



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 11:36 PM GMT

PDB ID : 1C96  
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 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 <http://wwpdb.org/ValidationPDFNotes.html>

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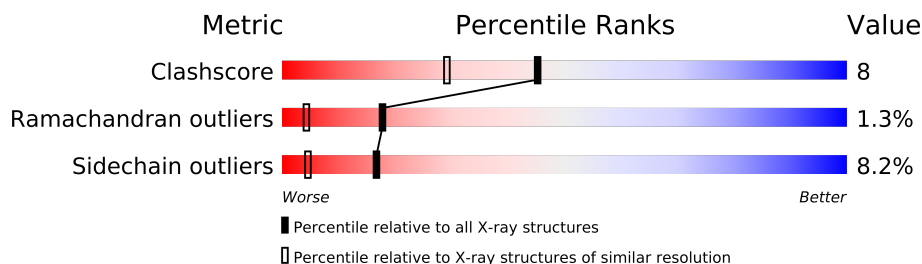
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : NOT EXECUTED  
EDS : NOT EXECUTED  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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	79885	5140 (1.84-1.80)
Ramachandran outliers	78287	5077 (1.84-1.80)
Sidechain outliers	78261	5077 (1.84-1.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	753	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6510 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

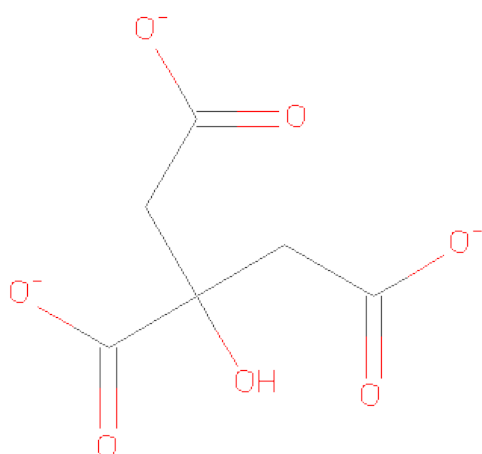
- Molecule 1 is a protein called MITOCHONDRIAL ACONITASE.

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:

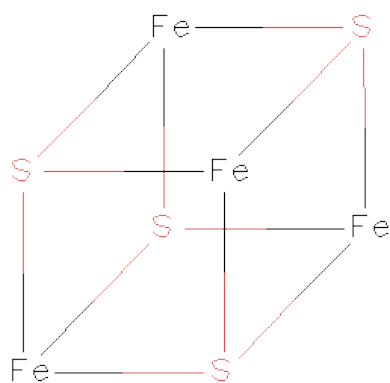
Chain	Residue	Modelled	Actual	Comment	Reference
A	13	HIS	ASN	CONFLICT	UNP P20004
A	26	ASP	ASN	CONFLICT	UNP P20004
A	303	PRO	SER	CONFLICT	UNP P20004
A	310	VAL	LEU	CONFLICT	UNP P20004
A	382	LYS	GLN	CONFLICT	UNP P20004
A	408	VAL	ILE	CONFLICT	UNP P20004
A	528	ARG	GLU	CONFLICT	UNP P20004
A	530	ALA	ASP	CONFLICT	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	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 (three-letter code: FLC) (formula: C<sub>6</sub>H<sub>5</sub>O<sub>7</sub>).



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

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



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

- Molecule 4 is OXYGEN ATOM (three-letter code: O) (formula: O).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	677	Total 677	O 677	0	0

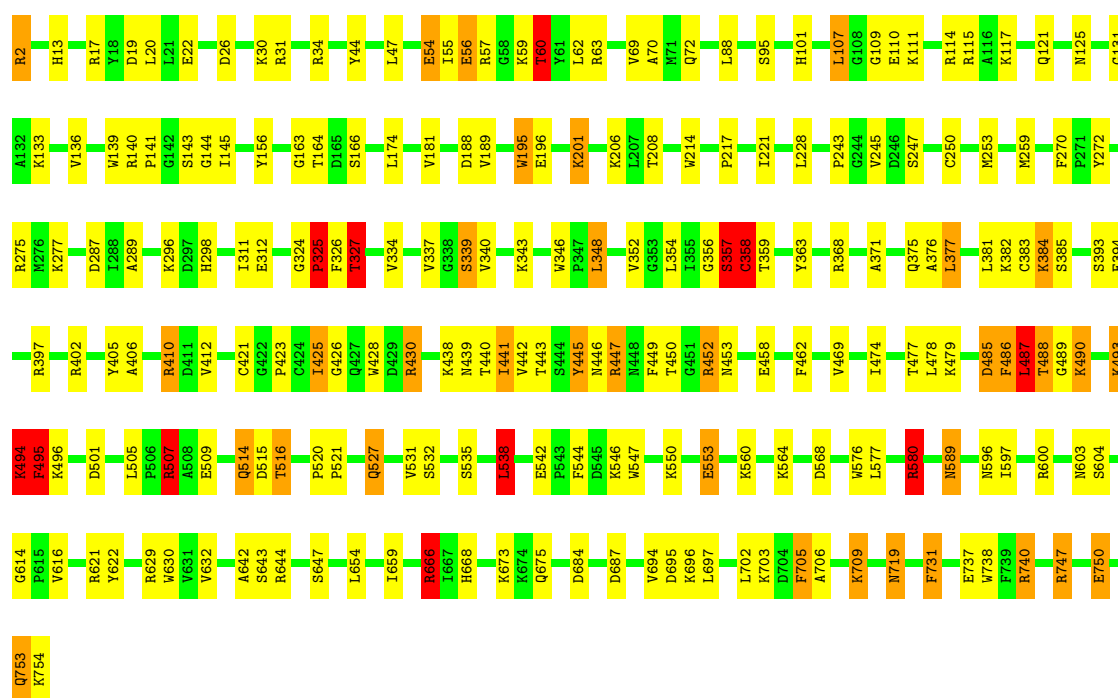
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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 will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	38.0	wwPDB-VP

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: FLC, SF4, 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	1.01	5/5938 (0.1%)	1.69	103/8045 (1.3%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	643	SER	N-CA	-8.97	1.28	1.46
1	A	195	TRP	CD1-NE1	-5.26	1.29	1.38
1	A	195	TRP	CG-CD2	-5.08	1.35	1.43
1	A	201	LYS	CD-CE	5.06	1.64	1.51
1	A	114	ARG	NE-CZ	5.02	1.39	1.33

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	666	ARG	NE-CZ-NH2	18.74	129.67	120.30
1	A	666	ARG	NE-CZ-NH1	-15.68	112.46	120.30
1	A	402	ARG	NE-CZ-NH1	-13.56	113.52	120.30
1	A	114	ARG	NE-CZ-NH2	12.58	126.59	120.30
1	A	195	TRP	CD1-CG-CD2	10.87	114.99	106.30
1	A	410	ARG	NE-CZ-NH1	-10.40	115.10	120.30
1	A	695	ASP	CB-CG-OD2	10.37	127.64	118.30
1	A	402	ARG	NE-CZ-NH2	10.30	125.45	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	580	ARG	NE-CZ-NH2	9.88	125.24	120.30
1	A	580	ARG	NE-CZ-NH1	-9.88	115.36	120.30
1	A	747	ARG	NE-CZ-NH1	-9.61	115.49	120.30
1	A	410	ARG	NE-CZ-NH2	9.56	125.08	120.30
1	A	644	ARG	NE-CZ-NH2	9.15	124.88	120.30
1	A	195	TRP	CE2-CD2-CG	-9.09	100.03	107.30
1	A	405	TYR	CB-CG-CD2	-8.93	115.64	121.00
1	A	576	TRP	CD1-CG-CD2	8.92	113.44	106.30
1	A	325	PRO	CA-C-N	8.87	136.71	117.20
1	A	430	ARG	NE-CZ-NH2	8.78	124.69	120.30
1	A	568	ASP	CB-CG-OD1	8.57	126.02	118.30
1	A	629	ARG	NE-CZ-NH2	8.53	124.56	120.30
1	A	397	ARG	NE-CZ-NH2	8.33	124.47	120.30
1	A	357	SER	CA-C-N	-8.31	98.91	117.20
1	A	214	TRP	CE2-CD2-CG	-7.95	100.94	107.30
1	A	490	LYS	CA-CB-CG	7.95	130.88	113.40
1	A	34	ARG	NE-CZ-NH1	-7.94	116.33	120.30
1	A	139	TRP	CD1-CG-CD2	7.83	112.56	106.30
1	A	115	ARG	NE-CZ-NH2	7.80	124.20	120.30
1	A	747	ARG	NE-CZ-NH2	7.65	124.12	120.30
1	A	358	CYS	CA-CB-SG	7.54	127.57	114.00
1	A	346	TRP	CE2-CD2-CG	-7.51	101.29	107.30
1	A	430	ARG	NE-CZ-NH1	-7.49	116.55	120.30
1	A	486	PHE	N-CA-C	7.41	130.99	111.00
1	A	547	TRP	CD1-CG-CD2	7.22	112.07	106.30
1	A	576	TRP	CE2-CD2-CG	-7.21	101.54	107.30
1	A	485	ASP	N-CA-C	7.03	129.97	111.00
1	A	287	ASP	CB-CG-OD1	6.98	124.58	118.30
1	A	57	ARG	NE-CZ-NH2	6.91	123.75	120.30
1	A	156	TYR	CB-CG-CD2	-6.90	116.86	121.00
1	A	740	ARG	NE-CZ-NH2	6.85	123.72	120.30
1	A	568	ASP	OD1-CG-OD2	-6.84	110.31	123.30
1	A	357	SER	O-C-N	6.80	133.59	122.70
1	A	214	TRP	CD1-CG-CD2	6.78	111.72	106.30
1	A	2	ARG	NE-CZ-NH2	6.75	123.68	120.30
1	A	63	ARG	NE-CZ-NH1	-6.74	116.93	120.30
1	A	705	PHE	CB-CG-CD1	-6.70	116.11	120.80
1	A	487	LEU	CA-CB-CG	6.69	130.69	115.30
1	A	114	ARG	NE-CZ-NH1	-6.58	117.01	120.30
1	A	687	ASP	CB-CG-OD2	6.58	124.22	118.30
1	A	695	ASP	CB-CG-OD1	-6.58	112.38	118.30
1	A	553	GLU	CA-CB-CG	6.57	127.86	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	428	TRP	CD1-CG-CD2	6.53	111.52	106.30
1	A	60	THR	N-CA-CB	-6.47	98.01	110.30
1	A	31	ARG	NE-CZ-NH2	6.45	123.53	120.30
1	A	346	TRP	CD1-CG-CD2	6.45	111.46	106.30
1	A	547	TRP	CE2-CD2-CG	-6.44	102.14	107.30
1	A	507	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	A	363	TYR	CB-CG-CD1	-6.40	117.16	121.00
1	A	576	TRP	CG-CD1-NE1	-6.37	103.73	110.10
1	A	630	TRP	CD1-CG-CD2	6.34	111.37	106.30
1	A	738	TRP	CD1-CG-CD2	6.31	111.35	106.30
1	A	629	ARG	NE-CZ-NH1	-6.26	117.17	120.30
1	A	195	TRP	CG-CD1-NE1	-6.26	103.84	110.10
1	A	494	LYS	CA-C-N	-6.24	103.47	117.20
1	A	188	ASP	CB-CG-OD2	6.20	123.88	118.30
1	A	445	TYR	CB-CG-CD2	-6.19	117.29	121.00
1	A	139	TRP	CE2-CD2-CG	-6.18	102.36	107.30
1	A	327	THR	N-CA-CB	6.14	121.97	110.30
1	A	405	TYR	CB-CG-CD1	6.12	124.67	121.00
1	A	495	PHE	N-CA-C	6.08	127.41	111.00
1	A	139	TRP	CG-CD1-NE1	-6.07	104.03	110.10
1	A	275	ARG	NE-CZ-NH2	6.07	123.33	120.30
1	A	538	LEU	CA-CB-CG	6.06	129.24	115.30
1	A	397	ARG	NE-CZ-NH1	-6.00	117.30	120.30
1	A	428	TRP	CE2-CD2-CG	-5.97	102.52	107.30
1	A	214	TRP	CG-CD2-CE3	5.89	139.20	133.90
1	A	750	GLU	CA-CB-CG	5.88	126.35	113.40
1	A	630	TRP	CE2-CD2-CG	-5.88	102.60	107.30
1	A	568	ASP	CB-CG-OD2	5.82	123.54	118.30
1	A	107	LEU	CA-CB-CG	5.79	128.62	115.30
1	A	348	LEU	CA-CB-CG	5.78	128.60	115.30
1	A	666	ARG	CG-CD-NE	-5.75	99.72	111.80
1	A	166	SER	CB-CA-C	-5.64	99.38	110.10
1	A	684	ASP	CB-CG-OD1	5.60	123.34	118.30
1	A	377	LEU	CA-CB-CG	5.55	128.07	115.30
1	A	514	GLN	N-CA-C	5.55	126.00	111.00
1	A	514	GLN	CB-CG-CD	5.54	126.00	111.60
1	A	2	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	A	34	ARG	NE-CZ-NH2	5.48	123.04	120.30
1	A	642	ALA	O-C-N	-5.45	113.99	122.70
1	A	695	ASP	CA-CB-CG	5.41	125.31	113.40
1	A	738	TRP	CE2-CD2-CG	-5.41	102.97	107.30
1	A	731	PHE	CB-CG-CD1	-5.39	117.03	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	440	THR	CA-CB-CG2	5.38	119.93	112.40
1	A	357	SER	C-N-CA	5.30	134.95	121.70
1	A	368	ARG	NE-CZ-NH2	5.25	122.92	120.30
1	A	488	THR	N-CA-CB	-5.24	100.34	110.30
1	A	440	THR	CA-CB-OG1	-5.18	98.12	109.00
1	A	356	GLY	CA-C-N	-5.18	105.80	117.20
1	A	57	ARG	CA-C-N	-5.17	105.85	116.20
1	A	447	ARG	NE-CZ-NH1	-5.15	117.73	120.30
1	A	687	ASP	OD1-CG-OD2	-5.14	113.53	123.30
1	A	384	LYS	CB-CG-CD	5.11	124.90	111.60
1	A	325	PRO	CA-C-O	-5.09	107.98	120.20

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5811	0	5805	98	0
2	A	13	0	5	3	0
3	A	8	0	0	3	0
4	A	1	0	0	0	0
5	A	677	0	0	8	0
All	All	6510	0	5810	98	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (98) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:S2	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:S4	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:326:PHE:HD1	1:A:450:THR:HG1	1.54	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:449:PHE:O	1:A:452:ARG:HB3	2.10	0.51
1:A:377:LEU:HD13	1:A:412:VAL:HG13	1.92	0.51
1:A:706:ALA:H	1:A:709:LYS:HZ2	1.57	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
1:A:26:ASP:HB3	5:A:1042:HOH:O	2.15	0.47
1:A:189:VAL:CG2	1:A:195:TRP:HB2	2.44	0.47
1:A:44:TYR:HA	1:A:47:LEU:HG	1.96	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:515:ASP:N	5:A:881:HOH:O	2.47	0.47
1:A:174:LEU:HD13	1:A:250:CYS:SG	2.55	0.47
1:A:55:ILE:HA	1:A:60:THR:HG21	1.97	0.47
1:A:488:THR:HG23	1:A:489:GLY:H	1.80	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:532:SER:HB3	1:A:535:SER:HB2	1.97	0.46
1:A:62:LEU:O	1:A:196:GLU:HA	2.16	0.46
1:A:442:VAL:HG23	1:A:469:VAL:HG13	1.98	0.46
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:425:ILE:CG1	3:A:755:SF4:S4	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:337:VAL:HA	1:A:340:VAL:HG22	1.98	0.44
1:A:245:VAL:HG13	1:A:270:PHE:HD1	1.81	0.44
1:A:449:PHE:HB3	5:A:1367:HOH:O	2.16	0.44
1:A:383:CYS:HA	1:A:474:ILE:HA	2.00	0.44
1:A:253:MET:SD	1:A:270:PHE:CD1	3.10	0.44
1:A:17:ARG:HD2	1:A:17:ARG:HA	1.86	0.44
1:A:580:ARG:HH12	2:A:756:FLC:CGC	2.30	0.44
1:A:208:THR:HG22	1:A:243:PRO:HG2	2.00	0.44
1:A:133:LYS:HB2	1:A:527:GLN:HB3	1.99	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:621:ARG:HG2	1:A:654:LEU:HD22	2.01	0.43
1:A:272:TYR:HD2	1:A:296:LYS:HG3	1.83	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:750:GLU:HA	1:A:754:LYS:HG2	2.01	0.42
1:A:311:ILE:HD13	1:A:311:ILE:HG21	1.82	0.42
1:A:376:ALA:O	1:A:381:LEU:HB2	2.19	0.42
1:A:371:ALA:O	1:A:375:GLN:HG3	2.19	0.42
1:A:56:GLU:HB3	1:A:59:LYS:HG2	2.02	0.42
1:A:589:ASN:C	1:A:589:ASN:HD22	2.24	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:HA	1:A:754:LYS:HD2	1.86	0.41
1:A:117:LYS:NZ	1:A:141:PRO:HB2	2.36	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:394:GLU:HG2	1:A:514:GLN:HG2	2.03	0.41
1:A:377:LEU:HD13	1:A:412:VAL:CG1	2.51	0.41
1:A:101:HIS:CD2	2:A:756:FLC:HG2	2.56	0.40
1:A:69:VAL:O	1:A:95:SER:HA	2.21	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%)	18 4

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%)	569 (92%)	51 (8%)	17 4

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	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	110	GLU
1	A	111	LYS
1	A	121	GLN
1	A	125	ASN
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	382	LYS
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	494	LYS
1	A	496	LYS

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Mol	Chain	Res	Type
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	546	LYS
1	A	550	LYS
1	A	553	GLU
1	A	589	ASN
1	A	694	VAL
1	A	696	LYS
1	A	697	LEU
1	A	702	LEU
1	A	703	LYS
1	A	705	PHE
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 (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	HIS
1	A	121	GLN
1	A	148	GLN
1	A	298	HIS
1	A	386	GLN
1	A	427	GLN
1	A	439	ASN
1	A	456	ASN
1	A	527	GLN
1	A	536	GLN
1	A	585	ASN
1	A	589	ASN
1	A	626	HIS
1	A	653	HIS
1	A	671	ASN
1	A	675	GLN
1	A	719	ASN
1	A	753	GLN



### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates 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$
3	SF4	A	755	1,2,4	12,12,12	139.29	11 (91%)	0,24,24	0.00	-
2	FLC	A	756	3	5,12,12	5.45	3 (60%)	7,17,17	3.02	3 (42%)

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
3	SF4	A	755	1,2,4	-	0/0/48/48	0/0/5/5
2	FLC	A	756	3	-	0/6/16/16	0/0/0/0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	755	SF4	S2-FE4	265.70	4.12	2.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	755	SF4	S4-FE1	257.72	4.06	2.33
3	A	755	SF4	S1-FE3	240.31	3.94	2.33
3	A	755	SF4	S3-FE2	191.09	3.61	2.33
3	A	755	SF4	S4-FE3	23.50	2.49	2.33
3	A	755	SF4	S4-FE2	20.54	2.47	2.33
3	A	755	SF4	S3-FE1	-13.20	2.24	2.33
3	A	755	SF4	S2-FE1	-12.40	2.24	2.33
3	A	755	SF4	S1-FE2	-11.46	2.25	2.33
2	A	756	FLC	CA-CAC	11.03	1.56	1.49
3	A	755	SF4	S2-FE3	-7.42	2.28	2.33
3	A	755	SF4	S1-FE4	-7.37	2.28	2.33
2	A	756	FLC	CA-CB	3.78	1.60	1.54
2	A	756	FLC	CG-CB	3.28	1.60	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	756	FLC	CB-CA-CAC	6.69	125.00	115.01
2	A	756	FLC	CB-CG-CGC	2.92	119.36	115.01
2	A	756	FLC	CG-CB-CA	-2.67	103.21	109.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.