



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 04:33 PM EDT

PDB ID : 1B0M
Title : ACONITASE R644Q:FLUOROCITRATE COMPLEX
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

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) : 2.23.2

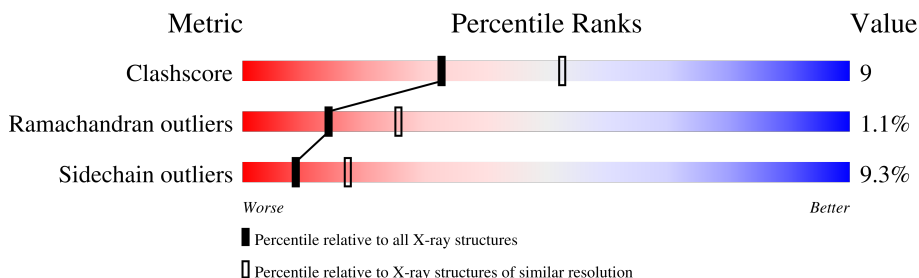
1 Overall quality at a glance

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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (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 of 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	753	 68% 26% 5%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6175 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.

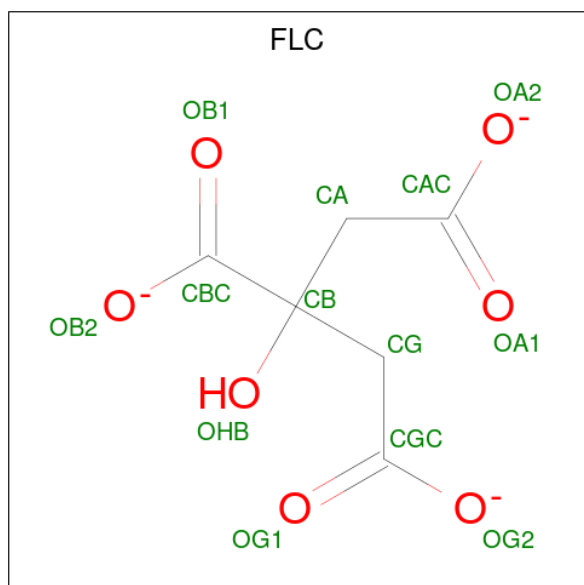
- Molecule 1 is a protein called PROTEIN (ACONITASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	753	5813	3665	1032	1094	22	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

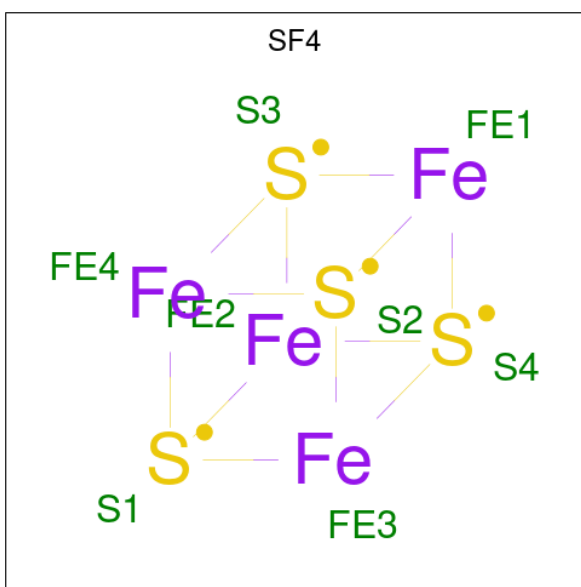
Chain	Residue	Modelled	Actual	Comment	Reference
A	644	GLN	ARG	engineered mutation	UNP P16276
A	647	SER	ARG	conflict	UNP P16276

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



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

- 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 water.

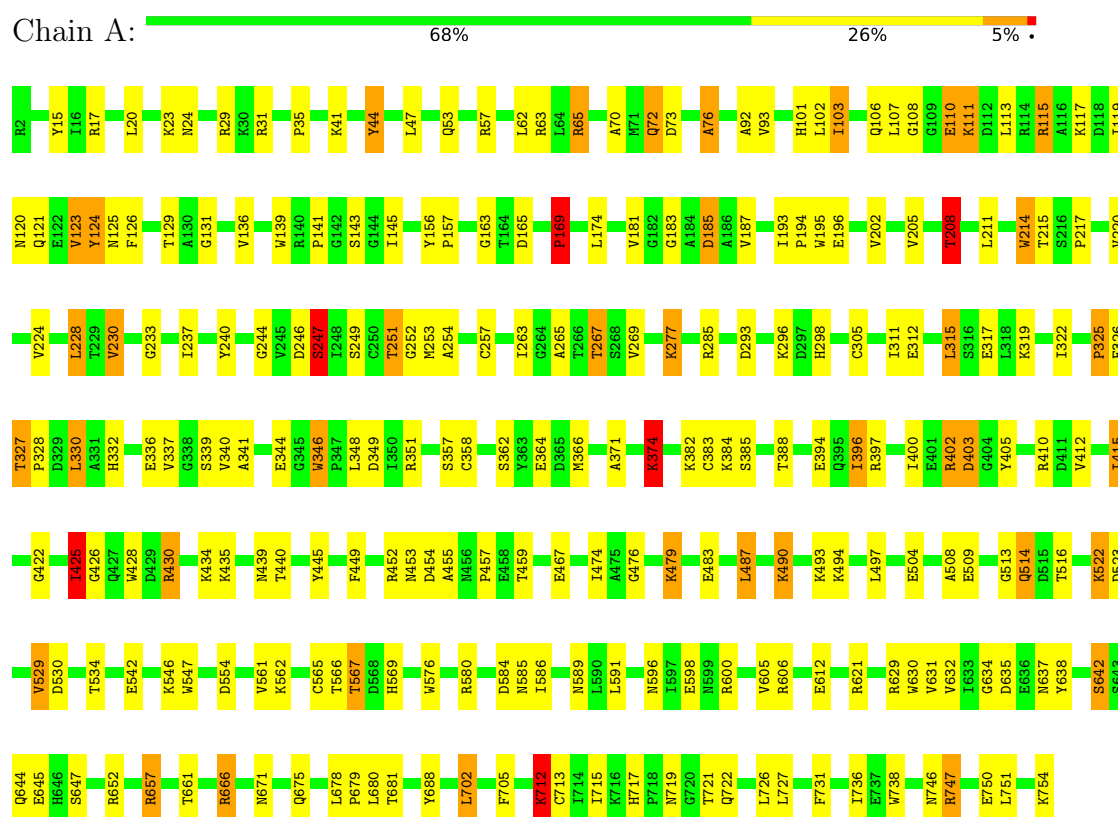
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	341	Total	O	0	0
			341	341		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	176.90Å 71.90Å 73.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50	Depositor
% Data completeness (in resolution range)	84.9 (20.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.193 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6175	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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, FLC

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	1.00	3/5940 (0.1%)	1.77	115/8048 (1.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	195	TRP	CD1-NE1	-5.20	1.29	1.38
1	A	346	TRP	CD1-NE1	-5.05	1.29	1.38
1	A	547	TRP	CG-CD2	-5.01	1.35	1.43

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	452	ARG	NE-CZ-NH2	-18.93	110.83	120.30
1	A	666	ARG	NE-CZ-NH1	15.86	128.23	120.30
1	A	666	ARG	NE-CZ-NH2	-15.28	112.66	120.30
1	A	402	ARG	NE-CZ-NH2	-14.59	113.00	120.30
1	A	402	ARG	NE-CZ-NH1	11.91	126.25	120.30
1	A	410	ARG	NE-CZ-NH2	-11.43	114.59	120.30
1	A	285	ARG	NE-CZ-NH1	11.25	125.92	120.30
1	A	57	ARG	NE-CZ-NH1	11.20	125.90	120.30
1	A	430	ARG	NE-CZ-NH2	-10.57	115.01	120.30
1	A	430	ARG	NE-CZ-NH1	10.57	125.59	120.30
1	A	65	ARG	NE-CZ-NH2	-10.48	115.06	120.30
1	A	580	ARG	NE-CZ-NH1	9.89	125.25	120.30
1	A	31	ARG	NE-CZ-NH2	-9.80	115.40	120.30
1	A	428	TRP	CD1-CG-CD2	9.73	114.09	106.30
1	A	156	TYR	CB-CG-CD2	-9.20	115.48	121.00
1	A	195	TRP	CD1-CG-CD2	9.20	113.66	106.30
1	A	195	TRP	CE2-CD2-CG	-9.10	100.02	107.30
1	A	285	ARG	NE-CZ-NH2	-8.85	115.87	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	738	TRP	CD1-CG-CD2	8.78	113.33	106.30
1	A	630	TRP	CD1-CG-CD2	8.76	113.31	106.30
1	A	346	TRP	CE2-CD2-CG	-8.69	100.35	107.30
1	A	403	ASP	CB-CG-OD2	8.43	125.89	118.30
1	A	428	TRP	CE2-CD2-CG	-8.40	100.58	107.30
1	A	267	THR	CA-CB-CG2	8.39	124.14	112.40
1	A	346	TRP	CD1-CG-CD2	8.17	112.83	106.30
1	A	346	TRP	CG-CD2-CE3	8.16	141.25	133.90
1	A	576	TRP	CD1-CG-CD2	7.95	112.66	106.30
1	A	397	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	A	139	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	A	652	ARG	NE-CZ-NH2	7.79	124.19	120.30
1	A	214	TRP	CD1-CG-CD2	7.78	112.52	106.30
1	A	738	TRP	CE2-CD2-CG	-7.58	101.24	107.30
1	A	214	TRP	CE2-CD2-CG	-7.53	101.28	107.30
1	A	586	ILE	CA-CB-CG1	-7.48	96.78	111.00
1	A	747	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	A	630	TRP	CE2-CD2-CG	-7.34	101.43	107.30
1	A	452	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	A	139	TRP	CE2-CD2-CG	-7.24	101.51	107.30
1	A	621	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	A	202	VAL	CG1-CB-CG2	-7.18	99.41	110.90
1	A	214	TRP	CG-CD2-CE3	7.13	140.31	133.90
1	A	547	TRP	CD1-CG-CD2	6.99	111.89	106.30
1	A	605	VAL	CG1-CB-CG2	-6.96	99.76	110.90
1	A	629	ARG	NE-CZ-NH2	6.95	123.78	120.30
1	A	195	TRP	CG-CD2-CE3	6.95	140.15	133.90
1	A	606	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	A	493	LYS	CA-C-N	-6.91	102.00	117.20
1	A	576	TRP	CE2-CD2-CG	-6.91	101.77	107.30
1	A	642	SER	N-CA-CB	-6.83	100.26	110.50
1	A	17	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	A	124	TYR	CB-CG-CD2	-6.76	116.94	121.00
1	A	547	TRP	CE2-CD2-CG	-6.71	101.93	107.30
1	A	63	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	A	514	GLN	CA-CB-CG	6.56	127.83	113.40
1	A	632	VAL	CG1-CB-CG2	-6.56	100.41	110.90
1	A	522	LYS	CA-C-N	-6.55	102.79	117.20
1	A	44	TYR	CB-CG-CD2	-6.54	117.08	121.00
1	A	115	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	A	629	ARG	CG-CD-NE	6.52	125.49	111.80
1	A	635	ASP	N-CA-CB	-6.48	98.94	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	THR	CA-CB-OG1	-6.42	95.51	109.00
1	A	410	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	A	452	ARG	CG-CD-NE	-6.39	98.38	111.80
1	A	652	ARG	NE-CZ-NH1	-6.35	117.12	120.30
1	A	688	TYR	CB-CG-CD1	-6.25	117.25	121.00
1	A	31	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	A	425	ILE	CB-CA-C	-6.14	99.31	111.60
1	A	208	THR	N-CA-CB	-6.13	98.65	110.30
1	A	205	VAL	CG1-CB-CG2	-6.10	101.14	110.90
1	A	680	LEU	CB-CG-CD1	-6.06	100.70	111.00
1	A	428	TRP	CG-CD1-NE1	-6.03	104.07	110.10
1	A	123	VAL	N-CA-CB	-6.01	98.28	111.50
1	A	397	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	A	449	PHE	CB-CG-CD2	-5.89	116.68	120.80
1	A	738	TRP	CG-CD2-CE3	5.86	139.17	133.90
1	A	346	TRP	CB-CG-CD1	-5.85	119.39	127.00
1	A	529	VAL	N-CA-C	-5.77	95.42	111.00
1	A	195	TRP	CG-CD1-NE1	-5.70	104.40	110.10
1	A	612	GLU	CA-CB-CG	5.68	125.89	113.40
1	A	374	LYS	CA-CB-CG	5.60	125.72	113.40
1	A	738	TRP	CG-CD1-NE1	-5.58	104.52	110.10
1	A	15	TYR	CB-CG-CD1	5.53	124.32	121.00
1	A	630	TRP	CG-CD1-NE1	-5.53	104.57	110.10
1	A	631	VAL	N-CA-CB	-5.52	99.35	111.50
1	A	247	SER	N-CA-CB	-5.50	102.25	110.50
1	A	428	TRP	CG-CD2-CE3	5.49	138.84	133.90
1	A	598	GLU	CA-CB-CG	5.47	125.44	113.40
1	A	467	GLU	OE1-CD-OE2	-5.36	116.87	123.30
1	A	103	ILE	CA-C-N	-5.36	105.42	117.20
1	A	405	TYR	CB-CG-CD2	-5.35	117.79	121.00
1	A	747	ARG	N-CA-CB	-5.34	100.98	110.60
1	A	452	ARG	NH1-CZ-NH2	5.31	125.24	119.40
1	A	15	TYR	CB-CG-CD2	-5.31	117.82	121.00
1	A	445	TYR	CB-CG-CD2	-5.28	117.83	121.00
1	A	92	ALA	N-CA-C	5.25	125.19	111.00
1	A	76	ALA	N-CA-CB	-5.25	102.76	110.10
1	A	123	VAL	CB-CA-C	5.23	121.33	111.40
1	A	657	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	A	214	TRP	CG-CD1-NE1	-5.20	104.90	110.10
1	A	638	TYR	CB-CG-CD1	-5.18	117.89	121.00
1	A	410	ARG	CG-CD-NE	-5.17	100.95	111.80
1	A	585	ASN	CB-CG-ND2	5.15	129.07	116.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	TYR	CB-CG-CD2	-5.14	117.92	121.00
1	A	430	ARG	CA-CB-CG	5.13	124.68	113.40
1	A	139	TRP	CG-CD2-CE3	5.12	138.50	133.90
1	A	452	ARG	N-CA-CB	-5.10	101.42	110.60
1	A	93	VAL	CA-CB-CG1	-5.10	103.25	110.90
1	A	106	GLN	N-CA-CB	-5.08	101.46	110.60
1	A	440	THR	CA-CB-CG2	5.07	119.50	112.40
1	A	346	TRP	CG-CD1-NE1	-5.07	105.03	110.10
1	A	497	LEU	CA-CB-CG	5.05	126.92	115.30
1	A	657	ARG	CG-CD-NE	-5.03	101.24	111.80
1	A	65	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	A	396	ILE	CB-CG1-CD1	-5.02	99.86	113.90
1	A	712	LYS	CA-CB-CG	-5.01	102.38	113.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	5813	0	5799	101	0
2	A	13	0	5	2	0
3	A	8	0	0	1	0
4	A	341	0	0	10	0
All	All	6175	0	5804	101	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 9.

All (101) 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:251:THR:HG23	4:A:846:HOH:O	1.74	0.87
1:A:731:PHE:HZ	4:A:1095:HOH:O	1.72	0.72
1:A:251:THR:HB	4:A:909:HOH:O	1.93	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:LYS:HD3	1:A:476:GLY:HA3	1.78	0.64
1:A:383:CYS:SG	1:A:474:ILE:HD12	2.39	0.62
1:A:228:LEU:HD11	1:A:311:ILE:HD11	1.81	0.62
1:A:220:VAL:O	1:A:224:VAL:HG23	2.00	0.62
1:A:348:LEU:HD12	1:A:479:LYS:HG2	1.82	0.61
1:A:567:THR:HG22	4:A:1056:HOH:O	2.02	0.60
1:A:430:ARG:HH22	1:A:439:ASN:ND2	1.99	0.60
1:A:584:ASP:HB2	4:A:1070:HOH:O	2.00	0.59
1:A:679:PRO:HD3	4:A:1095:HOH:O	2.01	0.59
1:A:336:GLU:O	1:A:340:VAL:HG23	2.02	0.59
1:A:73:ASP:OD1	1:A:101:HIS:HB2	2.04	0.58
1:A:108:GLY:HA3	1:A:415:ILE:HD11	1.86	0.57
1:A:402:ARG:HD2	1:A:403:ASP:OD1	2.04	0.57
1:A:143:SER:HB3	1:A:516:THR:HB	1.87	0.57
1:A:388:THR:HG22	1:A:415:ILE:HG23	1.86	0.56
1:A:634:GLY:O	1:A:661:THR:HA	2.05	0.56
1:A:396:ILE:O	1:A:400:ILE:HG12	2.05	0.56
1:A:566:THR:HB	1:A:569:HIS:ND1	2.19	0.56
1:A:35:PRO:HB2	1:A:305:CYS:HA	1.87	0.55
1:A:322:ILE:HG21	1:A:337:VAL:HG11	1.88	0.55
1:A:394:GLU:HG3	1:A:513:GLY:HA3	1.89	0.55
1:A:439:ASN:HD21	1:A:459:THR:HG23	1.72	0.55
1:A:44:TYR:HA	1:A:47:LEU:HG	1.88	0.54
1:A:62:LEU:O	1:A:196:GLU:HA	2.08	0.54
1:A:422:GLY:O	1:A:425:ILE:HG13	2.08	0.54
1:A:103:ILE:HD11	1:A:141:PRO:HB3	1.91	0.52
1:A:230:VAL:HA	1:A:263:ILE:HA	1.89	0.52
1:A:327:THR:HG22	1:A:328:PRO:HD2	1.90	0.52
1:A:357:SER:HB2	3:A:755:SF4:S2	2.50	0.52
1:A:165:ASP:OD2	2:A:756:FLC:HA1	2.10	0.51
1:A:487:LEU:O	1:A:494:LYS:HA	2.10	0.51
1:A:251:THR:HG22	1:A:362:SER:HB2	1.93	0.51
1:A:426:GLY:HA2	1:A:453:ASN:O	2.11	0.51
1:A:208:THR:O	1:A:315:LEU:HB2	2.12	0.50
1:A:115:ARG:HG2	1:A:119:ILE:HD12	1.94	0.50
1:A:388:THR:HG22	1:A:415:ILE:CG2	2.42	0.50
1:A:678:LEU:HD11	1:A:702:LEU:HD11	1.94	0.50
1:A:101:HIS:CD2	1:A:425:ILE:HD13	2.47	0.50
1:A:70:ALA:O	1:A:163:GLY:HA2	2.12	0.49
1:A:546:LYS:HD2	4:A:1092:HOH:O	2.11	0.49
1:A:647:SER:HB2	4:A:1056:HOH:O	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:THR:O	1:A:681:THR:HA	2.11	0.49
1:A:251:THR:CG2	1:A:362:SER:HB2	2.43	0.49
1:A:251:THR:O	1:A:254:ALA:HB3	2.11	0.49
1:A:145:ILE:HG21	1:A:358:CYS:HB3	1.95	0.48
1:A:211:LEU:HD22	1:A:215:THR:HG22	1.96	0.48
1:A:131:GLY:HA2	1:A:136:VAL:HB	1.95	0.48
1:A:596:ASN:O	1:A:600:ARG:HA	2.13	0.48
1:A:233:GLY:O	1:A:265:ALA:HA	2.14	0.48
1:A:385:SER:OG	1:A:476:GLY:HA2	2.14	0.48
1:A:181:VAL:HB	1:A:185:ASP:HB2	1.95	0.48
1:A:330:LEU:HD22	1:A:332:HIS:CE1	2.48	0.48
1:A:715:ILE:O	1:A:722:GLN:HA	2.15	0.47
1:A:169:PRO:O	1:A:257:CYS:HB3	2.14	0.47
1:A:362:SER:O	1:A:366:MET:HG2	2.15	0.47
1:A:237:ILE:HA	1:A:267:THR:O	2.15	0.46
1:A:249:SER:O	1:A:253:MET:HG3	2.16	0.46
1:A:430:ARG:HG2	1:A:454:ASP:HB2	1.98	0.46
1:A:455:ALA:O	1:A:457:PRO:HD3	2.16	0.46
1:A:642:SER:HA	2:A:756:FLC:OA1	2.15	0.46
1:A:341:ALA:HA	1:A:346:TRP:CE3	2.51	0.46
1:A:712:LYS:HG3	1:A:726:LEU:HD23	1.96	0.46
1:A:108:GLY:CA	1:A:415:ILE:HD11	2.45	0.46
1:A:183:GLY:O	1:A:187:VAL:HG23	2.16	0.46
1:A:217:PRO:HG2	1:A:252:GLY:HA3	1.98	0.45
1:A:751:LEU:HD12	4:A:918:HOH:O	2.16	0.45
1:A:675:GLN:HE21	1:A:675:GLN:HA	1.81	0.45
1:A:123:VAL:O	1:A:126:PHE:HB3	2.17	0.45
1:A:430:ARG:NH2	1:A:439:ASN:HD21	2.14	0.45
1:A:23:LYS:NZ	1:A:24:ASN:OD1	2.47	0.44
1:A:72:GLN:O	1:A:76:ALA:HB2	2.17	0.44
1:A:65:ARG:NH2	1:A:194:PRO:HG3	2.32	0.44
1:A:351:ARG:HG3	1:A:439:ASN:HB2	2.00	0.44
1:A:364:GLU:HB2	1:A:504:GLU:HA	2.00	0.43
1:A:47:LEU:HD22	1:A:53:GLN:HG2	2.01	0.43
1:A:120:ASN:HB2	1:A:124:TYR:CE2	2.54	0.43
1:A:129:THR:HG22	1:A:529:VAL:HG22	2.00	0.43
1:A:371:ALA:HA	1:A:374:LYS:HG3	2.01	0.43
1:A:705:PHE:CD2	1:A:736:ILE:HG23	2.53	0.43
1:A:41:LYS:HE2	1:A:298:HIS:HA	2.01	0.42
1:A:719:ASN:OD1	1:A:721:THR:HB	2.19	0.42
1:A:113:LEU:HG	1:A:117:LYS:HE3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:ARG:NH2	1:A:439:ASN:ND2	2.66	0.42
1:A:244:GLY:O	1:A:247:SER:HB3	2.20	0.42
1:A:277:LYS:NZ	1:A:293:ASP:OD2	2.52	0.42
1:A:384:LYS:CD	1:A:476:GLY:HA3	2.49	0.42
1:A:325:PRO:HG2	1:A:326:PHE:CD2	2.55	0.42
1:A:671:ASN:O	1:A:675:GLN:HG2	2.20	0.42
1:A:746:ASN:O	1:A:750:GLU:HG3	2.20	0.42
1:A:214:TRP:CD1	1:A:483:GLU:HG2	2.55	0.41
1:A:249:SER:HB2	1:A:504:GLU:HG3	2.02	0.41
1:A:439:ASN:ND2	1:A:459:THR:HG23	2.35	0.41
1:A:675:GLN:HA	1:A:675:GLN:NE2	2.36	0.40
1:A:717:HIS:CD2	1:A:721:THR:HG22	2.56	0.40
1:A:110:GLU:OE2	1:A:111:LYS:HG3	2.22	0.40
1:A:561:VAL:HG11	1:A:565:CYS:HB2	2.02	0.40
1:A:490:LYS:HD3	4:A:957:HOH:O	2.21	0.40
1:A:713:CYS:HB2	1:A:727:LEU:HD11	2.03	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%)	697 (93%)	46 (6%)	8 (1%)	14	26

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	591	LEU
1	A	230	VAL
1	A	296	LYS
1	A	169	PRO
1	A	508	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	554	ASP
1	A	479	LYS
1	A	645	GLU

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	622/622 (100%)	564 (91%)	58 (9%)	9 17

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	29	ARG
1	A	72	GLN
1	A	102	LEU
1	A	107	LEU
1	A	110	GLU
1	A	111	LYS
1	A	121	GLN
1	A	125	ASN
1	A	157	PRO
1	A	169	PRO
1	A	174	LEU
1	A	185	ASP
1	A	193	ILE
1	A	208	THR
1	A	228	LEU
1	A	246	ASP
1	A	247	SER
1	A	251	THR
1	A	269	VAL
1	A	277	LYS
1	A	312	GLU
1	A	315	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	317	GLU
1	A	319	LYS
1	A	325	PRO
1	A	327	THR
1	A	330	LEU
1	A	339	SER
1	A	344	GLU
1	A	349	ASP
1	A	374	LYS
1	A	382	LYS
1	A	412	VAL
1	A	415	ILE
1	A	425	ILE
1	A	434	LYS
1	A	435	LYS
1	A	487	LEU
1	A	490	LYS
1	A	509	GLU
1	A	514	GLN
1	A	522	LYS
1	A	523	ASP
1	A	530	ASP
1	A	534	THR
1	A	542	GLU
1	A	562	LYS
1	A	567	THR
1	A	589	ASN
1	A	637	ASN
1	A	644	GLN
1	A	657	ARG
1	A	666	ARG
1	A	702	LEU
1	A	712	LYS
1	A	747	ARG
1	A	754	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	386	GLN
1	A	427	GLN
1	A	439	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	514	GLN
1	A	536	GLN
1	A	585	ASN
1	A	589	ASN
1	A	671	ASN
1	A	675	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
2	FLC	A	756	-	3,12,12	3.40	2 (66%)	3,17,17	9.07	3 (100%)
3	SF4	A	755	4,1	0,12,12	-	-	-	-	-

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	756	FLC	CA-CB	-4.71	1.48	1.54
2	A	756	FLC	CG-CB	2.90	1.59	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	756	FLC	CB-CG-CGC	11.33	133.13	114.98
2	A	756	FLC	CB-CA-CAC	9.74	130.58	114.98
2	A	756	FLC	CG-CB-CA	-4.83	96.41	109.33

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	756	FLC	CAC-CA-CB-CBC
2	A	756	FLC	CAC-CA-CB-OHB
2	A	756	FLC	CA-CB-CG-CGC
2	A	756	FLC	CAC-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	756	FLC	2	0
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](#)

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.