



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 26, 2018 – 11:37 AM EDT

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

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

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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031021

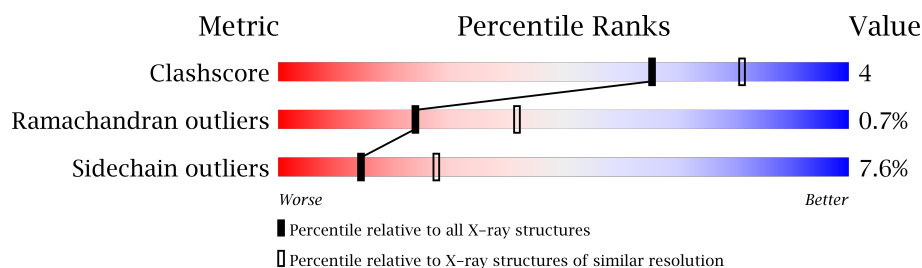
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	122126	4827 (2.50-2.50)
Ramachandran outliers	120053	4735 (2.50-2.50)
Sidechain outliers	120020	4737 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6139 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

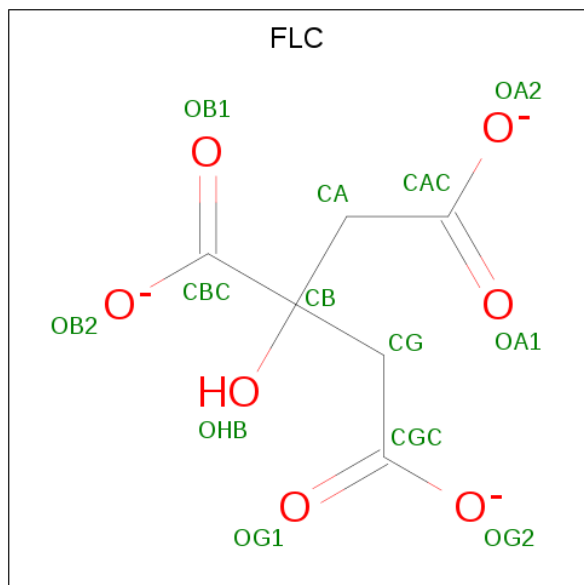
- Molecule 1 is a protein called PROTEIN (ACONITASE).

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

There are 2 discrepancies between the modelled and reference sequences:

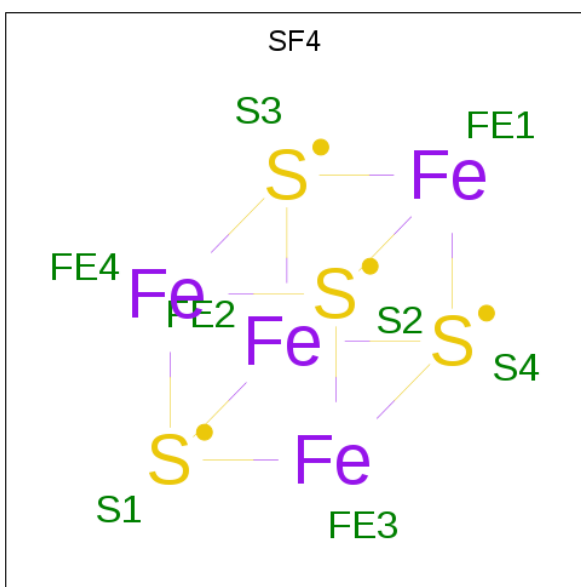
Chain	Residue	Modelled	Actual	Comment	Reference
A	642	ALA	SER	ENGINEERED	UNP P16276
A	647	SER	ARG	CONFLICT	UNP P16276

- Molecule 2 is CITRATE ANION (three-letter code: FLC) (formula:  $C_6H_5O_7^-$ ).



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

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: 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 (three-letter code: O) (formula: O).

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

- Molecule 5 is water.

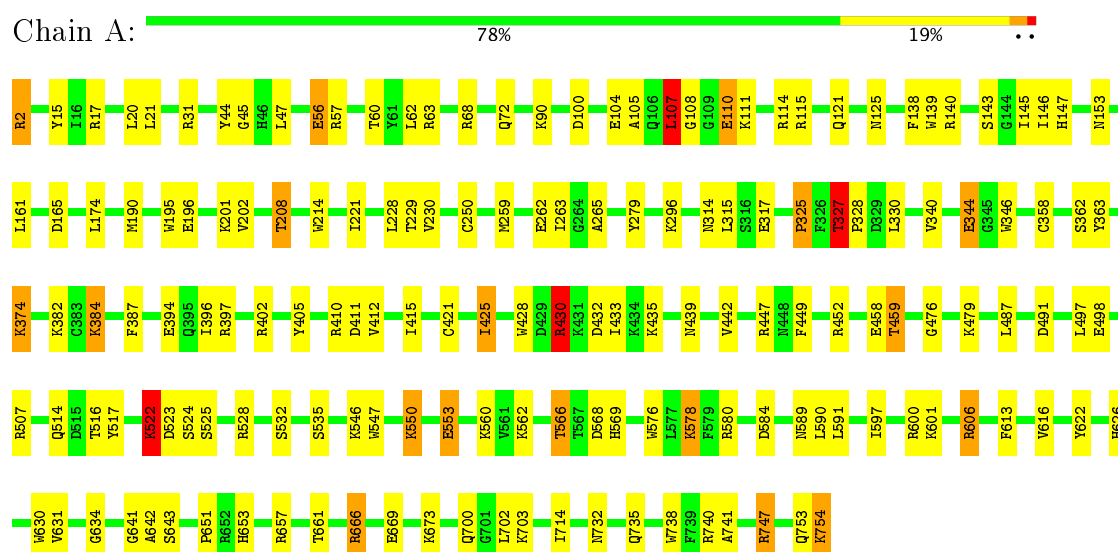
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	303	Total	O	0	0
			303	303		

### 3 Residue-property plots [i](#)

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: PROTEIN (ACONITASE)



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	B 1 1 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	187.80 Å   72.30 Å   74.10 Å 90.00°   90.00°   77.60°	Depositor
Resolution (Å)	20.00 – 2.50	Depositor
% Data completeness (in resolution range)	91.8 (20.00-2.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, $R_{free}$	0.172 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6139	wwPDB-VP
Average B, all atoms (Å <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: 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	0.93	2/5941 (0.0%)	1.63	81/8049 (1.0%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	641	GLY	C-N	-7.39	1.17	1.34
1	A	643	SER	N-CA	-6.83	1.32	1.46

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	430	ARG	NE-CZ-NH2	-14.44	113.08	120.30
1	A	580	ARG	NE-CZ-NH1	12.85	126.72	120.30
1	A	410	ARG	NE-CZ-NH1	12.58	126.59	120.30
1	A	666	ARG	NE-CZ-NH2	-11.96	114.32	120.30
1	A	115	ARG	NE-CZ-NH1	11.78	126.19	120.30
1	A	57	ARG	NE-CZ-NH1	10.71	125.65	120.30
1	A	580	ARG	NE-CZ-NH2	-10.34	115.13	120.30
1	A	115	ARG	NE-CZ-NH2	-10.21	115.19	120.30
1	A	402	ARG	NE-CZ-NH2	-9.37	115.62	120.30
1	A	740	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	A	402	ARG	NE-CZ-NH1	8.61	124.60	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	528	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	A	346	TRP	CD1-CG-CD2	8.52	113.11	106.30
1	A	428	TRP	CD1-CG-CD2	8.46	113.07	106.30
1	A	325	PRO	CA-C-N	8.42	135.72	117.20
1	A	666	ARG	NE-CZ-NH1	8.39	124.50	120.30
1	A	214	TRP	CD1-CG-CD2	8.35	112.98	106.30
1	A	195	TRP	CD1-CG-CD2	8.22	112.88	106.30
1	A	410	ARG	NE-CZ-NH2	-7.95	116.33	120.30
1	A	139	TRP	CD1-CG-CD2	7.92	112.64	106.30
1	A	630	TRP	CD1-CG-CD2	7.85	112.58	106.30
1	A	346	TRP	CE2-CD2-CG	-7.80	101.06	107.30
1	A	738	TRP	CD1-CG-CD2	7.79	112.53	106.30
1	A	100	ASP	CB-CG-OD1	7.72	125.25	118.30
1	A	547	TRP	CD1-CG-CD2	7.65	112.42	106.30
1	A	214	TRP	CE2-CD2-CG	-7.44	101.35	107.30
1	A	642	ALA	O-C-N	-7.29	111.04	122.70
1	A	325	PRO	N-CA-C	7.25	130.94	112.10
1	A	517	TYR	CB-CG-CD2	-7.17	116.70	121.00
1	A	428	TRP	CE2-CD2-CG	-7.16	101.57	107.30
1	A	522	LYS	CA-C-N	-7.16	101.44	117.20
1	A	547	TRP	CE2-CD2-CG	-7.07	101.64	107.30
1	A	279	TYR	CB-CG-CD1	-6.95	116.83	121.00
1	A	630	TRP	CE2-CD2-CG	-6.89	101.78	107.30
1	A	405	TYR	CB-CG-CD2	-6.88	116.87	121.00
1	A	576	TRP	CD1-CG-CD2	6.85	111.78	106.30
1	A	738	TRP	CE2-CD2-CG	-6.84	101.83	107.30
1	A	139	TRP	CE2-CD2-CG	-6.83	101.84	107.30
1	A	195	TRP	CE2-CD2-CG	-6.83	101.84	107.30
1	A	165	ASP	CB-CG-OD1	6.63	124.27	118.30
1	A	442	VAL	CG1-CB-CG2	-6.63	100.30	110.90
1	A	195	TRP	CG-CD1-NE1	-6.56	103.54	110.10
1	A	452	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	A	397	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	A	31	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	A	17	ARG	NE-CZ-NH2	-6.31	117.15	120.30
1	A	100	ASP	CB-CG-OD2	-6.11	112.81	118.30
1	A	576	TRP	CE2-CD2-CG	-6.04	102.47	107.30
1	A	265	ALA	CA-C-N	5.92	130.22	117.20
1	A	747	ARG	NE-CZ-NH1	5.89	123.24	120.30
1	A	642	ALA	C-N-CA	5.87	136.38	121.70
1	A	738	TRP	CG-CD1-NE1	-5.86	104.24	110.10
1	A	15	TYR	CB-CG-CD2	-5.83	117.50	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	TRP	O-C-N	-5.77	113.47	122.70
1	A	553	GLU	CA-CB-CG	5.72	125.98	113.40
1	A	459	THR	CA-CB-CG2	5.65	120.31	112.40
1	A	107	LEU	CA-CB-CG	5.62	128.24	115.30
1	A	700	GLN	N-CA-CB	-5.58	100.56	110.60
1	A	90	LYS	CA-CB-CG	5.54	125.60	113.40
1	A	580	ARG	CG-CD-NE	-5.53	100.19	111.80
1	A	606	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	A	161	LEU	CA-CB-CG	5.51	127.97	115.30
1	A	2	ARG	N-CA-C	-5.39	96.45	111.00
1	A	374	LYS	CA-CB-CG	5.36	125.20	113.40
1	A	754	LYS	CA-CB-CG	5.35	125.17	113.40
1	A	325	PRO	O-C-N	-5.31	114.21	122.70
1	A	547	TRP	CG-CD1-NE1	-5.27	104.83	110.10
1	A	327	THR	N-CA-CB	5.24	120.26	110.30
1	A	738	TRP	CG-CD2-CE3	5.24	138.61	133.90
1	A	195	TRP	CA-C-N	5.22	128.68	117.20
1	A	68	ARG	CA-CB-CG	5.20	124.83	113.40
1	A	228	LEU	CA-CB-CG	5.17	127.19	115.30
1	A	447	ARG	CG-CD-NE	-5.16	100.97	111.80
1	A	190	MET	CA-CB-CG	-5.14	104.56	113.30
1	A	452	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	387	PHE	N-CA-CB	-5.11	101.41	110.60
1	A	214	TRP	CG-CD1-NE1	-5.09	105.00	110.10
1	A	428	TRP	CG-CD1-NE1	-5.09	105.01	110.10
1	A	566	THR	N-CA-CB	-5.07	100.66	110.30
1	A	547	TRP	CG-CD2-CE3	5.06	138.46	133.90
1	A	202	VAL	CA-CB-CG1	-5.03	103.36	110.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	363	TYR	Sidechain

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5814	0	5803	51	0
2	A	13	0	3	0	0
3	A	8	0	0	1	0
4	A	1	0	0	0	0
5	A	303	0	0	1	0
All	All	6139	0	5806	51	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (51) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:LYS:HD3	1:A:476:GLY:HA3	1.49	0.94
1:A:566:THR:HG22	1:A:568:ASP:H	1.46	0.81
1:A:221:ILE:HG12	1:A:259:MET:HB3	1.73	0.69
1:A:107:LEU:HD23	1:A:111:LYS:HB3	1.77	0.67
1:A:430:ARG:HH22	1:A:439:ASN:HD21	1.40	0.66
1:A:430:ARG:HD2	1:A:432:ASP:OD1	1.99	0.63
1:A:63:ARG:HG3	5:A:897:HOH:O	1.97	0.63
1:A:550:LYS:HB2	1:A:550:LYS:NZ	2.14	0.62
1:A:566:THR:HB	1:A:569:HIS:ND1	2.15	0.61
1:A:550:LYS:HA	1:A:703:LYS:HE3	1.82	0.60
1:A:430:ARG:NH2	1:A:439:ASN:HD21	2.00	0.58
1:A:550:LYS:HB2	1:A:550:LYS:HZ2	1.68	0.58
1:A:174:LEU:HD13	1:A:250:CYS:SG	2.44	0.57
1:A:566:THR:HG22	1:A:568:ASP:N	2.18	0.57
1:A:362:SER:HA	1:A:396:ILE:HD13	1.89	0.54
1:A:425:ILE:HG13	3:A:755:SF4:S1	2.47	0.54
1:A:143:SER:HB3	1:A:516:THR:HB	1.90	0.54
1:A:208:THR:HG22	1:A:314:ASN:OD1	2.08	0.54
1:A:208:THR:O	1:A:315:LEU:HB2	2.07	0.54
1:A:532:SER:HB3	1:A:535:SER:HB2	1.90	0.54
1:A:560:LYS:HG2	1:A:597:ILE:HG21	1.91	0.51
1:A:121:GLN:O	1:A:125:ASN:HB2	2.12	0.50
1:A:449:PHE:CD2	1:A:566:THR:HG21	2.48	0.49
1:A:327:THR:HG22	1:A:328:PRO:HD2	1.95	0.48
1:A:606:ARG:HB2	1:A:613:PHE:CZ	2.48	0.48
1:A:110:GLU:O	1:A:114:ARG:HG3	2.14	0.47
1:A:108:GLY:HA3	1:A:415:ILE:HD11	1.97	0.46
1:A:382:LYS:NZ	1:A:411:ASP:O	2.48	0.46
1:A:732:ASN:OD1	1:A:735:GLN:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:LYS:HE3	1:A:522:LYS:HA	1.97	0.45
1:A:340:VAL:O	1:A:344:GLU:HB2	2.17	0.45
1:A:230:VAL:HA	1:A:263:ILE:HA	1.99	0.44
1:A:21:LEU:HD12	1:A:45:GLY:HA3	2.00	0.44
1:A:590:LEU:HD13	1:A:651:PRO:HD3	1.98	0.44
1:A:62:LEU:O	1:A:196:GLU:HA	2.19	0.43
1:A:421:CYS:HB2	1:A:425:ILE:HD11	2.01	0.43
1:A:634:GLY:HA3	1:A:661:THR:HG22	1.99	0.42
1:A:146:ILE:HD13	1:A:146:ILE:HG21	1.85	0.42
1:A:479:LYS:HB3	1:A:479:LYS:HE3	1.80	0.42
1:A:546:LYS:HD3	1:A:741:ALA:O	2.19	0.42
1:A:145:ILE:HG21	1:A:358:CYS:HB3	2.01	0.42
1:A:56:GLU:HB2	1:A:60:THR:HG23	2.01	0.42
1:A:622:TYR:O	1:A:626:HIS:HD2	2.03	0.42
1:A:104:GLU:HG2	1:A:105:ALA:N	2.35	0.42
1:A:44:TYR:HA	1:A:47:LEU:HG	2.01	0.41
1:A:138:PHE:HE2	1:A:140:ARG:HG2	1.85	0.41
1:A:591:LEU:HB2	1:A:616:VAL:HG11	2.03	0.41
1:A:584:ASP:OD1	1:A:653:HIS:HE1	2.03	0.41
1:A:714:ILE:N	1:A:714:ILE:HD12	2.36	0.40
1:A:669:GLU:O	1:A:673:LYS:HG3	2.21	0.40
1:A:147:HIS:HD2	1:A:358:CYS:SG	2.44	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	751/753 (100%)	709 (94%)	37 (5%)	5 (1%)	24 42

All (5) Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains ⓘ

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%)	14	28

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

Mol	Chain	Res	Type
1	A	2	ARG
1	A	20	LEU
1	A	56	GLU
1	A	72	GLN
1	A	107	LEU
1	A	110	GLU
1	A	153	ASN
1	A	201	LYS
1	A	208	THR
1	A	229	THR
1	A	262	GLU
1	A	317	GLU
1	A	325	PRO
1	A	327	THR
1	A	330	LEU
1	A	344	GLU
1	A	374	LYS
1	A	384	LYS
1	A	394	GLU
1	A	412	VAL
1	A	425	ILE
1	A	430	ARG

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Mol	Chain	Res	Type
1	A	433	ILE
1	A	435	LYS
1	A	458	GLU
1	A	459	THR
1	A	487	LEU
1	A	491	ASP
1	A	497	LEU
1	A	498	GLU
1	A	507	ARG
1	A	514	GLN
1	A	522	LYS
1	A	523	ASP
1	A	550	LYS
1	A	553	GLU
1	A	562	LYS
1	A	578	LYS
1	A	589	ASN
1	A	600	ARG
1	A	601	LYS
1	A	631	VAL
1	A	657	ARG
1	A	666	ARG
1	A	702	LEU
1	A	747	ARG
1	A	754	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	HIS
1	A	148	GLN
1	A	241	HIS
1	A	321	HIS
1	A	427	GLN
1	A	439	ASN
1	A	519	HIS
1	A	536	GLN
1	A	539	GLN
1	A	585	ASN
1	A	589	ASN
1	A	625	GLN
1	A	653	HIS

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Mol	Chain	Res	Type
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	$\# Z  > 2$
3	SF4	A	755	1,2,4	0,12,12	0.00	-	0,24,24	0.00	-
2	FLC	A	756	3	3,12,12	6.78	2 (66%)	3,17,17	10.68	2 (66%)

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	0/6/5/5
2	FLC	A	756	3	-	0/6/16/16	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	756	FLC	CA-CB	-10.46	1.39	1.54
2	A	756	FLC	OHB-CB	5.30	1.51	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	756	FLC	CB-CG-CGC	7.20	125.75	114.95
2	A	756	FLC	CB-CA-CAC	16.94	140.36	114.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

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

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.