



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 12:40 PM GMT

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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

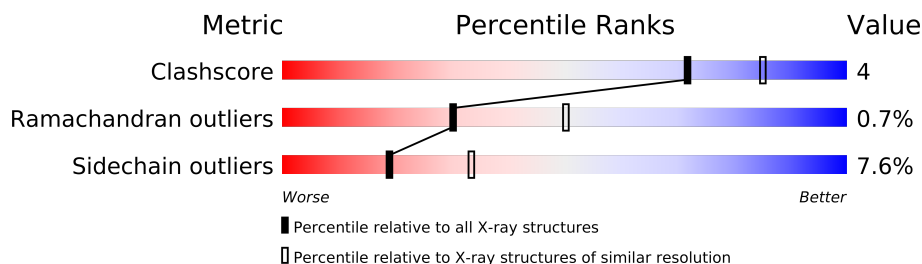
The following versions of software and data (see [references](#)) were used in the production of this report:

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 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	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (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 ≥ 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 i

There are 5 unique types of molecules in this entry. The entry contains 6139 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.

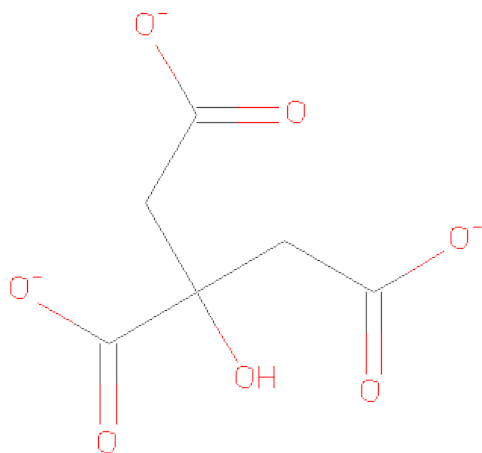
- Molecule 1 is a protein called PROTEIN (ACONITASE).

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		

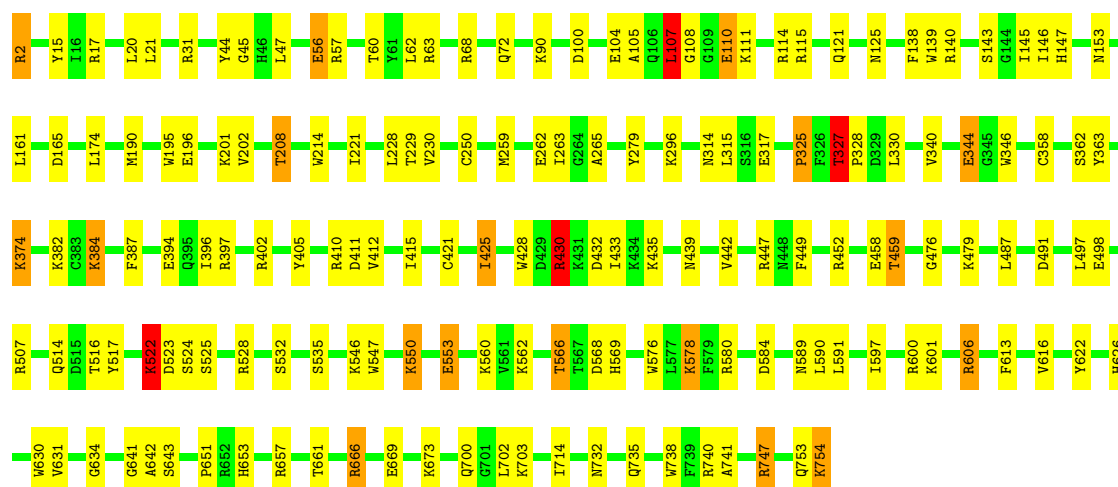
3 Residue-property plots

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: PROTEIN (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	B 1 1 2	Depositor
Cell constants a, b, c, α , β , γ	187.80Å 72.30Å 74.10Å 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 ²)	24.0	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	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 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	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

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 4.

All (51) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:532:SER:HB3	1:A:535:SER:HB2	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: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:732:ASN:OD1	1:A:735:GLN:HG3	2.15	0.46
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:421:CYS:HB2	1:A:425:ILE:HD11	2.01	0.43
1:A:62:LEU:O	1:A:196:GLU:HA	2.19	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:546:LYS:HD3	1:A:741:ALA:O	2.19	0.42
1:A:479:LYS:HB3	1:A:479:LYS:HE3	1.80	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

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%)	709 (94%)	37 (5%)	5 (1%)	30	50

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%)	19	33

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
1	A	433	ILE

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Mol	Chain	Res	Type
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
1	A	671	ASN

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	3.11	6 (50%)	0,24,24	0.00	-
2	FLC	A	756	3	5,12,12	12.82	4 (80%)	7,17,17	7.23	4 (57%)

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 (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	756	FLC	CA-CAC	-25.09	1.34	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	756	FLC	CA-CB	-9.67	1.39	1.54
2	A	756	FLC	CG-CGC	-8.67	1.44	1.49
3	A	755	SF4	S2-FE3	5.06	2.36	2.33
3	A	755	SF4	S3-FE4	4.90	2.36	2.33
3	A	755	SF4	S2-FE4	4.83	2.36	2.33
2	A	756	FLC	OHB-CB	4.81	1.51	1.43
3	A	755	SF4	S3-FE2	4.30	2.36	2.33
3	A	755	SF4	S3-FE1	-3.52	2.30	2.33
3	A	755	SF4	S1-FE2	2.57	2.35	2.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	756	FLC	CB-CA-CAC	16.97	140.36	115.01
2	A	756	FLC	CB-CG-CGC	7.19	125.75	115.01
2	A	756	FLC	OHB-CB-CA	-3.48	100.40	108.51
2	A	756	FLC	CA-CB-CBC	2.81	116.90	111.21

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.