	122.60
1	A	501	ASP	CA-CB-CG	-6.36	106.24	112.60
1	A	138	PHE	CA-CB-CG	6.30	120.11	113.80
1	A	82	GLN	CG-CD-NE2	6.30	125.85	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	ASN	CB-CG-ND2	6.23	125.75	116.40
1	A	327	THR	CB-CA-C	-6.23	98.64	108.91
1	A	542	GLU	N-CA-C	-6.22	100.93	110.32
1	A	254	ALA	CA-C-O	-6.21	114.30	120.82
1	A	368	ARG	N-CA-C	-6.18	104.62	111.36
1	A	46	HIS	CB-CG-ND1	6.16	131.93	122.70
1	A	296	LYS	N-CA-C	6.12	123.84	110.80
1	A	583	LEU	N-CA-C	6.08	118.41	111.11
1	A	495	PHE	CA-CB-CG	6.08	119.88	113.80
1	A	119	ILE	N-CA-C	6.06	117.53	110.62
1	A	287	ASP	CA-CB-CG	6.06	118.66	112.60
1	A	709	LYS	CA-C-N	6.01	125.98	120.21
1	A	709	LYS	C-N-CA	6.01	125.98	120.21
1	A	523	ASP	N-CA-C	-5.99	98.05	110.80
1	A	102	LEU	N-CA-C	5.97	119.53	112.72
1	A	605	VAL	O-C-N	5.97	129.39	123.00
1	A	387	PHE	N-CA-CB	-5.96	101.41	110.77
1	A	9	HIS	CB-CG-ND1	5.96	131.63	122.70
1	A	256	ILE	CA-C-O	-5.94	114.77	120.95
1	A	553	GLU	CA-CB-CG	5.94	125.98	114.10
1	A	569	HIS	CB-CG-ND1	5.92	131.58	122.70
1	A	332	HIS	CB-CG-CD2	-5.92	123.50	131.20
1	A	372	VAL	N-CA-C	-5.92	105.08	110.82
1	A	545	ASP	CA-CB-CG	5.91	118.51	112.60
1	A	700	GLN	N-CA-CB	-5.91	100.56	111.13
1	A	390	THR	CA-C-N	5.89	125.65	119.76
1	A	390	THR	C-N-CA	5.89	125.65	119.76
1	A	319	LYS	CA-C-N	5.84	125.86	119.90
1	A	319	LYS	C-N-CA	5.84	125.86	119.90
1	A	118	ASP	CA-CB-CG	5.80	118.40	112.60
1	A	274	HIS	CB-CG-ND1	5.79	131.38	122.70
1	A	522	LYS	CA-C-O	5.78	128.78	120.51
1	A	572	ALA	O-C-N	-5.78	115.99	122.75
1	A	459	THR	CA-CB-CG2	5.77	120.31	110.50
1	A	90	LYS	CA-CB-CG	5.75	125.60	114.10
1	A	589	ASN	CA-CB-CG	5.74	118.34	112.60
1	A	265	ALA	O-C-N	-5.72	115.84	122.87
1	A	348	LEU	N-CA-C	5.69	119.39	112.23
1	A	354	LEU	N-CA-C	5.68	119.58	107.70
1	A	459	THR	CA-CB-OG1	-5.67	101.10	109.60
1	A	692	HIS	CB-CG-CD2	-5.67	123.83	131.20
1	A	332	HIS	CA-CB-CG	-5.65	108.15	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	ILE	N-CA-C	-5.65	100.28	108.36
1	A	603	ASN	OD1-CG-ND2	-5.64	116.95	122.60
1	A	93	VAL	O-C-N	-5.63	116.56	121.57
1	A	323	ASN	OD1-CG-ND2	-5.63	116.97	122.60
1	A	522	LYS	CG-CD-CE	5.62	124.22	111.30
1	A	675	GLN	CG-CD-NE2	5.61	124.82	116.40
1	A	59	LYS	N-CA-C	5.59	119.88	112.72
1	A	344	GLU	N-CA-C	5.59	119.96	113.20
1	A	36	LEU	CA-C-O	-5.58	114.80	120.71
1	A	645	GLU	N-CA-C	5.57	119.56	112.87
1	A	433	ILE	O-C-N	-5.57	116.65	123.00
1	A	491	ASP	CA-CB-CG	5.56	118.16	112.60
1	A	185	ASP	CA-C-O	-5.55	114.98	120.70
1	A	346	TRP	CA-C-N	5.55	125.87	119.93
1	A	346	TRP	C-N-CA	5.55	125.87	119.93
1	A	374	LYS	CA-CB-CG	5.55	125.20	114.10
1	A	754	LYS	CA-CB-CG	5.53	125.17	114.10
1	A	83	PHE	CA-CB-CG	-5.52	108.28	113.80
1	A	140	ARG	CA-C-N	5.51	125.83	119.93
1	A	140	ARG	C-N-CA	5.51	125.83	119.93
1	A	241	HIS	CB-CG-CD2	-5.50	124.05	131.20
1	A	410	ARG	CB-CA-C	-5.50	102.22	110.90
1	A	331	ALA	N-CA-C	5.49	118.58	109.46
1	A	319	LYS	O-C-N	-5.49	116.68	121.35
1	A	278	LYS	CG-CD-CE	5.49	123.92	111.30
1	A	684	ASP	CA-C-N	5.49	125.20	119.82
1	A	684	ASP	C-N-CA	5.49	125.20	119.82
1	A	88	LEU	CD1-CG-CD2	-5.48	98.74	110.80
1	A	732	ASN	OD1-CG-ND2	-5.46	117.14	122.60
1	A	306	HIS	CB-CG-CD2	-5.46	124.11	131.20
1	A	439	ASN	CA-CB-CG	5.46	118.06	112.60
1	A	687	ASP	CA-CB-CG	-5.44	107.16	112.60
1	A	13	HIS	CB-CG-ND1	5.44	130.86	122.70
1	A	666	ARG	NE-CZ-NH2	-5.42	114.32	119.20
1	A	574	GLY	CA-C-N	5.42	125.08	119.56
1	A	574	GLY	C-N-CA	5.42	125.08	119.56
1	A	73	ASP	CA-CB-CG	5.41	118.01	112.60
1	A	311	ILE	N-CA-C	-5.41	100.05	108.86
1	A	150	ILE	CA-C-O	-5.40	115.06	121.05
1	A	59	LYS	CB-CA-C	-5.40	101.52	110.37
1	A	642	ALA	N-CA-C	5.38	117.23	110.24
1	A	650	GLU	CA-C-O	-5.37	112.80	120.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	580	ARG	CG-CD-NE	-5.37	100.19	112.00
1	A	68	ARG	CA-CB-CG	5.37	124.83	114.10
1	A	528	ARG	N-CA-C	-5.36	101.44	109.95
1	A	104	GLU	N-CA-C	5.34	117.97	109.96
1	A	566	THR	CA-C-O	-5.31	116.03	121.87
1	A	263	ILE	N-CA-C	-5.28	107.97	113.10
1	A	410	ARG	CA-C-O	-5.27	115.27	120.70
1	A	542	GLU	CB-CA-C	5.26	115.96	108.76
1	A	745	LEU	CA-C-O	-5.24	114.87	120.42
1	A	498	GLU	CB-CG-CD	5.24	121.50	112.60
1	A	519	HIS	CA-C-O	-5.23	115.25	120.64
1	A	320	PRO	N-CA-C	5.23	119.41	111.15
1	A	33	ASN	CA-CB-CG	-5.22	107.38	112.60
1	A	580	ARG	NE-CZ-NH1	5.22	126.72	121.50
1	A	2	ARG	N-CA-C	-5.20	96.45	111.00
1	A	153	ASN	N-CA-C	5.20	120.55	114.62
1	A	267	THR	CA-CB-CG2	5.18	119.31	110.50
1	A	668	HIS	CA-CB-CG	-5.18	108.62	113.80
1	A	37	THR	CA-C-O	-5.17	116.03	121.88
1	A	511	ASP	N-CA-C	-5.16	102.06	109.24
1	A	608	ALA	N-CA-C	5.16	117.57	111.33
1	A	519	HIS	CB-CG-CD2	-5.16	124.50	131.20
1	A	147	HIS	CB-CG-CD2	-5.15	124.50	131.20
1	A	626	HIS	CA-CB-CG	-5.15	108.65	113.80
1	A	149	ILE	N-CA-C	5.14	115.87	110.62
1	A	335	ALA	N-CA-C	5.14	116.96	111.36
1	A	119	ILE	N-CA-CB	-5.14	104.05	110.47
1	A	469	VAL	CA-C-O	-5.13	115.93	121.27
1	A	431	LYS	N-CA-C	5.13	120.66	113.02
1	A	566	THR	O-C-N	-5.12	116.75	122.75
1	A	195	TRP	CG-CD1-NE1	-5.12	103.54	110.20
1	A	254	ALA	CA-C-N	5.12	127.91	120.79
1	A	254	ALA	C-N-CA	5.12	127.91	120.79
1	A	346	TRP	CE2-CD2-CG	-5.11	101.06	107.20
1	A	481	ASN	OD1-CG-ND2	-5.10	117.50	122.60
1	A	732	ASN	CA-CB-CG	5.09	117.69	112.60
1	A	410	ARG	NE-CZ-NH1	5.09	126.59	121.50
1	A	411	ASP	CA-C-O	-5.09	114.35	120.10
1	A	621	ARG	CA-C-O	-5.08	115.47	120.70
1	A	523	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	342	GLU	N-CA-CB	-5.06	102.40	109.94
1	A	424	CYS	CA-C-O	-5.05	115.06	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	424	CYS	N-CA-CB	-5.05	102.69	110.16
1	A	646	HIS	CB-CG-ND1	5.05	130.27	122.70
1	A	327	THR	N-CA-CB	5.04	120.26	111.19
1	A	223	LYS	CA-C-O	-5.03	115.08	120.42
1	A	498	GLU	N-CA-C	-5.03	103.89	110.53
1	A	394	GLU	CB-CA-C	-5.03	102.77	110.81
1	A	49	ASP	CA-C-N	5.02	124.62	119.05
1	A	49	ASP	C-N-CA	5.02	124.62	119.05
1	A	717	HIS	CA-C-N	5.02	124.68	119.56
1	A	717	HIS	C-N-CA	5.02	124.68	119.56
1	A	447	ARG	CG-CD-NE	-5.01	100.97	112.00
1	A	482	PRO	O-C-N	5.01	128.68	122.22
1	A	12	PRO	N-CA-C	5.00	120.20	114.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	363	TYR	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	5803	51	0
2	A	13	0	3	0	0
3	A	8	0	0	1	0
4	A	1	0	0	0	0
5	A	303	0	0	1	0
All	All	6139	0	5806	51	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 (51) 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:384:LYS:HD3	1:A:476:GLY:HA3	1.49	0.94
1:A:566:THR:HG22	1:A:568:ASP:H	1.46	0.81
1:A:221:ILE:HG12	1:A:259:MET:HB3	1.73	0.69
1:A:107:LEU:HD23	1:A:111:LYS:HB3	1.77	0.67
1:A:430:ARG:HH22	1:A:439:ASN:HD21	1.40	0.66
1:A:430:ARG:HD2	1:A:432:ASP:OD1	1.99	0.63
1:A:63:ARG:HG3	5:A:897:HOH:O	1.97	0.63
1:A:550:LYS:HB2	1:A:550:LYS:NZ	2.14	0.62
1:A:566:THR:HB	1:A:569:HIS:ND1	2.15	0.61
1:A:550:LYS:HA	1:A:703:LYS:HE3	1.82	0.60
1:A:430:ARG:NH2	1:A:439:ASN:HD21	2.00	0.58
1:A:174:LEU:HD13	1:A:250:CYS:SG	2.44	0.57
1:A:566:THR:HG22	1:A:568:ASP:N	2.18	0.57
1:A:362:SER:HA	1:A:396:ILE:HD13	1.89	0.54
1:A:425:ILE:HG13	3:A:755:SF4:S1	2.47	0.54
1:A:143:SER:HB3	1:A:516:THR:HB	1.90	0.54
1:A:208:THR:O	1:A:315:LEU:HB2	2.07	0.54
1:A:208:THR:HG22	1:A:314:ASN:OD1	2.08	0.54
1:A:532:SER:HB3	1:A:535:SER:HB2	1.90	0.54
1:A:560:LYS:HG2	1:A:597:ILE:HG21	1.91	0.51
1:A:121:GLN:O	1:A:125:ASN:HB2	2.12	0.50
1:A:449:PHE:CD2	1:A:566:THR:HG21	2.48	0.49
1:A:327:THR:HG22	1:A:328:PRO:HD2	1.95	0.48
1:A:606:ARG:HB2	1:A:613:PHE:CZ	2.48	0.48
1:A:110:GLU:O	1:A:114:ARG:HG3	2.14	0.47
1:A:108:GLY:HA3	1:A:415:ILE:HD11	1.97	0.46
1:A:382:LYS:NZ	1:A:411:ASP:O	2.48	0.46
1:A:732:ASN:OD1	1:A:735:GLN:HG3	2.15	0.46
1:A:522:LYS:HE3	1:A:522:LYS:HA	1.97	0.45
1:A:340:VAL:O	1:A:344:GLU:HB2	2.17	0.45
1:A:550:LYS:HB2	1:A:550:LYS:HZ2	1.79	0.45
1:A:230:VAL:HA	1:A:263:ILE:HA	1.99	0.44
1:A:21:LEU:HD12	1:A:45:GLY:HA3	2.00	0.44
1:A:590:LEU:HD13	1:A:651:PRO:HD3	1.98	0.44
1:A:62:LEU:O	1:A:196:GLU:HA	2.19	0.43
1:A:421:CYS:HB2	1:A:425:ILE:HD11	2.01	0.43
1:A:634:GLY:HA3	1:A:661:THR:HG22	1.99	0.42
1:A:146:ILE:HD13	1:A:146:ILE:HG21	1.85	0.42
1:A:479:LYS:HE3	1:A:479:LYS:HB3	1.80	0.42
1:A:546:LYS:HD3	1:A:741:ALA:O	2.19	0.42
1:A:56:GLU:HB2	1:A:60:THR:HG23	2.01	0.42
1:A:145:ILE:HG21	1:A:358:CYS:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:622:TYR:O	1:A:626:HIS:HD2	2.03	0.42
1:A:104:GLU:HG2	1:A:105:ALA:N	2.35	0.42
1:A:44:TYR:HA	1:A:47:LEU:HG	2.01	0.41
1:A:138:PHE:HE2	1:A:140:ARG:HG2	1.85	0.41
1:A:591:LEU:HB2	1:A:616:VAL:HG11	2.03	0.41
1:A:584:ASP:OD1	1:A:653:HIS:HE1	2.03	0.41
1:A:714:ILE:HD12	1:A:714:ILE:N	2.36	0.40
1:A:669:GLU:O	1:A:673:LYS:HG3	2.21	0.40
1:A:147:HIS:HD2	1:A:358:CYS:SG	2.44	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	751/753 (100%)	709 (94%)	37 (5%)	5 (1%)	18	34

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	524	SER
1	A	753	GLN
1	A	296	LYS
1	A	525	SER
1	A	578	LYS

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

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

Mol	Chain	Res	Type
1	A	2	ARG
1	A	20	LEU
1	A	56	GLU
1	A	72	GLN
1	A	107	LEU
1	A	110	GLU
1	A	153	ASN
1	A	198	LYS
1	A	201	LYS
1	A	208	THR
1	A	229	THR
1	A	262	GLU
1	A	311	ILE
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	336	GLU
1	A	344	GLU
1	A	355	ILE
1	A	374	LYS
1	A	384	LYS
1	A	394	GLU
1	A	412	VAL
1	A	425	ILE
1	A	430	ARG
1	A	433	ILE
1	A	435	LYS
1	A	458	GLU
1	A	459	THR
1	A	487	LEU
1	A	491	ASP
1	A	497	LEU

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Mol	Chain	Res	Type
1	A	498	GLU
1	A	514	GLN
1	A	522	LYS
1	A	523	ASP
1	A	550	LYS
1	A	553	GLU
1	A	562	LYS
1	A	589	ASN
1	A	600	ARG
1	A	601	LYS
1	A	631	VAL
1	A	702	LEU
1	A	712	LYS
1	A	724	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	77	GLN
1	A	147	HIS
1	A	153	ASN
1	A	241	HIS
1	A	306	HIS
1	A	321	HIS
1	A	419	ASN
1	A	439	ASN
1	A	481	ASN
1	A	519	HIS
1	A	536	GLN
1	A	539	GLN
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 ⓘ

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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	FLC	A	756	3	12,12,12	4.41	7 (58%)	17,17,17	3.29	7 (41%)
3	SF4	A	755	1,4,2	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
2	FLC	A	756	3	-	7/16/16/16	-
3	SF4	A	755	1,4,2	-	-	0/6/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	756	FLC	CA-CB	-11.67	1.39	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	756	FLC	CB-CBC	-5.55	1.47	1.53
2	A	756	FLC	CA-CAC	-5.36	1.34	1.50
2	A	756	FLC	OHB-CB	4.33	1.51	1.43
2	A	756	FLC	OG2-CGC	-2.71	1.21	1.30
2	A	756	FLC	CG-CGC	-2.07	1.44	1.50
2	A	756	FLC	OB1-CBC	2.05	1.28	1.22

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	756	FLC	CB-CA-CAC	9.67	140.36	113.92
2	A	756	FLC	OHB-CB-CBC	4.68	115.59	108.96
2	A	756	FLC	CB-CG-CGC	4.33	125.75	113.92
2	A	756	FLC	OHB-CB-CA	-3.94	100.40	109.38
2	A	756	FLC	OA1-CAC-CA	-3.21	113.86	122.95
2	A	756	FLC	CA-CB-CBC	3.10	116.90	110.03
2	A	756	FLC	OHB-CB-CG	-2.14	104.50	109.38

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	756	FLC	CAC-CA-CB-OHB
2	A	756	FLC	CA-CB-CG-CGC
2	A	756	FLC	CBC-CB-CG-CGC
2	A	756	FLC	CAC-CA-CB-CBC
2	A	756	FLC	CAC-CA-CB-CG
2	A	756	FLC	OHB-CB-CG-CGC
2	A	756	FLC	CB-CA-CAC-OA1

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	641:GLY	C	642:ALA	N	1.17

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.