



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 12:33 pm BST

PDB ID : 1FGH
Title : COMPLEX WITH 4-HYDROXY-TRANS-ACONITATE
Authors : Lauble, H.; Kennedy, M.C.; Emptage, M.H.; Beinert, H.; Stout, C.D.
Deposited on : 1996-09-14
Resolution : 2.05 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 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

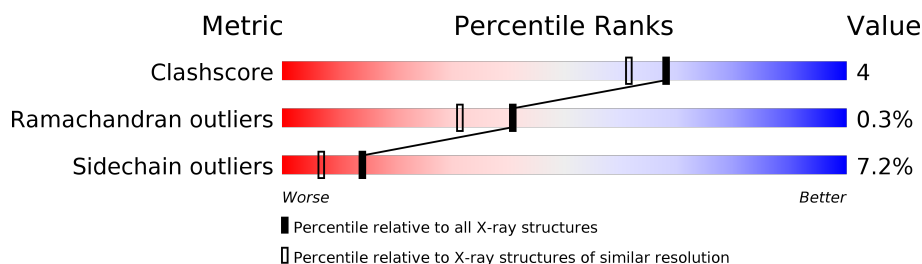
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)

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 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	754	 83% 13% . .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6093 atoms, of which 4 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.

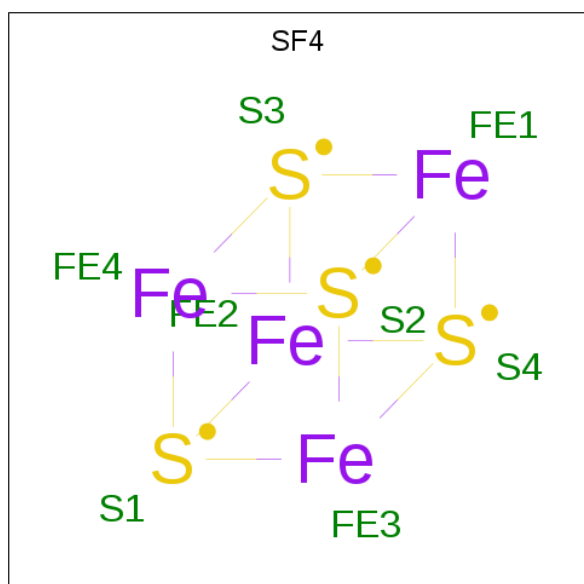
- Molecule 1 is a protein called ACONITASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	753	5812	3663	1031	1096	22	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

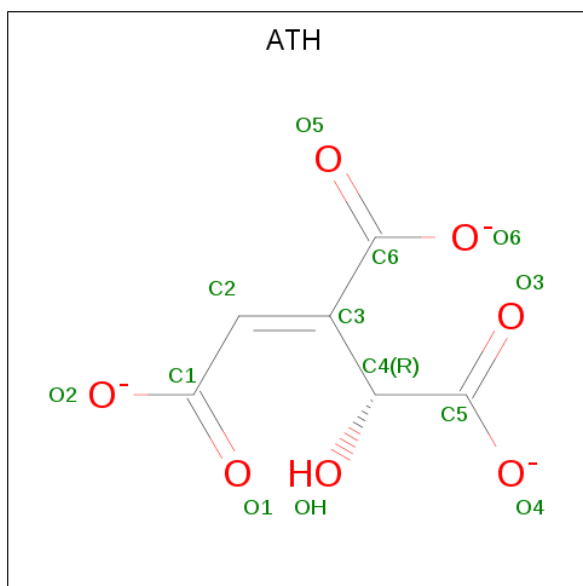
Chain	Residue	Modelled	Actual	Comment	Reference
A	303	SER	PRO	CONFLICT	UNP P20004
A	310	LEU	VAL	CONFLICT	UNP P20004
A	597	SER	ILE	CONFLICT	UNP P20004
A	647	SER	ARG	CONFLICT	UNP P20004
A	653	PHE	HIS	CONFLICT	UNP P20004
A	712	THR	LYS	CONFLICT	UNP P20004

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

- Molecule 3 is 4-HYDROXY-ACONITATE ION (three-letter code: ATH) (formula: $C_6H_3O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			15	6	2	7		

- Molecule 4 is water.

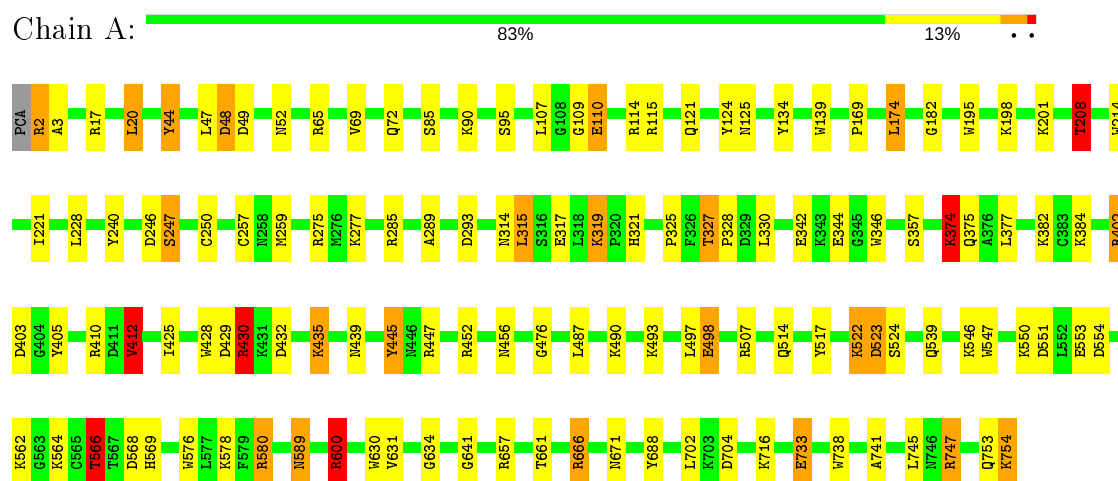
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	256	Total	H	O	0	0
			258	2	256		

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: 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, α , β , γ	185.90 Å 71.80 Å 72.20 Å 90.00° 90.00° 77.70°	Depositor
Resolution (Å)	8.00 – 2.05	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.05)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.177 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6093	wwPDB-VP
Average B, all atoms (Å ²)	16.0	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, ATH

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	0.84	0/5938	1.58	77/8044 (1.0%)

There are no bond length outliers.

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	580	ARG	NE-CZ-NH2	-28.66	105.97	120.30
1	A	580	ARG	NE-CZ-NH1	26.49	133.54	120.30
1	A	402	ARG	NE-CZ-NH2	-18.34	111.13	120.30
1	A	430	ARG	NE-CZ-NH2	-17.74	111.43	120.30
1	A	430	ARG	NE-CZ-NH1	15.99	128.30	120.30
1	A	410	ARG	NE-CZ-NH1	15.28	127.94	120.30
1	A	410	ARG	NE-CZ-NH2	-14.80	112.90	120.30
1	A	402	ARG	NE-CZ-NH1	12.72	126.66	120.30
1	A	65	ARG	NE-CZ-NH1	11.96	126.28	120.30
1	A	600	ARG	NE-CZ-NH1	11.43	126.02	120.30
1	A	452	ARG	NE-CZ-NH2	-11.08	114.76	120.30
1	A	666	ARG	NE-CZ-NH2	-10.87	114.86	120.30
1	A	65	ARG	NE-CZ-NH2	-10.24	115.18	120.30
1	A	195	TRP	CD1-CG-CD2	9.27	113.72	106.30
1	A	630	TRP	CD1-CG-CD2	9.21	113.67	106.30
1	A	346	TRP	CD1-CG-CD2	8.87	113.39	106.30
1	A	325	PRO	CA-C-N	8.64	136.20	117.20
1	A	600	ARG	NE-CZ-NH2	-8.46	116.07	120.30
1	A	517	TYR	CB-CG-CD1	-8.44	115.94	121.00
1	A	566	THR	N-CA-CB	-8.39	94.35	110.30
1	A	115	ARG	NE-CZ-NH2	-8.31	116.15	120.30
1	A	428	TRP	CD1-CG-CD2	7.88	112.60	106.30
1	A	630	TRP	CE2-CD2-CG	-7.77	101.09	107.30
1	A	139	TRP	CD1-CG-CD2	7.76	112.51	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	576	TRP	CD1-CG-CD2	7.60	112.38	106.30
1	A	195	TRP	CE2-CD2-CG	-7.40	101.38	107.30
1	A	214	TRP	CD1-CG-CD2	7.39	112.21	106.30
1	A	522	LYS	CA-C-N	-7.35	101.03	117.20
1	A	214	TRP	CE2-CD2-CG	-7.25	101.50	107.30
1	A	346	TRP	CE2-CD2-CG	-7.20	101.54	107.30
1	A	498	GLU	CA-CB-CG	6.98	128.77	113.40
1	A	195	TRP	CG-CD1-NE1	-6.97	103.13	110.10
1	A	580	ARG	CG-CD-NE	-6.88	97.35	111.80
1	A	551	ASP	CB-CG-OD1	6.82	124.44	118.30
1	A	547	TRP	CD1-CG-CD2	6.82	111.75	106.30
1	A	447	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	A	666	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	A	139	TRP	CE2-CD2-CG	-6.63	102.00	107.30
1	A	405	TYR	CB-CG-CD2	-6.58	117.05	121.00
1	A	576	TRP	CE2-CD2-CG	-6.51	102.09	107.30
1	A	428	TRP	CE2-CD2-CG	-6.38	102.20	107.30
1	A	547	TRP	CE2-CD2-CG	-6.37	102.21	107.30
1	A	738	TRP	CD1-CG-CD2	6.33	111.37	106.30
1	A	580	ARG	CD-NE-CZ	6.30	132.42	123.60
1	A	523	ASP	N-CA-C	-6.16	94.37	111.00
1	A	630	TRP	CG-CD1-NE1	-6.07	104.03	110.10
1	A	666	ARG	CG-CD-NE	-5.99	99.22	111.80
1	A	374	LYS	CA-CB-CG	5.98	126.56	113.40
1	A	44	TYR	CB-CG-CD2	-5.94	117.43	121.00
1	A	412	VAL	CB-CA-C	-5.88	100.24	111.40
1	A	600	ARG	CA-CB-CG	5.84	126.25	113.40
1	A	346	TRP	CG-CD1-NE1	-5.78	104.32	110.10
1	A	498	GLU	OE1-CD-OE2	-5.77	116.37	123.30
1	A	139	TRP	CG-CD1-NE1	-5.74	104.36	110.10
1	A	688	TYR	CB-CG-CD1	-5.71	117.57	121.00
1	A	124	TYR	CB-CG-CD2	-5.61	117.63	121.00
1	A	410	ARG	CG-CD-NE	-5.59	100.05	111.80
1	A	738	TRP	CE2-CD2-CG	-5.59	102.83	107.30
1	A	428	TRP	CG-CD1-NE1	-5.59	104.51	110.10
1	A	139	TRP	CG-CD2-CE3	5.58	138.92	133.90
1	A	747	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	A	346	TRP	CG-CD2-CE3	5.53	138.88	133.90
1	A	507	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	A	733	GLU	OE1-CD-OE2	-5.42	116.80	123.30
1	A	445	TYR	CB-CG-CD2	-5.41	117.76	121.00
1	A	293	ASP	CB-CG-OD1	5.36	123.13	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	325	PRO	O-C-N	-5.35	114.14	122.70
1	A	208	THR	N-CA-CB	-5.31	100.20	110.30
1	A	247	SER	CA-CB-OG	5.27	125.43	111.20
1	A	48	ASP	CB-CG-OD1	5.25	123.03	118.30
1	A	342	GLU	OE1-CD-OE2	-5.25	117.00	123.30
1	A	240	TYR	CB-CG-CD2	-5.22	117.87	121.00
1	A	429	ASP	CB-CG-OD1	5.21	122.98	118.30
1	A	539	GLN	CG-CD-NE2	5.18	129.13	116.70
1	A	285	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	A	214	TRP	CG-CD2-CE3	5.04	138.44	133.90
1	A	115	ARG	NE-CZ-NH1	5.02	122.81	120.30

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	5812	0	5794	44	2
2	A	8	0	0	0	0
3	A	13	2	2	1	0
4	A	256	2	0	1	0
All	All	6089	4	5796	44	2

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 (44) 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:430:ARG:HH22	1:A:439:ASN:HD21	1.33	0.76
1:A:430:ARG:HD2	1:A:432:ASP:OD1	1.95	0.65
1:A:600:ARG:HH11	1:A:600:ARG:HG3	1.68	0.58
1:A:384:LYS:HD3	1:A:476:GLY:HA3	1.88	0.56
1:A:430:ARG:HH22	1:A:439:ASN:ND2	2.01	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:LYS:HG3	1:A:289:ALA:HB1	1.89	0.54
1:A:402:ARG:HD2	1:A:403:ASP:OD1	2.08	0.54
1:A:580:ARG:HH22	3:A:755:ATH:C1	2.21	0.54
1:A:566:THR:HB	1:A:569:HIS:ND1	2.24	0.53
1:A:641:GLY:HA2	4:A:1056:HOH:O	2.09	0.53
1:A:208:THR:HG22	1:A:314:ASN:HA	1.91	0.53
1:A:182:GLY:HA3	1:A:671:ASN:HD21	1.75	0.52
1:A:377:LEU:HG	1:A:412:VAL:HG13	1.92	0.51
1:A:85:SER:HB2	1:A:745:LEU:HD21	1.93	0.50
1:A:221:ILE:HG12	1:A:259:MET:HB3	1.95	0.48
1:A:600:ARG:NH1	1:A:600:ARG:HG3	2.28	0.48
1:A:201:LYS:HD2	1:A:201:LYS:HA	1.72	0.48
1:A:546:LYS:HD3	1:A:741:ALA:O	2.14	0.47
1:A:90:LYS:HD2	1:A:134:TYR:O	2.15	0.47
1:A:17:ARG:HB3	1:A:20:LEU:HB2	1.97	0.47
1:A:374:LYS:HD2	1:A:375:GLN:HG3	1.97	0.47
1:A:327:THR:HG22	1:A:328:PRO:HD2	1.96	0.46
1:A:246:ASP:O	1:A:275:ARG:NH1	2.49	0.46
1:A:357:SER:HB3	1:A:445:TYR:CD1	2.50	0.46
1:A:110:GLU:O	1:A:114:ARG:HG3	2.16	0.46
1:A:319:LYS:O	1:A:321:HIS:HD2	1.99	0.45
1:A:44:TYR:HA	1:A:47:LEU:HG	1.99	0.45
1:A:169:PRO:O	1:A:257:CYS:HB3	2.17	0.44
1:A:17:ARG:NH2	1:A:20:LEU:HD23	2.33	0.44
1:A:435:LYS:HD2	1:A:456:ASN:HA	1.99	0.44
1:A:754:LYS:C	1:A:754:LYS:HZ2	2.21	0.43
1:A:327:THR:HG23	1:A:564:LYS:NZ	2.33	0.43
1:A:174:LEU:HD13	1:A:250:CYS:SG	2.58	0.43
1:A:566:THR:CG2	1:A:568:ASP:H	2.32	0.42
1:A:550:LYS:HB2	1:A:550:LYS:NZ	2.35	0.42
1:A:589:ASN:C	1:A:589:ASN:HD22	2.23	0.42
1:A:208:THR:O	1:A:315:LEU:HB2	2.20	0.42
1:A:2:ARG:HE	1:A:3:ALA:N	2.18	0.42
1:A:49:ASP:OD2	1:A:52:ASN:HB2	2.19	0.41
1:A:430:ARG:NH2	1:A:439:ASN:HD21	2.09	0.41
1:A:554:ASP:OD1	1:A:716:LYS:NZ	2.51	0.41
1:A:382:LYS:HE3	1:A:382:LYS:HB3	1.92	0.41
1:A:69:VAL:O	1:A:95:SER:HA	2.21	0.40
1:A:634:GLY:O	1:A:661:THR:HA	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ASP:OD2	1:A:493:LYS:NZ[1_556]	2.01	0.19
1:A:48:ASP:OD1	1:A:493:LYS:NZ[1_556]	2.10	0.10

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	751/754 (100%)	723 (96%)	26 (4%)	2 (0%)	41 31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	GLY
1	A	524	SER

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	622/622 (100%)	577 (93%)	45 (7%)	14 7

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	20	LEU
1	A	72	GLN

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Mol	Chain	Res	Type
1	A	107	LEU
1	A	110	GLU
1	A	121	GLN
1	A	125	ASN
1	A	174	LEU
1	A	198	LYS
1	A	208	THR
1	A	228	LEU
1	A	247	SER
1	A	315	LEU
1	A	317	GLU
1	A	319	LYS
1	A	327	THR
1	A	330	LEU
1	A	344	GLU
1	A	374	LYS
1	A	412	VAL
1	A	425	ILE
1	A	430	ARG
1	A	435	LYS
1	A	487	LEU
1	A	490	LYS
1	A	497	LEU
1	A	498	GLU
1	A	514	GLN
1	A	522	LYS
1	A	523	ASP
1	A	553	GLU
1	A	562	LYS
1	A	566	THR
1	A	578	LYS
1	A	589	ASN
1	A	600	ARG
1	A	631	VAL
1	A	657	ARG
1	A	666	ARG
1	A	702	LEU
1	A	704	ASP
1	A	733	GLU
1	A	747	ARG
1	A	753	GLN
1	A	754	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	148	GLN
1	A	321	HIS
1	A	439	ASN
1	A	514	GLN
1	A	519	HIS
1	A	536	GLN
1	A	585	ASN
1	A	589	ASN
1	A	625	GLN
1	A	637	ASN
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](#)

2 ligands are modelled in this entry.

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	ATH	A	755	2	3,12,12	2.55	1 (33%)	2,16,16	0.37	0
2	SF4	A	999	1,3,4	0,12,12	0.00	-	-		

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	ATH	A	755	2	-	0/6/16/16	-
2	SF4	A	999	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)
3	A	755	ATH	C4-C3	4.26	1.56	1.51

There are no bond angle outliers.

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	ATH	1	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.