



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 07:42 PM EDT

PDB ID : 1C97 / pdb_00001c97
Title : S642A:ISOCITRATE COMPLEX OF ACONITASE
Authors : Lloyd, S.J.; Lauble, H.; Prasad, G.S.; Stout, C.D.
Deposited on : 1999-07-31
Resolution : 1.98 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

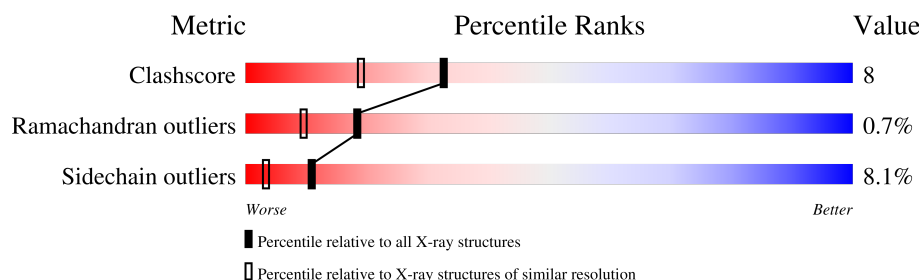
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)

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	SF4	A	755	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6429 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.

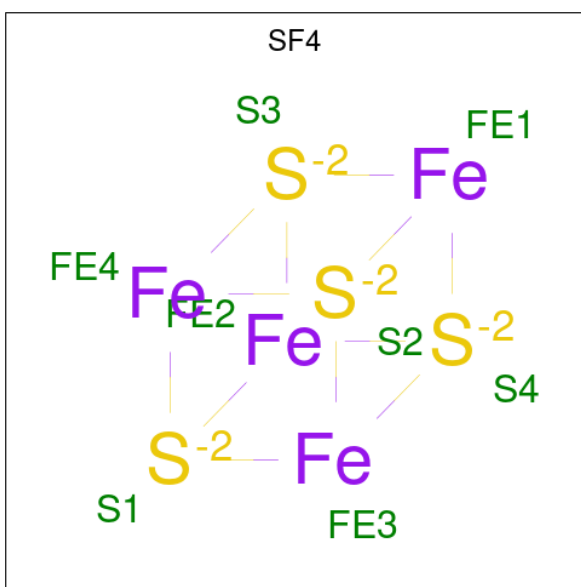
- Molecule 1 is a protein called MITOCHONDRIAL ACONITASE.

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

There are 16 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	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 IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).

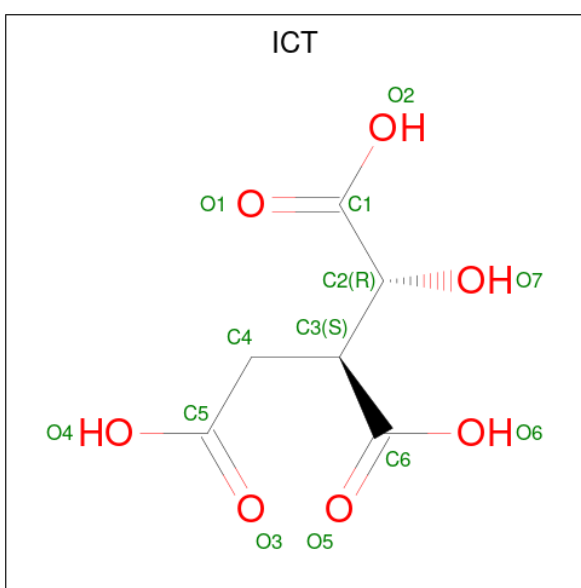


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 3 is OXYGEN ATOM (CCD ID: O) (formula: O).

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

- Molecule 4 is ISOCITRIC ACID (CCD ID: ICT) (formula: C₆H₈O₇).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	593	Total	O	0	0
			593	593		

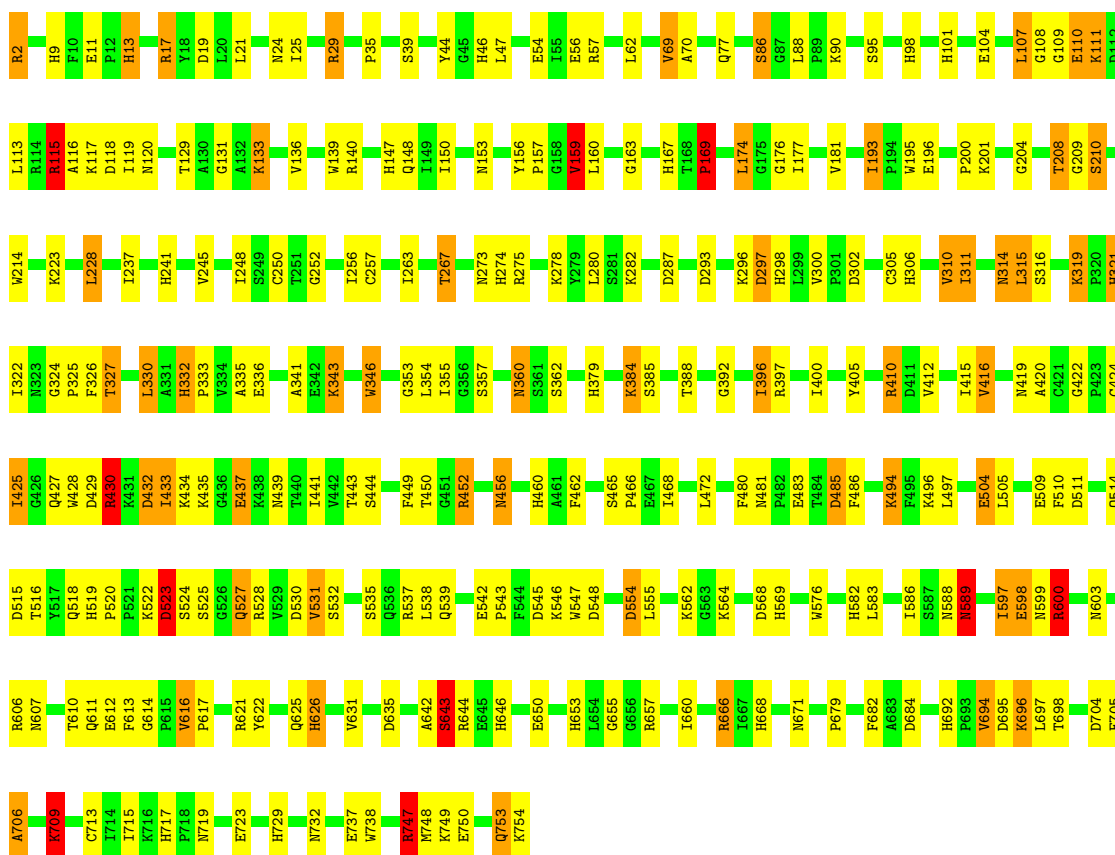
3 Residue-property plots

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: MITOCHONDRIAL ACONITASE

Chain A: 



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	176.40Å 71.40Å 71.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.98	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-1.98)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.218 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6429	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: O, 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	1.32	43/5941 (0.7%)	2.02	200/8049 (2.5%)

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	531	VAL	CA-CB	9.99	1.66	1.54
1	A	310	VAL	CA-CB	9.13	1.66	1.54
1	A	321	HIS	CD2-NE2	-7.92	1.29	1.37
1	A	692	HIS	CD2-NE2	-7.84	1.29	1.37
1	A	379	HIS	CD2-NE2	-7.23	1.29	1.37
1	A	147	HIS	CD2-NE2	-7.15	1.29	1.37
1	A	582	HIS	CD2-NE2	-7.10	1.30	1.37
1	A	9	HIS	CG-ND1	-7.02	1.30	1.38
1	A	668	HIS	CD2-NE2	-7.02	1.30	1.37
1	A	416	VAL	CA-CB	6.77	1.62	1.54
1	A	193	ILE	CA-CB	6.70	1.62	1.54
1	A	519	HIS	CD2-NE2	-6.68	1.30	1.37
1	A	13	HIS	CD2-NE2	-6.58	1.30	1.37
1	A	626	HIS	CD2-NE2	-6.55	1.30	1.37
1	A	460	HIS	CD2-NE2	-6.54	1.30	1.37
1	A	306	HIS	CD2-NE2	-6.53	1.30	1.37
1	A	616	VAL	CA-CB	6.45	1.58	1.53
1	A	717	HIS	CD2-NE2	-6.43	1.30	1.37
1	A	569	HIS	CD2-NE2	-6.40	1.30	1.37
1	A	569	HIS	CG-ND1	-6.38	1.31	1.38
1	A	210	SER	N-CA	-6.30	1.38	1.46
1	A	653	HIS	CD2-NE2	-6.29	1.30	1.37
1	A	9	HIS	CD2-NE2	-6.24	1.30	1.37
1	A	646	HIS	CD2-NE2	-6.23	1.30	1.37
1	A	46	HIS	CG-ND1	-6.23	1.31	1.38
1	A	167	HIS	CG-ND1	-6.12	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	98	HIS	CD2-NE2	-6.12	1.31	1.37
1	A	717	HIS	CG-ND1	-6.01	1.31	1.38
1	A	302	ASP	CA-C	-6.01	1.46	1.53
1	A	167	HIS	CD2-NE2	-5.96	1.31	1.37
1	A	46	HIS	CD2-NE2	-5.95	1.31	1.37
1	A	332	HIS	CD2-NE2	-5.88	1.31	1.37
1	A	159	VAL	CA-CB	5.74	1.60	1.54
1	A	692	HIS	CG-ND1	-5.66	1.32	1.38
1	A	321	HIS	CG-ND1	-5.65	1.32	1.38
1	A	729	HIS	CD2-NE2	-5.61	1.31	1.37
1	A	274	HIS	CD2-NE2	-5.60	1.31	1.37
1	A	668	HIS	CG-ND1	-5.47	1.32	1.38
1	A	298	HIS	CD2-NE2	-5.44	1.31	1.37
1	A	379	HIS	CG-ND1	-5.43	1.32	1.38
1	A	101	HIS	CD2-NE2	-5.27	1.32	1.37
1	A	200	PRO	CA-CB	-5.18	1.46	1.53
1	A	433	ILE	CA-CB	5.05	1.62	1.54

All (200) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	666	ARG	NE-CZ-NH2	15.48	133.13	119.20
1	A	666	ARG	NE-CZ-NH1	-15.00	106.50	121.50
1	A	209	GLY	CA-C-N	11.02	140.85	122.33
1	A	209	GLY	C-N-CA	11.02	140.85	122.33
1	A	545	ASP	CA-CB-CG	11.00	123.60	112.60
1	A	523	ASP	CA-CB-CG	10.49	123.09	112.60
1	A	518	GLN	OE1-CD-NE2	-9.94	112.66	122.60
1	A	209	GLY	O-C-N	-9.88	113.51	122.90
1	A	607	ASN	CA-CB-CG	9.72	122.32	112.60
1	A	465	SER	CA-C-O	-9.23	112.29	120.60
1	A	548	ASP	CA-CB-CG	8.86	121.46	112.60
1	A	147	HIS	CA-CB-CG	-8.45	105.35	113.80
1	A	539	GLN	CA-CB-CG	8.31	130.72	114.10
1	A	523	ASP	N-CA-C	-8.30	93.13	110.80
1	A	732	ASN	CA-CB-CG	8.24	120.84	112.60
1	A	599	ASN	OD1-CG-ND2	-8.19	114.41	122.60
1	A	115	ARG	CA-CB-CG	8.04	130.17	114.10
1	A	57	ARG	NE-CZ-NH2	7.98	126.39	119.20
1	A	626	HIS	CA-CB-CG	-7.90	105.90	113.80
1	A	77	GLN	OE1-CD-NE2	-7.88	114.72	122.60
1	A	589	ASN	OD1-CG-ND2	-7.78	114.82	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	643	SER	CA-CB-OG	-7.71	95.69	111.10
1	A	530	ASP	CA-CB-CG	7.69	120.29	112.60
1	A	569	HIS	CB-CG-ND1	7.61	134.12	122.70
1	A	297	ASP	CA-CB-CG	7.42	120.02	112.60
1	A	518	GLN	CA-CB-CG	7.30	128.71	114.10
1	A	603	ASN	OD1-CG-ND2	-7.29	115.31	122.60
1	A	24	ASN	CA-C-O	-7.25	112.73	120.42
1	A	582	HIS	CB-CG-CD2	-7.23	121.80	131.20
1	A	481	ASN	CA-C-O	-7.15	113.01	119.59
1	A	671	ASN	OD1-CG-ND2	-7.13	115.47	122.60
1	A	753	GLN	CA-CB-CG	6.95	128.00	114.10
1	A	589	ASN	CA-CB-CG	6.93	119.53	112.60
1	A	430	ARG	CA-CB-CG	-6.91	100.29	114.10
1	A	263	ILE	O-C-N	-6.85	115.92	122.09
1	A	156	TYR	O-C-N	-6.83	116.67	121.65
1	A	101	HIS	N-CA-C	6.82	121.59	113.28
1	A	278	LYS	CA-CB-CG	6.81	127.71	114.10
1	A	481	ASN	OD1-CG-ND2	-6.68	115.92	122.60
1	A	419	ASN	CA-CB-CG	6.67	119.27	112.60
1	A	293	ASP	CA-CB-CG	6.66	119.26	112.60
1	A	110	GLU	O-C-N	6.64	129.16	122.12
1	A	69	VAL	CA-C-O	-6.63	113.50	120.39
1	A	278	LYS	CG-CD-CE	6.62	126.53	111.30
1	A	280	LEU	O-C-N	6.56	128.83	122.07
1	A	460	HIS	CB-CG-CD2	-6.55	122.69	131.20
1	A	625	GLN	CB-CG-CD	6.52	123.69	112.60
1	A	410	ARG	NE-CZ-NH1	-6.51	114.98	121.50
1	A	631	VAL	CG1-CB-CG2	-6.51	96.49	110.80
1	A	598	GLU	CA-CB-CG	6.50	127.09	114.10
1	A	118	ASP	CA-CB-CG	-6.46	106.14	112.60
1	A	644	ARG	N-CA-C	6.45	120.19	110.64
1	A	296	LYS	CA-C-N	6.42	129.18	120.38
1	A	296	LYS	C-N-CA	6.42	129.18	120.38
1	A	694	VAL	CB-CA-C	-6.42	101.70	112.16
1	A	101	HIS	CB-CG-CD2	-6.39	122.89	131.20
1	A	120	ASN	CA-CB-CG	6.37	118.97	112.60
1	A	614	GLY	CA-C-N	6.36	126.74	119.93
1	A	614	GLY	C-N-CA	6.36	126.74	119.93
1	A	116	ALA	O-C-N	-6.36	115.38	122.12
1	A	706	ALA	CA-C-N	6.32	126.69	119.93
1	A	706	ALA	C-N-CA	6.32	126.69	119.93
1	A	635	ASP	N-CA-CB	-6.30	99.84	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	ASP	CA-CB-CG	6.28	118.88	112.60
1	A	430	ARG	NE-CZ-NH2	6.24	124.82	119.20
1	A	657	ARG	NE-CZ-NH2	6.24	124.81	119.20
1	A	616	VAL	CA-C-N	6.23	125.72	119.24
1	A	616	VAL	C-N-CA	6.23	125.72	119.24
1	A	422	GLY	CA-C-N	6.21	127.60	119.84
1	A	422	GLY	C-N-CA	6.21	127.60	119.84
1	A	181	VAL	CA-C-O	-6.20	115.56	121.64
1	A	569	HIS	CB-CG-CD2	-6.16	123.19	131.20
1	A	603	ASN	CB-CG-ND2	6.16	125.64	116.40
1	A	195	TRP	CE2-CD2-CG	-6.16	99.81	107.20
1	A	2	ARG	CA-CB-CG	6.16	126.41	114.10
1	A	56	GLU	CA-CB-CG	-6.13	101.83	114.10
1	A	267	THR	CA-CB-OG1	-6.10	100.45	109.60
1	A	510	PHE	CA-CB-CG	6.08	119.88	113.80
1	A	310	VAL	CA-C-O	6.08	126.81	120.36
1	A	481	ASN	CA-C-N	6.08	125.70	119.56
1	A	481	ASN	C-N-CA	6.08	125.70	119.56
1	A	273	ASN	CA-CB-CG	6.04	118.64	112.60
1	A	282	LYS	CB-CG-CD	5.98	125.05	111.30
1	A	287	ASP	CA-CB-CG	5.97	118.57	112.60
1	A	705	PHE	CA-CB-CG	5.96	119.76	113.80
1	A	245	VAL	N-CA-C	5.96	117.41	110.62
1	A	568	ASP	CA-CB-CG	5.95	118.55	112.60
1	A	519	HIS	CB-CG-ND1	5.92	131.59	122.70
1	A	612	GLU	CB-CG-CD	5.91	122.65	112.60
1	A	646	HIS	CB-CG-CD2	-5.90	123.53	131.20
1	A	588	ASN	OD1-CG-ND2	-5.88	116.72	122.60
1	A	644	ARG	NE-CZ-NH2	5.87	124.48	119.20
1	A	167	HIS	CB-CG-ND1	5.86	131.50	122.70
1	A	397	ARG	CA-C-O	-5.84	114.69	120.82
1	A	748	MET	CA-C-O	-5.83	114.87	121.00
1	A	452	ARG	CA-C-N	5.79	130.52	120.68
1	A	452	ARG	C-N-CA	5.79	130.52	120.68
1	A	278	LYS	CB-CG-CD	-5.78	98.01	111.30
1	A	537	ARG	NE-CZ-NH2	5.78	124.40	119.20
1	A	241	HIS	CA-CB-CG	5.76	119.56	113.80
1	A	153	ASN	OD1-CG-ND2	-5.74	116.86	122.60
1	A	343	LYS	CA-CB-CG	5.74	125.58	114.10
1	A	750	GLU	CA-CB-CG	5.74	125.58	114.10
1	A	719	ASN	OD1-CG-ND2	-5.72	116.88	122.60
1	A	167	HIS	CB-CG-CD2	-5.72	123.77	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	682	PHE	CA-CB-CG	5.71	119.52	113.80
1	A	717	HIS	CB-CG-CD2	-5.71	123.77	131.20
1	A	274	HIS	CB-CG-CD2	-5.71	123.78	131.20
1	A	660	ILE	N-CA-C	-5.70	100.18	108.17
1	A	111	LYS	O-C-N	5.70	127.94	122.07
1	A	468	ILE	N-CA-C	-5.69	104.80	111.00
1	A	539	GLN	OE1-CD-NE2	-5.68	116.92	122.60
1	A	554	ASP	N-CA-C	5.67	119.47	111.52
1	A	668	HIS	CA-CB-CG	-5.66	108.14	113.80
1	A	511	ASP	CA-CB-CG	5.66	118.26	112.60
1	A	717	HIS	CA-C-N	5.64	125.49	119.28
1	A	717	HIS	C-N-CA	5.64	125.49	119.28
1	A	160	LEU	CA-C-O	5.63	126.31	120.40
1	A	729	HIS	CB-CG-CD2	-5.60	123.92	131.20
1	A	332	HIS	CB-CG-CD2	-5.60	123.92	131.20
1	A	611	GLN	OE1-CD-NE2	-5.59	117.01	122.60
1	A	542	GLU	CA-C-N	5.58	125.91	119.93
1	A	542	GLU	C-N-CA	5.58	125.91	119.93
1	A	420	ALA	O-C-N	-5.58	117.45	123.42
1	A	600	ARG	NE-CZ-NH2	5.58	124.22	119.20
1	A	360	ASN	N-CA-CB	-5.58	105.09	111.79
1	A	204	GLY	O-C-N	-5.57	119.32	123.61
1	A	696	LYS	O-C-N	-5.57	116.69	123.10
1	A	410	ARG	NE-CZ-NH2	5.57	124.21	119.20
1	A	200	PRO	N-CA-C	5.54	120.18	111.38
1	A	449	PHE	CA-CB-CG	5.53	119.33	113.80
1	A	314	ASN	OD1-CG-ND2	-5.52	117.08	122.60
1	A	311	ILE	CB-CG1-CD1	-5.51	102.22	113.80
1	A	133	LYS	CA-C-O	-5.50	115.03	120.70
1	A	666	ARG	CD-NE-CZ	5.50	132.10	124.40
1	A	709	LYS	CA-CB-CG	5.49	125.08	114.10
1	A	327	THR	CB-CA-C	-5.47	100.67	108.88
1	A	655	GLY	CA-C-N	5.47	125.54	120.34
1	A	655	GLY	C-N-CA	5.47	125.54	120.34
1	A	543	PRO	N-CA-CB	5.47	108.11	103.19
1	A	17	ARG	NE-CZ-NH1	-5.43	116.07	121.50
1	A	679	PRO	O-C-N	-5.43	117.28	123.03
1	A	195	TRP	CD1-CG-CD2	5.42	114.97	106.30
1	A	564	LYS	CA-CB-CG	5.41	124.93	114.10
1	A	300	VAL	O-C-N	-5.41	117.93	121.72
1	A	732	ASN	OD1-CG-ND2	-5.40	117.20	122.60
1	A	432	ASP	N-CA-C	5.37	119.53	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	509	GLU	CB-CG-CD	5.36	121.72	112.60
1	A	314	ASN	CB-CG-ND2	5.36	124.44	116.40
1	A	481	ASN	CB-CG-ND2	5.36	124.44	116.40
1	A	150	ILE	CA-C-O	-5.33	115.41	120.95
1	A	335	ALA	N-CA-C	5.33	117.50	111.11
1	A	576	TRP	CG-CD1-NE1	-5.31	103.30	110.20
1	A	427	GLN	OE1-CD-NE2	-5.30	117.30	122.60
1	A	444	SER	N-CA-C	-5.30	106.58	112.57
1	A	362	SER	CA-CB-OG	5.30	121.70	111.10
1	A	621	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	A	201	LYS	O-C-N	-5.28	116.16	122.65
1	A	437	GLU	CB-CG-CD	5.27	121.56	112.60
1	A	396	ILE	CA-C-O	-5.26	115.27	120.85
1	A	695	ASP	N-CA-C	5.26	117.50	110.35
1	A	504	GLU	CB-CG-CD	5.25	121.53	112.60
1	A	441	ILE	CA-C-O	-5.25	114.79	120.36
1	A	738	TRP	CE2-CD2-CG	-5.25	100.90	107.20
1	A	321	HIS	CB-CG-CD2	-5.24	124.39	131.20
1	A	603	ASN	CA-CB-CG	5.23	117.83	112.60
1	A	195	TRP	CG-CD2-CE3	5.22	139.12	133.90
1	A	527	GLN	N-CA-C	5.21	117.90	110.24
1	A	514	GLN	CA-C-O	5.20	127.45	121.47
1	A	657	ARG	CB-CG-CD	5.20	123.25	111.30
1	A	666	ARG	CG-CD-NE	-5.19	100.58	112.00
1	A	747	ARG	NE-CZ-NH1	-5.18	116.32	121.50
1	A	424	CYS	CA-C-O	-5.18	115.39	120.82
1	A	357	SER	O-C-N	-5.17	115.72	122.59
1	A	343	LYS	N-CA-CB	-5.17	102.31	110.06
1	A	456	ASN	CA-C-N	5.16	124.82	119.56
1	A	456	ASN	C-N-CA	5.16	124.82	119.56
1	A	684	ASP	CA-C-N	5.16	124.82	119.56
1	A	684	ASP	C-N-CA	5.16	124.82	119.56
1	A	599	ASN	CB-CG-ND2	5.15	124.12	116.40
1	A	485	ASP	CA-CB-CG	5.11	117.71	112.60
1	A	518	GLN	CB-CA-C	5.11	118.49	111.23
1	A	704	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	29	ARG	CD-NE-CZ	-5.09	117.27	124.40
1	A	642	ALA	N-CA-C	5.09	116.86	110.24
1	A	692	HIS	CB-CG-CD2	-5.08	124.59	131.20
1	A	195	TRP	CG-CD1-NE1	-5.08	103.60	110.20
1	A	11	GLU	CA-C-N	5.07	124.85	119.28
1	A	11	GLU	C-N-CA	5.07	124.85	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	684	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	747	ARG	NE-CZ-NH2	5.06	123.75	119.20
1	A	518	GLN	N-CA-CB	-5.06	102.20	110.95
1	A	576	TRP	CE2-CD2-CG	-5.04	101.16	107.20
1	A	610	THR	N-CA-C	5.03	119.47	113.23
1	A	346	TRP	N-CA-C	-5.03	103.37	110.31
1	A	46	HIS	CB-CG-ND1	5.01	130.22	122.70
1	A	101	HIS	CB-CG-ND1	5.01	130.21	122.70
1	A	267	THR	CA-CB-CG2	5.01	119.01	110.50
1	A	353	GLY	O-C-N	-5.01	119.19	123.80
1	A	139	TRP	CG-CD2-CE3	5.01	138.91	133.90

There are no chirality outliers.

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	5814	0	5804	91	0
2	A	8	0	0	2	0
3	A	1	0	0	1	0
4	A	13	0	4	4	0
5	A	593	0	0	4	0
All	All	6429	0	5808	92	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 8.

All (92) 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:643:SER:HB2	4:A:756:ICT:O6	1.71	0.90
1:A:504:GLU:HG2	1:A:505:LEU:HG	1.58	0.85
3:A:1500:O:O	4:A:756:ICT:O1	1.97	0.83
1:A:433:ILE:HD12	1:A:456:ASN:HD22	1.47	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:PRO:HB2	1:A:522:LYS:HG2	1.68	0.74
1:A:113:LEU:HG	1:A:117:LYS:HE2	1.71	0.71
1:A:643:SER:H	4:A:756:ICT:C6	2.10	0.65
1:A:425:ILE:HG12	2:A:755:SF4:S1	2.40	0.62
1:A:86:SER:HB2	1:A:88:LEU:HD12	1.82	0.62
1:A:333:PRO:HD2	1:A:336:GLU:HG2	1.82	0.61
1:A:108:GLY:HA3	1:A:415:ILE:HD11	1.82	0.61
1:A:430:ARG:HH12	1:A:439:ASN:HD21	1.50	0.59
1:A:107:LEU:HD23	1:A:111:LYS:HB3	1.84	0.58
1:A:354:LEU:HD13	1:A:443:THR:HG22	1.87	0.56
1:A:104:GLU:OE2	1:A:429:ASP:HB2	2.05	0.56
1:A:325:PRO:HB3	1:A:462:PHE:CE2	2.42	0.55
1:A:643:SER:CB	4:A:756:ICT:O6	2.52	0.55
1:A:706:ALA:H	1:A:709:LYS:HZ2	1.56	0.54
1:A:35:PRO:HB2	1:A:305:CYS:HA	1.90	0.54
1:A:13:HIS:H	1:A:13:HIS:CD2	2.26	0.53
1:A:208:THR:O	1:A:315:LEU:HB2	2.09	0.53
1:A:13:HIS:HB3	5:A:1017:HOH:O	2.08	0.53
1:A:606:ARG:HB2	1:A:613:PHE:CZ	2.45	0.51
1:A:433:ILE:HB	1:A:437:GLU:HB3	1.94	0.50
1:A:2:ARG:NH1	1:A:17:ARG:HD2	2.26	0.50
1:A:177:ILE:HG23	1:A:267:THR:HG21	1.93	0.49
1:A:341:ALA:HA	1:A:346:TRP:CE3	2.47	0.49
1:A:480:PHE:CE2	1:A:485:ASP:HB2	2.47	0.49
1:A:115:ARG:O	1:A:119:ILE:HG12	2.14	0.48
1:A:535:SER:HB3	1:A:538:LEU:O	2.14	0.48
1:A:325:PRO:HG2	1:A:326:PHE:HD2	1.80	0.47
1:A:70:ALA:O	1:A:163:GLY:HA2	2.15	0.47
1:A:400:ILE:HB	1:A:405:TYR:HB2	1.97	0.47
1:A:589:ASN:C	1:A:589:ASN:HD22	2.23	0.46
1:A:148:GLN:HG3	1:A:392:GLY:HA3	1.97	0.46
1:A:622:TYR:O	1:A:626:HIS:HD2	1.98	0.46
1:A:69:VAL:O	1:A:95:SER:HA	2.14	0.46
1:A:140:ARG:HH21	1:A:516:THR:HA	1.80	0.46
1:A:737:GLU:HB3	1:A:747:ARG:HD2	1.98	0.46
1:A:430:ARG:HD3	1:A:432:ASP:OD1	2.16	0.46
1:A:90:LYS:HG2	1:A:522:LYS:NZ	2.30	0.46
1:A:44:TYR:HA	1:A:47:LEU:HG	1.98	0.46
1:A:214:TRP:CD1	1:A:483:GLU:HG2	2.51	0.45
1:A:428:TRP:CZ2	1:A:430:ARG:HG3	2.52	0.45
1:A:354:LEU:CD1	1:A:443:THR:HG22	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:ILE:O	1:A:275:ARG:HG3	2.17	0.45
1:A:562:LYS:HA	1:A:562:LYS:HD2	1.64	0.45
1:A:697:LEU:HD23	1:A:715:ILE:HA	1.97	0.45
1:A:360:ASN:HB3	1:A:466:PRO:HG3	1.99	0.45
1:A:425:ILE:CG1	2:A:755:SF4:S1	3.05	0.45
1:A:583:LEU:HA	1:A:586:ILE:HG22	1.98	0.45
1:A:110:GLU:HG2	5:A:965:HOH:O	2.18	0.44
1:A:228:LEU:HD13	1:A:311:ILE:HD11	1.99	0.44
1:A:494:LYS:HD3	5:A:980:HOH:O	2.18	0.44
1:A:237:ILE:HG12	1:A:267:THR:HG22	2.00	0.44
1:A:546:LYS:HG2	1:A:547:TRP:N	2.33	0.44
1:A:29:ARG:HG3	1:A:29:ARG:NH2	2.33	0.43
1:A:384:LYS:HE2	1:A:384:LYS:HB3	1.82	0.43
1:A:252:GLY:O	1:A:256:ILE:HG13	2.18	0.43
1:A:643:SER:HB3	5:A:790:HOH:O	2.17	0.43
1:A:698:THR:O	1:A:713:CYS:HA	2.19	0.43
1:A:388:THR:HG22	1:A:415:ILE:CG2	2.48	0.43
1:A:485:ASP:O	1:A:496:LYS:HG3	2.19	0.43
1:A:21:LEU:O	1:A:25:ILE:HG13	2.18	0.43
1:A:62:LEU:O	1:A:196:GLU:HA	2.19	0.43
1:A:129:THR:O	1:A:133:LYS:HB2	2.18	0.43
1:A:589:ASN:ND2	1:A:650:GLU:OE2	2.52	0.43
1:A:523:ASP:HB2	1:A:524:SER:H	1.68	0.42
1:A:324:GLY:O	1:A:330:LEU:HD13	2.20	0.42
1:A:330:LEU:HD22	1:A:332:HIS:CE1	2.55	0.42
1:A:749:LYS:O	1:A:754:LYS:HB2	2.17	0.42
1:A:113:LEU:O	1:A:117:LYS:HG3	2.18	0.42
1:A:228:LEU:CD1	1:A:311:ILE:HD11	2.49	0.42
1:A:131:GLY:HA2	1:A:136:VAL:HB	2.01	0.42
1:A:486:PHE:CE2	1:A:496:LYS:HD3	2.55	0.42
1:A:597:ILE:O	1:A:600:ARG:HD3	2.19	0.42
1:A:355:ILE:HG21	1:A:355:ILE:HD13	1.82	0.41
1:A:715:ILE:HD12	1:A:723:GLU:HG3	2.02	0.41
1:A:749:LYS:HD2	1:A:754:LYS:HE3	2.03	0.41
1:A:325:PRO:HG2	1:A:326:PHE:CD2	2.56	0.41
1:A:107:LEU:N	1:A:107:LEU:HD22	2.35	0.41
1:A:148:GLN:OE1	1:A:396:ILE:HD11	2.21	0.41
1:A:322:ILE:HD11	1:A:462:PHE:HB3	2.02	0.41
1:A:319:LYS:O	1:A:321:HIS:HD2	2.04	0.41
1:A:532:SER:HB3	1:A:535:SER:HB2	2.02	0.41
1:A:39:SER:HB3	1:A:237:ILE:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:LEU:O	1:A:696:LYS:HA	2.20	0.41
1:A:616:VAL:HB	1:A:617:PRO:HD3	2.01	0.41
1:A:174:LEU:HD13	1:A:250:CYS:SG	2.60	0.40
1:A:169:PRO:O	1:A:257:CYS:HB3	2.21	0.40
1:A:159:VAL:HG12	1:A:176:GLY:HA3	2.03	0.40
1:A:228:LEU:HD12	1:A:228:LEU:HA	1.96	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%)	712 (95%)	34 (4%)	5 (1%)	18 9

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	450	THR
1	A	452	ARG
1	A	169	PRO
1	A	525	SER
1	A	109	GLY

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%)	571 (92%)	50 (8%)	11 3

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

Mol	Chain	Res	Type
1	A	54	GLU
1	A	86	SER
1	A	107	LEU
1	A	115	ARG
1	A	157	PRO
1	A	159	VAL
1	A	169	PRO
1	A	174	LEU
1	A	193	ILE
1	A	208	THR
1	A	210	SER
1	A	223	LYS
1	A	228	LEU
1	A	297	ASP
1	A	310	VAL
1	A	314	ASN
1	A	315	LEU
1	A	316	SER
1	A	319	LYS
1	A	327	THR
1	A	330	LEU
1	A	343	LYS
1	A	384	LYS
1	A	385	SER
1	A	410	ARG
1	A	412	VAL
1	A	416	VAL
1	A	425	ILE
1	A	430	ARG
1	A	434	LYS
1	A	435	LYS
1	A	472	LEU
1	A	494	LYS
1	A	497	LEU
1	A	515	ASP
1	A	523	ASP
1	A	527	GLN
1	A	528	ARG

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Mol	Chain	Res	Type
1	A	531	VAL
1	A	554	ASP
1	A	589	ASN
1	A	597	ILE
1	A	598	GLU
1	A	600	ARG
1	A	643	SER
1	A	666	ARG
1	A	694	VAL
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 (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	HIS
1	A	77	GLN
1	A	82	GLN
1	A	106	GLN
1	A	121	GLN
1	A	314	ASN
1	A	321	HIS
1	A	332	HIS
1	A	439	ASN
1	A	481	ASN
1	A	518	GLN
1	A	519	HIS
1	A	536	GLN
1	A	556	GLN
1	A	589	ASN
1	A	626	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 [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	SF4	A	755	4,3,1	0,12,12	-	-	-		
4	ICT	A	756	2	12,12,12	1.98	5 (41%)	13,16,16	4.79	7 (53%)

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	755	4,3,1	-	-	0/6/5/5
4	ICT	A	756	2	-	5/16/16/16	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	756	ICT	O7-C2	3.42	1.48	1.42
4	A	756	ICT	C2-C1	-2.97	1.48	1.52
4	A	756	ICT	C3-C6	-2.85	1.46	1.51
4	A	756	ICT	O6-C6	-2.30	1.23	1.30
4	A	756	ICT	O1-C1	2.17	1.28	1.22

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	756	ICT	C4-C3-C6	-10.73	94.20	111.25
4	A	756	ICT	O6-C6-C3	7.27	132.81	113.93
4	A	756	ICT	O7-C2-C3	5.85	123.82	110.63
4	A	756	ICT	O7-C2-C1	-5.62	98.69	110.69
4	A	756	ICT	C3-C4-C5	-4.87	104.84	113.95
4	A	756	ICT	O5-C6-C3	-4.66	112.01	123.01
4	A	756	ICT	O6-C6-O5	-3.99	115.04	124.08

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	755	SF4	2	0
4	A	756	ICT	4	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.