



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:57 PM UTC

PDB ID : 1C96 / pdb_00001c96
Title : S642A:CITRATE COMPLEX OF ACONITASE
Authors : Lloyd, S.J.; Lauble, H.; Prasad, G.S.; Stout, C.D.
Deposited on : 1999-07-31
Resolution : 1.81 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

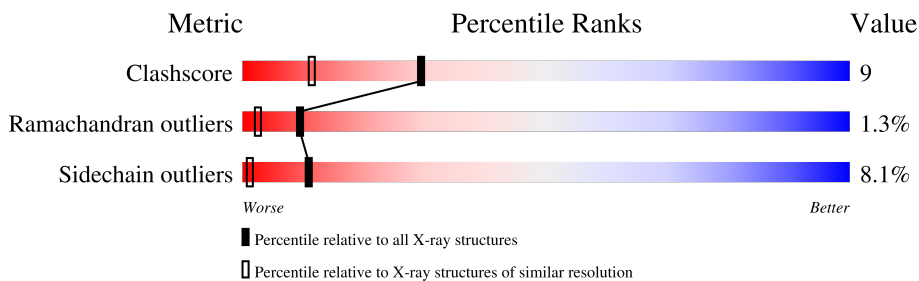
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.81 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	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)

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
3	SF4	A	755	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6510 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 MITOCHONDRIAL ACONITASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	753	5811	3665	1034	1090	22	0	0	0

There are 17 discrepancies between the modelled and reference sequences:

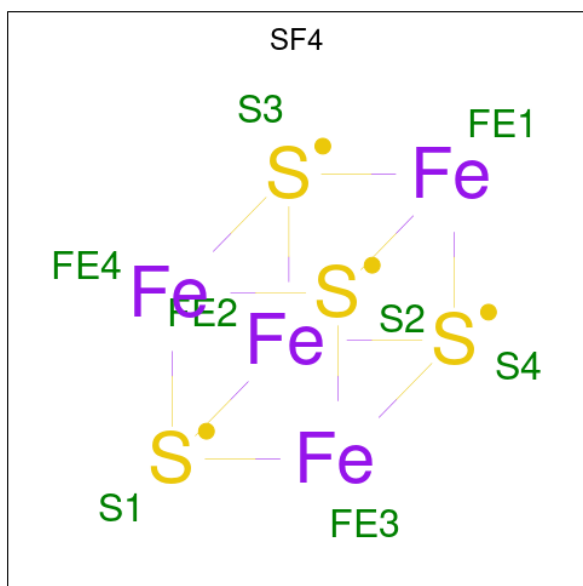
Chain	Residue	Modelled	Actual	Comment	Reference
A	13	HIS	ASN	conflict	UNP P20004
A	26	ASP	ASN	conflict	UNP P20004
A	303	PRO	SER	conflict	UNP P20004
A	310	VAL	LEU	conflict	UNP P20004
A	382	LYS	GLN	conflict	UNP P20004
A	408	VAL	ILE	conflict	UNP P20004
A	528	ARG	GLU	conflict	UNP P20004
A	530	ALA	ASP	conflict	UNP P20004
A	550	LYS	ARG	conflict	UNP P20004
A	597	ILE	VAL	conflict	UNP P20004
A	600	ARG	GLY	conflict	UNP P20004
A	625	GLN	LYS	conflict	UNP P20004
A	642	ALA	SER	engineered mutation	UNP P20004
A	647	SER	ALA	conflict	UNP P20004
A	700	GLN	LYS	conflict	UNP P20004
A	712	LYS	THR	conflict	UNP P20004
A	753	GLN	LYS	conflict	UNP P20004

- Molecule 2 is CITRATE ANION (CCD ID: FLC) (formula: C₆H₅O₇).



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	677	Total	O	0	0
			677	677		

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	176.10Å 71.40Å 71.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.81	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-1.81)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.225 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6510	wwPDB-VP
Average B, all atoms (Å ²)	38.0	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	1.30	41/5938 (0.7%)	2.02	202/8045 (2.5%)

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	4

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	643	SER	N-CA	-13.36	1.28	1.46
1	A	46	HIS	CD2-NE2	-7.47	1.29	1.37
1	A	626	HIS	CD2-NE2	-7.38	1.29	1.37
1	A	313	ILE	CA-CB	7.03	1.63	1.54
1	A	646	HIS	CD2-NE2	-6.96	1.30	1.37
1	A	668	HIS	CD2-NE2	-6.91	1.30	1.37
1	A	298	HIS	CD2-NE2	-6.69	1.30	1.37
1	A	241	HIS	CD2-NE2	-6.66	1.30	1.37
1	A	460	HIS	CD2-NE2	-6.65	1.30	1.37
1	A	379	HIS	CD2-NE2	-6.61	1.30	1.37
1	A	13	HIS	CD2-NE2	-6.35	1.30	1.37
1	A	9	HIS	CD2-NE2	-6.32	1.30	1.37
1	A	692	HIS	CD2-NE2	-6.27	1.30	1.37
1	A	579	PHE	C-N	-6.27	1.25	1.33
1	A	717	HIS	CD2-NE2	-6.22	1.31	1.37
1	A	582	HIS	CD2-NE2	-6.21	1.31	1.37
1	A	514	GLN	CA-CB	6.18	1.64	1.53
1	A	93	VAL	CA-CB	6.14	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	332	HIS	CD2-NE2	-6.13	1.31	1.37
1	A	653	HIS	CD2-NE2	-6.04	1.31	1.37
1	A	729	HIS	CD2-NE2	-5.98	1.31	1.37
1	A	114	ARG	NE-CZ	5.93	1.39	1.33
1	A	147	HIS	CD2-NE2	-5.93	1.31	1.37
1	A	666	ARG	CD-NE	-5.90	1.38	1.46
1	A	569	HIS	CD2-NE2	-5.88	1.31	1.37
1	A	101	HIS	CD2-NE2	-5.87	1.31	1.37
1	A	46	HIS	CG-ND1	-5.84	1.31	1.38
1	A	306	HIS	CD2-NE2	-5.75	1.31	1.37
1	A	167	HIS	CD2-NE2	-5.71	1.31	1.37
1	A	519	HIS	CD2-NE2	-5.69	1.31	1.37
1	A	653	HIS	CG-ND1	-5.60	1.32	1.38
1	A	597	ILE	CA-CB	5.56	1.61	1.54
1	A	379	HIS	CG-ND1	-5.41	1.32	1.38
1	A	317	GLU	CA-CB	-5.39	1.44	1.53
1	A	710	PRO	CA-CB	-5.31	1.46	1.53
1	A	668	HIS	CG-ND1	-5.30	1.32	1.38
1	A	425	ILE	CA-CB	5.25	1.61	1.54
1	A	321	HIS	CD2-NE2	-5.17	1.32	1.37
1	A	196	GLU	CA-CB	-5.16	1.46	1.53
1	A	274	HIS	CG-CD2	5.08	1.41	1.35
1	A	312	GLU	CA-CB	-5.02	1.45	1.53

All (202) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	486	PHE	N-CA-C	14.02	130.99	109.96
1	A	695	ASP	CA-CB-CG	12.71	125.31	112.60
1	A	666	ARG	NE-CZ-NH2	11.63	129.67	119.20
1	A	515	ASP	CA-CB-CG	10.03	122.63	112.60
1	A	666	ARG	NE-CZ-NH1	-9.04	112.46	121.50
1	A	485	ASP	N-CA-C	9.00	129.97	110.80
1	A	273	ASN	CA-CB-CG	8.76	121.36	112.60
1	A	485	ASP	CA-C-N	8.60	132.99	120.95
1	A	485	ASP	C-N-CA	8.60	132.99	120.95
1	A	490	LYS	CA-CB-CG	8.39	130.88	114.10
1	A	357	SER	O-C-N	8.27	133.59	122.59
1	A	114	ARG	NE-CZ-NH2	8.21	126.59	119.20
1	A	402	ARG	NE-CZ-NH1	-7.98	113.52	121.50
1	A	411	ASP	CA-CB-CG	7.94	120.54	112.60
1	A	509	GLU	CB-CG-CD	7.91	126.05	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	514	GLN	CB-CG-CD	7.88	126.00	112.60
1	A	147	HIS	CA-CB-CG	-7.87	105.93	113.80
1	A	495	PHE	N-CA-C	7.80	127.41	110.80
1	A	501	ASP	CA-CB-CG	-7.74	104.86	112.60
1	A	60	THR	N-CA-CB	-7.74	98.01	110.63
1	A	460	HIS	CB-CG-CD2	-7.73	121.16	131.20
1	A	440	THR	CA-CB-OG1	-7.66	98.12	109.60
1	A	154	TYR	N-CA-C	7.65	123.53	114.04
1	A	491	ASP	CA-CB-CG	7.61	120.21	112.60
1	A	485	ASP	CA-CB-CG	7.33	119.93	112.60
1	A	717	HIS	CB-CG-CD2	-7.17	121.87	131.20
1	A	706	ALA	CA-C-N	7.17	127.60	119.93
1	A	706	ALA	C-N-CA	7.17	127.60	119.93
1	A	314	ASN	OD1-CG-ND2	-7.17	115.43	122.60
1	A	366	MET	CA-C-O	-7.14	112.85	120.42
1	A	514	GLN	N-CA-C	7.13	126.00	110.80
1	A	603	ASN	N-CA-C	7.13	121.36	111.74
1	A	732	ASN	OD1-CG-ND2	-7.02	115.58	122.60
1	A	357	SER	CA-C-N	7.02	134.95	121.54
1	A	357	SER	C-N-CA	7.02	134.95	121.54
1	A	545	ASP	CA-CB-CG	7.00	119.60	112.60
1	A	449	PHE	CA-CB-CG	6.98	120.78	113.80
1	A	402	ARG	NE-CZ-NH2	6.95	125.45	119.20
1	A	82	GLN	OE1-CD-NE2	-6.91	115.69	122.60
1	A	263	ILE	N-CA-C	-6.90	106.00	112.83
1	A	642	ALA	O-C-N	-6.90	113.99	122.82
1	A	553	GLU	CA-CB-CG	6.88	127.86	114.10
1	A	166	SER	CB-CA-C	-6.88	99.38	110.79
1	A	580	ARG	NE-CZ-NH2	6.71	125.24	119.20
1	A	699	ILE	N-CA-CB	6.69	119.04	111.21
1	A	510	PHE	CA-CB-CG	6.67	120.47	113.80
1	A	153	ASN	OD1-CG-ND2	-6.67	115.93	122.60
1	A	121	GLN	CB-CG-CD	6.62	123.86	112.60
1	A	327	THR	CB-CA-C	-6.62	99.27	109.20
1	A	152	GLU	CB-CG-CD	6.57	123.76	112.60
1	A	306	HIS	CB-CG-CD2	-6.56	122.67	131.20
1	A	599	ASN	OD1-CG-ND2	-6.55	116.05	122.60
1	A	535	SER	O-C-N	-6.54	114.82	122.87
1	A	410	ARG	NE-CZ-NH2	6.53	125.08	119.20
1	A	582	HIS	CB-CG-CD2	-6.47	122.79	131.20
1	A	410	ARG	NE-CZ-NH1	-6.40	115.10	121.50
1	A	528	ARG	N-CA-C	-6.33	98.93	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	11	GLU	CA-C-N	6.31	125.93	119.56
1	A	11	GLU	C-N-CA	6.31	125.93	119.56
1	A	644	ARG	NE-CZ-NH2	6.30	124.88	119.20
1	A	646	HIS	CB-CG-CD2	-6.30	123.01	131.20
1	A	493	LYS	N-CA-C	6.29	124.21	110.80
1	A	125	ASN	CB-CG-ND2	6.28	125.83	116.40
1	A	702	LEU	N-CA-C	-6.27	104.54	111.82
1	A	422	GLY	CA-C-N	6.19	127.58	119.84
1	A	422	GLY	C-N-CA	6.19	127.58	119.84
1	A	548	ASP	CA-CB-CG	6.18	118.78	112.60
1	A	460	HIS	CB-CG-ND1	6.17	131.95	122.70
1	A	167	HIS	CB-CG-CD2	-6.16	123.19	131.20
1	A	580	ARG	NE-CZ-NH1	-6.14	115.36	121.50
1	A	108	GLY	CA-C-O	6.13	126.46	122.23
1	A	111	LYS	N-CA-C	-6.13	104.51	111.07
1	A	750	GLU	CA-CB-CG	6.12	126.35	114.10
1	A	430	ARG	NE-CZ-NH2	6.10	124.69	119.20
1	A	61	TYR	CA-C-O	6.10	126.88	120.36
1	A	481	ASN	OD1-CG-ND2	-6.09	116.51	122.60
1	A	574	GLY	CA-C-N	6.08	125.70	119.56
1	A	574	GLY	C-N-CA	6.08	125.70	119.56
1	A	359	THR	CA-CB-OG1	-6.05	100.53	109.60
1	A	689	ASN	OD1-CG-ND2	-6.04	116.56	122.60
1	A	453	ASN	N-CA-C	6.02	119.09	111.69
1	A	747	ARG	NE-CZ-NH1	-6.01	115.49	121.50
1	A	488	THR	N-CA-CB	-6.00	100.34	110.49
1	A	332	HIS	CB-CG-CD2	-5.98	123.42	131.20
1	A	195	TRP	CE2-CD2-CG	-5.97	100.03	107.20
1	A	46	HIS	CB-CG-CD2	-5.97	123.44	131.20
1	A	629	ARG	NE-CZ-NH2	5.96	124.56	119.20
1	A	85	SER	O-C-N	-5.92	115.46	122.20
1	A	384	LYS	CB-CG-CD	5.91	124.90	111.30
1	A	604	SER	CA-C-O	5.90	128.19	120.11
1	A	589	ASN	OD1-CG-ND2	-5.89	116.71	122.60
1	A	166	SER	N-CA-C	5.86	117.66	111.28
1	A	397	ARG	NE-CZ-NH2	5.85	124.47	119.20
1	A	625	GLN	OE1-CD-NE2	-5.83	116.77	122.60
1	A	311	ILE	CB-CG1-CD1	-5.83	101.56	113.80
1	A	514	GLN	OE1-CD-NE2	-5.82	116.78	122.60
1	A	699	ILE	CB-CA-C	-5.82	103.01	110.98
1	A	140	ARG	CA-C-N	5.80	126.14	119.93
1	A	140	ARG	C-N-CA	5.80	126.14	119.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	THR	CA-CB-OG1	-5.80	100.90	109.60
1	A	242	GLY	CA-C-N	5.78	125.25	119.24
1	A	242	GLY	C-N-CA	5.78	125.25	119.24
1	A	246	ASP	CA-CB-CG	-5.78	106.82	112.60
1	A	310	VAL	N-CA-C	5.78	116.20	108.11
1	A	505	LEU	CA-C-O	-5.77	114.92	120.64
1	A	201	LYS	N-CA-C	-5.76	102.77	110.55
1	A	516	THR	N-CA-C	5.75	122.11	114.12
1	A	344	GLU	N-CA-C	5.75	120.14	113.18
1	A	141	PRO	O-C-N	5.74	129.86	122.85
1	A	358	CYS	CA-CB-SG	5.72	127.57	114.40
1	A	551	ASP	CA-CB-CG	5.72	118.33	112.60
1	A	23	LYS	CA-CB-CG	-5.68	102.74	114.10
1	A	753	GLN	CA-C-N	5.65	131.88	121.70
1	A	753	GLN	C-N-CA	5.65	131.88	121.70
1	A	73	ASP	CA-CB-CG	5.63	118.23	112.60
1	A	216	SER	CA-C-N	5.63	126.88	119.84
1	A	216	SER	C-N-CA	5.63	126.88	119.84
1	A	364	GLU	CA-CB-CG	-5.63	102.85	114.10
1	A	666	ARG	CG-CD-NE	-5.58	99.72	112.00
1	A	358	CYS	N-CA-C	5.57	122.67	110.80
1	A	115	ARG	NE-CZ-NH2	5.56	124.20	119.20
1	A	60	THR	CB-CA-C	5.55	118.88	109.50
1	A	440	THR	CA-CB-CG2	5.55	119.93	110.50
1	A	717	HIS	N-CA-C	5.54	116.87	109.83
1	A	258	ASN	OD1-CG-ND2	-5.52	117.08	122.60
1	A	505	LEU	O-C-N	-5.52	117.25	121.55
1	A	319	LYS	CA-C-N	5.50	125.43	119.76
1	A	319	LYS	C-N-CA	5.50	125.43	119.76
1	A	728	ASN	CA-CB-CG	5.50	118.10	112.60
1	A	519	HIS	CB-CG-CD2	-5.49	124.07	131.20
1	A	747	ARG	NE-CZ-NH2	5.47	124.12	119.20
1	A	120	ASN	CA-CB-CG	5.46	118.06	112.60
1	A	441	ILE	CA-C-O	-5.46	114.48	120.43
1	A	327	THR	CA-C-N	5.45	125.16	119.82
1	A	327	THR	C-N-CA	5.45	125.16	119.82
1	A	481	ASN	CA-C-N	5.44	125.78	119.47
1	A	481	ASN	C-N-CA	5.44	125.78	119.47
1	A	195	TRP	CD1-CG-CD2	5.43	114.99	106.30
1	A	123	VAL	N-CA-CB	-5.43	103.62	110.57
1	A	376	ALA	CA-C-N	5.39	127.51	120.28
1	A	376	ALA	C-N-CA	5.39	127.51	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	346	TRP	N-CA-C	-5.39	102.18	110.32
1	A	362	SER	CA-C-O	-5.38	116.36	122.01
1	A	147	HIS	CB-CG-CD2	-5.36	124.23	131.20
1	A	699	ILE	N-CA-C	-5.36	100.17	107.99
1	A	494	LYS	O-C-N	5.35	129.70	122.59
1	A	694	VAL	CB-CA-C	-5.35	103.45	112.16
1	A	274	HIS	CB-CG-CD2	-5.33	124.28	131.20
1	A	214	TRP	CG-CD2-CE3	5.30	139.20	133.90
1	A	738	TRP	N-CA-C	-5.30	105.42	111.14
1	A	717	HIS	CB-CG-ND1	5.27	130.61	122.70
1	A	306	HIS	CA-CB-CG	5.26	119.06	113.80
1	A	88	LEU	CA-C-N	5.25	124.94	119.64
1	A	88	LEU	C-N-CA	5.25	124.94	119.64
1	A	568	ASP	OD1-CG-OD2	-5.25	110.31	122.90
1	A	92	ALA	N-CA-C	5.23	118.82	112.23
1	A	310	VAL	O-C-N	-5.22	117.62	123.26
1	A	513	GLY	CA-C-N	5.22	131.51	121.54
1	A	513	GLY	C-N-CA	5.22	131.51	121.54
1	A	214	TRP	CE2-CD2-CG	-5.22	100.94	107.20
1	A	554	ASP	N-CA-C	5.22	118.64	111.54
1	A	654	LEU	N-CA-C	5.21	118.77	112.93
1	A	165	ASP	CA-C-N	5.21	127.25	120.28
1	A	165	ASP	C-N-CA	5.21	127.25	120.28
1	A	57	ARG	CA-C-O	5.20	126.79	120.81
1	A	604	SER	CA-CB-OG	5.20	121.50	111.10
1	A	319	LYS	CB-CA-C	5.19	117.39	109.56
1	A	10	PHE	CA-CB-CG	-5.17	108.63	113.80
1	A	34	ARG	NE-CZ-NH1	-5.17	116.33	121.50
1	A	553	GLU	CB-CG-CD	5.17	121.39	112.60
1	A	136	VAL	CA-C-N	5.17	125.25	120.34
1	A	136	VAL	C-N-CA	5.17	125.25	120.34
1	A	531	VAL	CA-C-N	5.16	127.67	120.65
1	A	531	VAL	C-N-CA	5.16	127.67	120.65
1	A	293	ASP	CA-CB-CG	5.15	117.75	112.60
1	A	717	HIS	CA-C-N	5.14	125.18	119.32
1	A	717	HIS	C-N-CA	5.14	125.18	119.32
1	A	167	HIS	CA-CB-CG	-5.14	108.66	113.80
1	A	167	HIS	CB-CG-ND1	5.13	130.40	122.70
1	A	488	THR	CB-CA-C	5.13	120.62	110.42
1	A	734	THR	CA-CB-OG1	-5.12	101.92	109.60
1	A	84	ILE	CA-C-N	5.12	127.85	120.38
1	A	84	ILE	C-N-CA	5.12	127.85	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	325	PRO	CA-C-O	-5.09	107.98	120.20
1	A	672	LEU	N-CA-C	-5.09	105.81	111.36
1	A	431	LYS	N-CA-C	5.09	121.64	110.80
1	A	692	HIS	ND1-CG-CD2	5.09	111.19	106.10
1	A	46	HIS	CB-CG-ND1	5.08	130.32	122.70
1	A	90	LYS	CB-CG-CD	-5.08	99.62	111.30
1	A	753	GLN	O-C-N	5.08	129.35	122.59
1	A	168	THR	CA-C-N	5.07	126.18	119.84
1	A	168	THR	C-N-CA	5.07	126.18	119.84
1	A	57	ARG	NE-CZ-NH2	5.06	123.75	119.20
1	A	28	VAL	CA-C-O	-5.06	115.30	120.71
1	A	351	ARG	N-CA-C	5.06	116.48	111.07
1	A	589	ASN	CA-CB-CG	5.05	117.65	112.60
1	A	740	ARG	NE-CZ-NH2	5.03	123.72	119.20
1	A	49	ASP	CA-C-N	5.02	124.80	119.28
1	A	49	ASP	C-N-CA	5.02	124.80	119.28
1	A	241	HIS	CB-CG-CD2	-5.01	124.69	131.20
1	A	484	THR	CA-C-N	5.01	131.11	121.54
1	A	484	THR	C-N-CA	5.01	131.11	121.54

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	324	GLY	Peptide
1	A	580	ARG	Sidechain
1	A	622	TYR	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	5811	0	5805	100	0
2	A	13	0	5	3	0
3	A	8	0	0	3	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	677	0	0	8	0
All	All	6510	0	5810	100	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 9.

All (100) 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:632:VAL:HB	1:A:659:ILE:HG23	1.70	0.72
1:A:145:ILE:HG21	1:A:358:CYS:HB2	1.74	0.69
1:A:737:GLU:HG2	1:A:740:ARG:HH11	1.61	0.65
1:A:358:CYS:HB3	3:A:755:SF4:S4	2.37	0.64
1:A:430:ARG:HH22	1:A:439:ASN:HD21	1.46	0.64
1:A:560:LYS:HD3	1:A:597:ILE:HG21	1.86	0.58
1:A:334:VAL:O	1:A:337:VAL:HG12	2.05	0.56
1:A:425:ILE:HG13	3:A:755:SF4:S1	2.45	0.55
1:A:339:SER:O	1:A:343:LYS:HG3	2.07	0.55
1:A:505:LEU:H	1:A:507:ARG:NH2	2.05	0.54
1:A:406:ALA:O	1:A:410:ARG:HB2	2.08	0.54
1:A:376:ALA:HB2	1:A:474:ILE:HD13	1.90	0.54
1:A:354:LEU:HD13	1:A:443:THR:HG22	1.89	0.54
1:A:352:VAL:O	1:A:441:ILE:HG22	2.08	0.54
1:A:487:LEU:HD22	1:A:494:LYS:O	2.08	0.54
1:A:327:THR:HG23	1:A:564:LYS:NZ	2.24	0.53
1:A:221:ILE:HG12	1:A:259:MET:HB3	1.92	0.52
1:A:487:LEU:HB3	1:A:495:PHE:O	2.09	0.52
1:A:377:LEU:HD13	1:A:412:VAL:HG13	1.92	0.51
1:A:449:PHE:O	1:A:452:ARG:HB3	2.10	0.51
1:A:13:HIS:CD2	1:A:13:HIS:H	2.28	0.51
1:A:577:LEU:HA	1:A:580:ARG:HG2	1.91	0.51
1:A:477:THR:OG1	1:A:479:LYS:HG2	2.10	0.51
1:A:505:LEU:H	1:A:507:ARG:HH22	1.59	0.51
1:A:425:ILE:HG21	2:A:756:FLC:HG1	1.93	0.50
1:A:327:THR:HG23	1:A:564:LYS:HZ3	1.77	0.50
1:A:201:LYS:HG3	5:A:1308:HOH:O	2.12	0.49
1:A:22:GLU:HG3	1:A:298:HIS:CE1	2.48	0.48
1:A:438:LYS:HA	1:A:458:GLU:HB3	1.94	0.48
1:A:486:PHE:HA	1:A:495:PHE:HB2	1.94	0.48
1:A:719:ASN:ND2	1:A:719:ASN:H	2.11	0.48
1:A:357:SER:HB2	1:A:445:TYR:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:ASP:HB3	5:A:1042:HOH:O	2.15	0.47
1:A:44:TYR:HA	1:A:47:LEU:HG	1.96	0.47
1:A:189:VAL:CG2	1:A:195:TRP:HB2	2.44	0.47
1:A:426:GLY:HA2	1:A:453:ASN:O	2.14	0.47
1:A:206:LYS:HB3	1:A:312:GLU:HG2	1.97	0.47
1:A:55:ILE:HA	1:A:60:THR:HG21	1.97	0.47
1:A:174:LEU:HD13	1:A:250:CYS:SG	2.55	0.47
1:A:515:ASP:N	5:A:881:HOH:O	2.47	0.47
1:A:488:THR:HG23	1:A:489:GLY:H	1.80	0.46
1:A:144:GLY:HA3	1:A:393:SER:HA	1.96	0.46
1:A:544:PHE:HE2	1:A:675:GLN:HE21	1.63	0.46
1:A:62:LEU:O	1:A:196:GLU:HA	2.16	0.46
1:A:532:SER:HB3	1:A:535:SER:HB2	1.97	0.46
1:A:706:ALA:H	1:A:709:LYS:HZ2	1.63	0.46
1:A:442:VAL:HG23	1:A:469:VAL:HG13	1.98	0.46
1:A:589:ASN:C	1:A:589:ASN:HD22	2.24	0.45
1:A:143:SER:HB3	1:A:516:THR:HB	1.97	0.45
1:A:604:SER:HA	1:A:614:GLY:O	2.16	0.45
1:A:666:ARG:HD3	5:A:793:HOH:O	2.15	0.45
1:A:277:LYS:HG3	1:A:289:ALA:HB1	1.97	0.45
1:A:514:GLN:HA	5:A:1263:HOH:O	2.17	0.45
1:A:381:LEU:C	1:A:382:LYS:HD2	2.42	0.45
1:A:425:ILE:CG1	3:A:755:SF4:S1	3.05	0.45
1:A:348:LEU:HD23	1:A:478:LEU:HB2	1.99	0.45
1:A:531:VAL:HG13	1:A:538:LEU:HB3	1.99	0.45
1:A:131:GLY:HA2	1:A:136:VAL:HB	1.99	0.44
1:A:245:VAL:HG13	1:A:270:PHE:HD1	1.81	0.44
1:A:337:VAL:HA	1:A:340:VAL:HG22	1.98	0.44
1:A:117:LYS:HZ3	1:A:141:PRO:HB2	1.82	0.44
1:A:449:PHE:HB3	5:A:1367:HOH:O	2.16	0.44
1:A:17:ARG:HA	1:A:17:ARG:HD2	1.86	0.44
1:A:253:MET:SD	1:A:270:PHE:CD1	3.10	0.44
1:A:383:CYS:HA	1:A:474:ILE:HA	2.00	0.44
1:A:133:LYS:HB2	1:A:527:GLN:HB3	1.99	0.44
1:A:208:THR:HG22	1:A:243:PRO:HG2	2.00	0.44
1:A:580:ARG:HH12	2:A:756:FLC:CGC	2.30	0.44
1:A:70:ALA:O	1:A:163:GLY:HA2	2.18	0.44
1:A:666:ARG:HD2	5:A:828:HOH:O	2.18	0.43
1:A:359:THR:OG1	1:A:446:ASN:ND2	2.52	0.43
1:A:272:TYR:HD2	1:A:296:LYS:HG3	1.83	0.43
1:A:621:ARG:HG2	1:A:654:LEU:HD22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:LEU:HB3	1:A:495:PHE:C	2.43	0.43
1:A:647:SER:HB3	1:A:668:HIS:CE1	2.52	0.43
1:A:325:PRO:HB3	1:A:462:PHE:CZ	2.54	0.43
1:A:603:ASN:HA	1:A:616:VAL:HG23	2.01	0.43
1:A:54:GLU:O	1:A:60:THR:HG21	2.19	0.43
1:A:673:LYS:HG2	1:A:731:PHE:CZ	2.54	0.43
1:A:311:ILE:HG21	1:A:311:ILE:HD13	1.82	0.42
1:A:750:GLU:HA	1:A:754:LYS:HG2	2.01	0.42
1:A:371:ALA:O	1:A:375:GLN:HG3	2.19	0.42
1:A:376:ALA:O	1:A:381:LEU:HB2	2.19	0.42
1:A:56:GLU:HB3	1:A:59:LYS:HG2	2.02	0.42
1:A:325:PRO:HG2	1:A:326:PHE:CD2	2.55	0.42
1:A:140:ARG:HD3	5:A:1056:HOH:O	2.19	0.41
1:A:596:ASN:O	1:A:600:ARG:HA	2.19	0.41
1:A:383:CYS:HB3	1:A:385:SER:O	2.20	0.41
1:A:352:VAL:HB	1:A:441:ILE:HG22	2.01	0.41
1:A:17:ARG:NH2	1:A:19:ASP:OD2	2.53	0.41
1:A:754:LYS:HD2	1:A:754:LYS:HA	1.86	0.41
1:A:117:LYS:NZ	1:A:141:PRO:HB2	2.36	0.41
1:A:394:GLU:HG2	1:A:514:GLN:HG2	2.03	0.41
1:A:421:CYS:HB2	1:A:425:ILE:HD11	2.02	0.41
1:A:493:LYS:HB3	1:A:494:LYS:H	1.63	0.41
1:A:377:LEU:HD13	1:A:412:VAL:CG1	2.51	0.41
1:A:69:VAL:O	1:A:95:SER:HA	2.21	0.40
1:A:101:HIS:CD2	2:A:756:FLC:HG2	2.56	0.40
1:A:520:PRO:HA	1:A:521:PRO:HD2	1.99	0.40
1:A:164:THR:HA	1:A:181:VAL:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	751/753 (100%)	706 (94%)	35 (5%)	10 (1%)	9 2

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	357	SER
1	A	495	PHE
1	A	485	ASP
1	A	109	GLY
1	A	494	LYS
1	A	358	CYS
1	A	753	GLN
1	A	493	LYS
1	A	719	ASN
1	A	325	PRO

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	620/620 (100%)	570 (92%)	50 (8%)	11 1

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	20	LEU
1	A	23	LYS
1	A	30	LYS
1	A	54	GLU
1	A	56	GLU
1	A	60	THR
1	A	72	GLN
1	A	88	LEU
1	A	107	LEU
1	A	121	GLN

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Mol	Chain	Res	Type
1	A	125	ASN
1	A	174	LEU
1	A	217	PRO
1	A	228	LEU
1	A	247	SER
1	A	325	PRO
1	A	327	THR
1	A	339	SER
1	A	358	CYS
1	A	377	LEU
1	A	384	LYS
1	A	423	PRO
1	A	425	ILE
1	A	441	ILE
1	A	447	ARG
1	A	452	ARG
1	A	487	LEU
1	A	490	LYS
1	A	496	LYS
1	A	501	ASP
1	A	507	ARG
1	A	509	GLU
1	A	516	THR
1	A	527	GLN
1	A	538	LEU
1	A	542	GLU
1	A	550	LYS
1	A	553	GLU
1	A	567	THR
1	A	589	ASN
1	A	659	ILE
1	A	694	VAL
1	A	696	LYS
1	A	697	LEU
1	A	702	LEU
1	A	703	LYS
1	A	709	LYS
1	A	747	ARG
1	A	753	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	HIS
1	A	52	ASN
1	A	77	GLN
1	A	121	GLN
1	A	274	HIS
1	A	298	HIS
1	A	386	GLN
1	A	419	ASN
1	A	439	ASN
1	A	456	ASN
1	A	518	GLN
1	A	527	GLN
1	A	536	GLN
1	A	585	ASN
1	A	589	ASN
1	A	626	HIS
1	A	671	ASN
1	A	675	GLN
1	A	689	ASN
1	A	719	ASN
1	A	746	ASN
1	A	753	GLN

5.3.3 RNA [i](#)

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](#)

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	4.11	5 (41%)	17,17,17	1.94	5 (29%)
3	SF4	A	755	1,2,4	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	-	3/16/16/16	-
3	SF4	A	755	1,2,4	-	-	0/6/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	756	FLC	CB-CBC	11.04	1.64	1.53
2	A	756	FLC	CA-CB	5.51	1.60	1.54
2	A	756	FLC	CG-CB	4.88	1.60	1.54
2	A	756	FLC	OA1-CAC	3.09	1.32	1.22
2	A	756	FLC	OG2-CGC	-2.41	1.22	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	756	FLC	CB-CA-CAC	4.05	125.00	113.92
2	A	756	FLC	OB2-CBC-CB	3.42	119.70	113.14
2	A	756	FLC	OHB-CB-CBC	3.20	113.50	108.96
2	A	756	FLC	CG-CB-CA	-2.38	103.21	109.31
2	A	756	FLC	OG1-CGC-CG	-2.14	116.88	122.95

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	756	FLC	CA-CB-CG-CGC

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

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	756	FLC	3	0
3	A	755	SF4	3	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.