



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 04:30 pm BST

PDB ID : 1C97  
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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

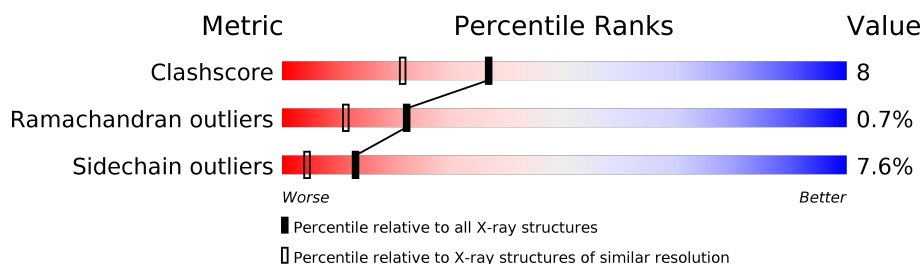
# 1 Overall quality at a glance

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	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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
1	A	753	Total	C	N	O	S	0	0	0
			5814	3666	1034	1092	22			

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 (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).

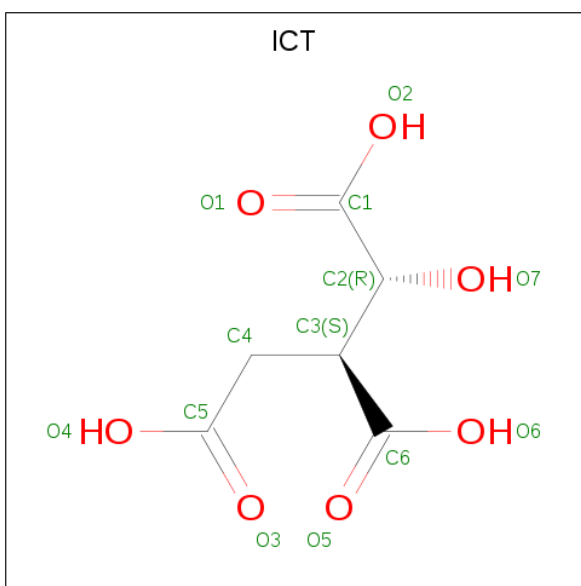


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 3 is OXYGEN ATOM (three-letter code: O) (formula: O).

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

- Molecule 4 is ISOCITRIC ACID (three-letter code: ICT) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).



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

- Molecule 5 is water.

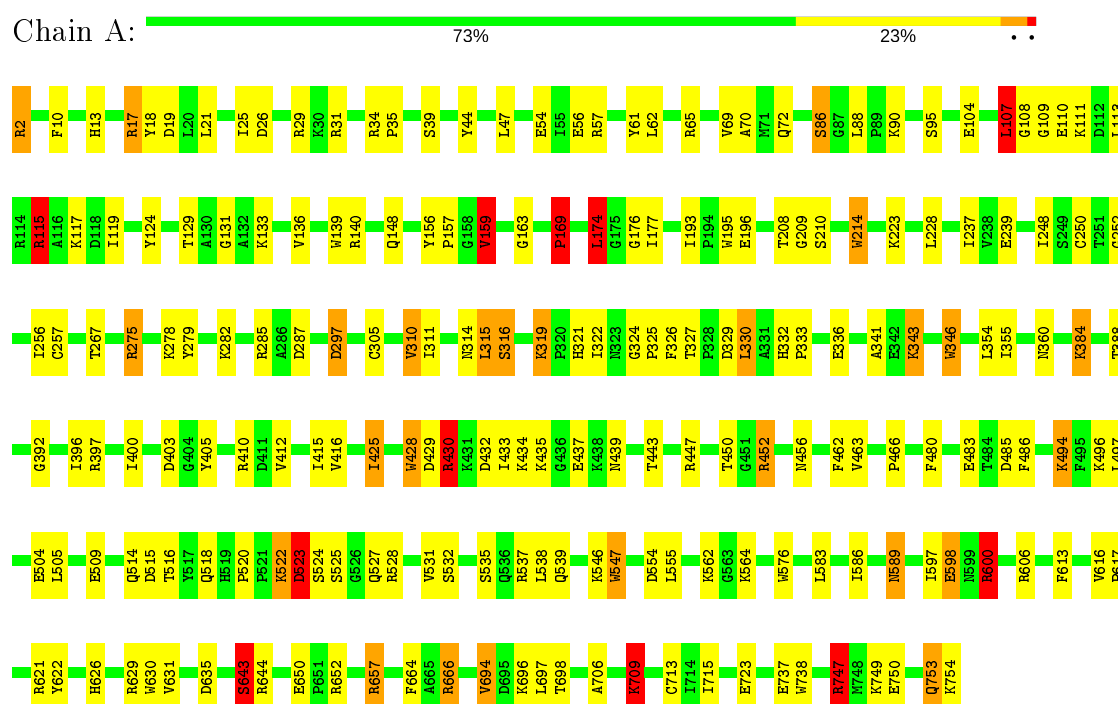
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	593	Total	O	0	0
			593	593		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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



## 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, $\alpha$ , $\beta$ , $\gamma$	176.40 Å   71.40 Å   71.90 Å 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 <sup>2</sup> )	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, O, 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	1.01	5/5941 (0.1%)	1.68	99/8049 (1.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	531	VAL	CA-CB	5.72	1.66	1.54
1	A	239	GLU	CB-CG	-5.63	1.41	1.52
1	A	310	VAL	CA-CB	5.49	1.66	1.54
1	A	316	SER	CB-OG	-5.40	1.35	1.42
1	A	195	TRP	CD1-NE1	-5.24	1.29	1.38

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	666	ARG	NE-CZ-NH1	-27.59	106.50	120.30
1	A	666	ARG	NE-CZ-NH2	25.67	133.13	120.30
1	A	57	ARG	NE-CZ-NH2	12.17	126.39	120.30
1	A	195	TRP	CD1-CG-CD2	10.84	114.97	106.30
1	A	410	ARG	NE-CZ-NH1	-10.63	114.98	120.30
1	A	195	TRP	CE2-CD2-CG	-9.36	99.81	107.30
1	A	430	ARG	NE-CZ-NH2	9.04	124.82	120.30
1	A	657	ARG	NE-CZ-NH2	9.03	124.81	120.30
1	A	631	VAL	CG1-CB-CG2	-9.01	96.49	110.90
1	A	576	TRP	CD1-CG-CD2	8.62	113.20	106.30
1	A	17	ARG	NE-CZ-NH1	-8.46	116.07	120.30
1	A	644	ARG	NE-CZ-NH2	8.36	124.48	120.30
1	A	124	TYR	CB-CG-CD2	-8.31	116.02	121.00
1	A	537	ARG	NE-CZ-NH2	8.20	124.40	120.30
1	A	738	TRP	CE2-CD2-CG	-8.00	100.90	107.30
1	A	738	TRP	CD1-CG-CD2	8.00	112.70	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	747	ARG	NE-CZ-NH1	-7.96	116.32	120.30
1	A	346	TRP	CD1-CG-CD2	7.96	112.67	106.30
1	A	539	GLN	CA-CB-CG	7.87	130.72	113.40
1	A	600	ARG	NE-CZ-NH2	7.84	124.22	120.30
1	A	410	ARG	NE-CZ-NH2	7.83	124.21	120.30
1	A	630	TRP	CD1-CG-CD2	7.72	112.48	106.30
1	A	214	TRP	CD1-CG-CD2	7.70	112.46	106.30
1	A	576	TRP	CE2-CD2-CG	-7.68	101.16	107.30
1	A	209	GLY	C-N-CA	7.66	140.85	121.70
1	A	115	ARG	CA-CB-CG	7.62	130.17	113.40
1	A	547	TRP	CD1-CG-CD2	7.58	112.36	106.30
1	A	329	ASP	CB-CG-OD2	7.46	125.02	118.30
1	A	156	TYR	CB-CG-CD2	-7.33	116.60	121.00
1	A	621	ARG	NE-CZ-NH2	7.31	123.96	120.30
1	A	346	TRP	CE2-CD2-CG	-7.28	101.47	107.30
1	A	26	ASP	CB-CG-OD1	7.15	124.74	118.30
1	A	10	PHE	CB-CG-CD2	-7.14	115.80	120.80
1	A	518	GLN	CA-CB-CG	6.96	128.71	113.40
1	A	747	ARG	NE-CZ-NH2	6.91	123.75	120.30
1	A	285	ARG	NE-CZ-NH1	-6.86	116.87	120.30
1	A	576	TRP	CG-CD1-NE1	-6.80	103.30	110.10
1	A	214	TRP	CE2-CD2-CG	-6.80	101.86	107.30
1	A	34	ARG	NE-CZ-NH2	6.76	123.68	120.30
1	A	139	TRP	CD1-CG-CD2	6.75	111.70	106.30
1	A	547	TRP	CE2-CD2-CG	-6.73	101.92	107.30
1	A	522	LYS	CA-C-N	-6.72	102.41	117.20
1	A	403	ASP	CB-CG-OD1	6.70	124.33	118.30
1	A	753	GLN	CA-CB-CG	6.64	128.00	113.40
1	A	523	ASP	N-CA-C	-6.62	93.13	111.00
1	A	57	ARG	NE-CZ-NH1	-6.58	117.01	120.30
1	A	657	ARG	NE-CZ-NH1	-6.55	117.03	120.30
1	A	278	LYS	CA-CB-CG	6.51	127.71	113.40
1	A	195	TRP	CG-CD1-NE1	-6.50	103.60	110.10
1	A	428	TRP	CD1-CG-CD2	6.38	111.41	106.30
1	A	19	ASP	CB-CG-OD2	6.37	124.03	118.30
1	A	598	GLU	CA-CB-CG	6.22	127.09	113.40
1	A	630	TRP	CG-CD1-NE1	-6.20	103.90	110.10
1	A	630	TRP	CE2-CD2-CG	-6.13	102.39	107.30
1	A	65	ARG	NE-CZ-NH2	6.11	123.35	120.30
1	A	34	ARG	NE-CZ-NH1	-6.07	117.27	120.30
1	A	666	ARG	CD-NE-CZ	6.07	132.10	123.60
1	A	139	TRP	CE2-CD2-CG	-6.03	102.47	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	635	ASP	N-CA-CB	-5.98	99.84	110.60
1	A	430	ARG	CA-CB-CG	-5.96	100.29	113.40
1	A	514	GLN	CA-C-N	-5.92	104.19	117.20
1	A	2	ARG	CA-CB-CG	5.92	126.41	113.40
1	A	195	TRP	CG-CD2-CE3	5.79	139.12	133.90
1	A	430	ARG	NE-CZ-NH1	-5.79	117.40	120.30
1	A	643	SER	CA-CB-OG	-5.75	95.69	111.20
1	A	209	GLY	O-C-N	-5.74	113.51	122.70
1	A	297	ASP	CB-CG-OD1	5.71	123.44	118.30
1	A	652	ARG	NE-CZ-NH2	5.68	123.14	120.30
1	A	107	LEU	CA-CB-CG	5.66	128.32	115.30
1	A	447	ARG	NE-CZ-NH2	5.66	123.13	120.30
1	A	18	TYR	CB-CG-CD2	-5.64	117.62	121.00
1	A	463	VAL	CG1-CB-CG2	-5.63	101.89	110.90
1	A	174	LEU	CB-CG-CD2	-5.59	101.50	111.00
1	A	139	TRP	CG-CD2-CE3	5.56	138.91	133.90
1	A	343	LYS	CA-CB-CG	5.54	125.58	113.40
1	A	397	ARG	NE-CZ-NH2	5.54	123.07	120.30
1	A	750	GLU	CA-CB-CG	5.54	125.58	113.40
1	A	738	TRP	CG-CD2-CE3	5.49	138.84	133.90
1	A	664	PHE	CB-CG-CD1	-5.48	116.96	120.80
1	A	287	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	403	ASP	OD1-CG-OD2	-5.40	113.05	123.30
1	A	447	ARG	NE-CZ-NH1	-5.37	117.62	120.30
1	A	630	TRP	CB-CG-CD1	-5.36	120.03	127.00
1	A	666	ARG	CG-CD-NE	-5.34	100.58	111.80
1	A	61	TYR	CB-CG-CD2	-5.33	117.80	121.00
1	A	709	LYS	CA-CB-CG	5.31	125.08	113.40
1	A	428	TRP	CG-CD1-NE1	-5.31	104.79	110.10
1	A	159	VAL	CG1-CB-CG2	-5.26	102.48	110.90
1	A	56	GLU	CA-CB-CG	-5.26	101.83	113.40
1	A	564	LYS	CA-CB-CG	5.24	124.93	113.40
1	A	576	TRP	CD1-NE1-CE2	5.23	113.71	109.00
1	A	278	LYS	CB-CG-CD	-5.23	98.01	111.60
1	A	629	ARG	NE-CZ-NH2	5.22	122.91	120.30
1	A	738	TRP	CG-CD1-NE1	-5.21	104.89	110.10
1	A	282	LYS	CB-CG-CD	5.17	125.05	111.60
1	A	31	ARG	NE-CZ-NH2	5.11	122.86	120.30
1	A	694	VAL	CB-CA-C	-5.11	101.70	111.40
1	A	275	ARG	NE-CZ-NH2	5.02	122.81	120.30
1	A	279	TYR	CB-CG-CD1	-5.00	118.00	121.00

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	5803	91	0
2	A	8	0	0	2	0
3	A	1	0	0	0	0
4	A	13	0	4	3	0
5	A	593	0	0	4	0
All	All	6429	0	5807	91	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 (91) 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
1:A:433:ILE:HD12	1:A:456:ASN:HD22	1.47	0.78
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:706:ALA:H	1:A:709:LYS:HZ2	1.54	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:35:PRO:HB2	1:A:305:CYS:HA	1.90	0.54
1:A:13:HIS:CD2	1:A:13:HIS:H	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:400:ILE:HB	1:A:405:TYR:HB2	1.97	0.47
1:A:70:ALA:O	1:A:163:GLY:HA2	2.15	0.47
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
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:HB3	1:A:384:LYS:HE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:ASP:O	1:A:496:LYS:HG3	2.19	0.43
1:A:129:THR:O	1:A:133:LYS:HB2	2.18	0.43
1:A:62:LEU:O	1:A:196:GLU:HA	2.19	0.43
1:A:21:LEU:O	1:A:25:ILE:HG13	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:589:ASN:HD22	1:A:589:ASN:C	2.23	0.41
1:A:325:PRO:HG2	1:A:326:PHE:CD2	2.56	0.41
1:A:107:LEU:HD22	1:A:107:LEU:N	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:616:VAL:HB	1:A:617:PRO:HD3	2.01	0.41
1:A:39:SER:HB3	1:A:237:ILE:HG21	2.02	0.41
1:A:555:LEU:O	1:A:696:LYS:HA	2.20	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%)	22	11

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 ⓘ

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%)	574 (92%)	47 (8%)	13	4

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	GLU
1	A	72	GLN
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	210	SER
1	A	223	LYS
1	A	297	ASP
1	A	310	VAL

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Mol	Chain	Res	Type
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	412	VAL
1	A	416	VAL
1	A	425	ILE
1	A	430	ARG
1	A	434	LYS
1	A	435	LYS
1	A	452	ARG
1	A	494	LYS
1	A	497	LEU
1	A	509	GLU
1	A	515	ASP
1	A	523	ASP
1	A	527	GLN
1	A	528	ARG
1	A	554	ASP
1	A	589	ASN
1	A	598	GLU
1	A	600	ARG
1	A	643	SER
1	A	657	ARG
1	A	666	ARG
1	A	694	VAL
1	A	709	LYS
1	A	747	ARG
1	A	753	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	HIS
1	A	82	GLN
1	A	314	ASN
1	A	321	HIS
1	A	332	HIS

*Continued on next page...*

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Mol	Chain	Res	Type
1	A	439	ASN
1	A	481	ASN
1	A	519	HIS
1	A	536	GLN
1	A	556	GLN
1	A	589	ASN
1	A	626	HIS
1	A	671	ASN

### 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 carbohydrates 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	1,3,4	0,12,12	0.00	-	-		
4	ICT	A	756	3,2	2,12,12	2.25	1 (50%)	5,16,16	8.13	4 (80%)

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
4	ICT	A	756	3,2	-	4/6/16/16	-
2	SF4	A	755	1,3,4	-	-	0/6/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	756	ICT	O7-C2	3.17	1.48	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	756	ICT	C4-C3-C6	-13.66	94.20	112.70
4	A	756	ICT	C1-C2-C3	-9.37	101.70	112.25
4	A	756	ICT	O7-C2-C3	5.45	123.82	108.56
4	A	756	ICT	O7-C2-C1	-5.16	98.69	111.10

There are no chirality outliers.

All (4) 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	O7-C2-C3-C6
4	A	756	ICT	C6-C3-C4-C5

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	755	SF4	2	0
4	A	756	ICT	3	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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.