



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 12:40 PM GMT

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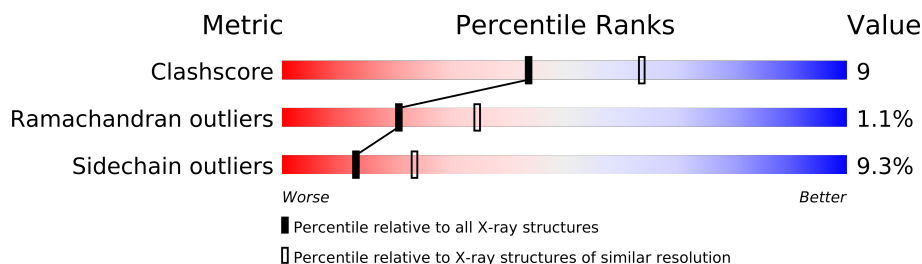
The following versions of software and data (see [references](#)) were used in the production of this report:

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 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  $\geq 3$ , 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 i

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

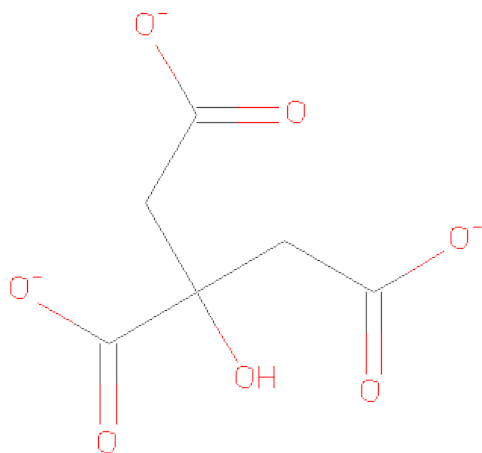
- Molecule 1 is a protein called PROTEIN (ACONITASE).

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

There are 2 discrepancies between the modelled and reference sequences:

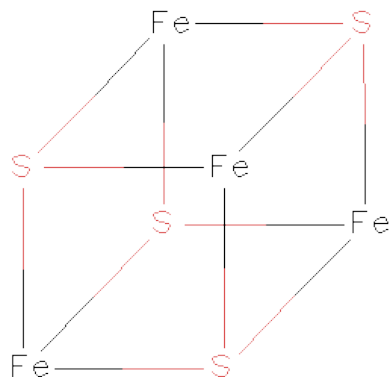
Chain	Residue	Modelled	Actual	Comment	Reference
A	644	GLN	ARG	ENGINEERED	UNP P16276
A	647	SER	ARG	CONFLICT	UNP P16276

- 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 water.

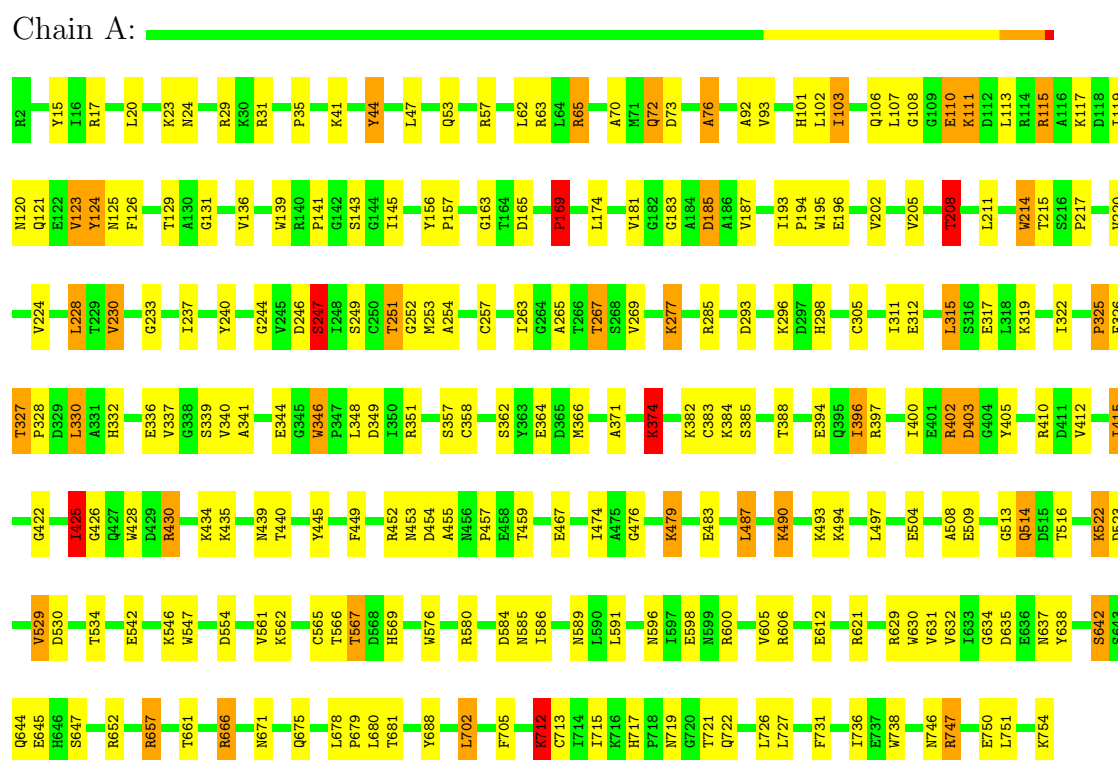
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	341	Total	O	0	0
			341	341		

### 3 Residue-property plots

These plots are drawn for all protein, RNA 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)



## 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, $\alpha$ , $\beta$ , $\gamma$	176.90Å 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 <sup>2</sup> )	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

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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

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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

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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 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	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

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 9.

All (101) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

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Atom-1	Atom-2	Distance(Å)	Clash(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:679:PRO:HD3	4:A:1095:HOH:O	2.01	0.59
1:A:584:ASP:HB2	4:A:1070:HOH:O	2.00	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:566:THR:HB	1:A:569:HIS:ND1	2.19	0.56
1:A:396:ILE:O	1:A:400:ILE:HG12	2.05	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:439:ASN:HD21	1:A:459:THR:HG23	1.72	0.55
1:A:394:GLU:HG3	1:A:513:GLY:HA3	1.89	0.55
1:A:62:LEU:O	1:A:196:GLU:HA	2.08	0.54
1:A:44:TYR:HA	1:A:47:LEU:HG	1.88	0.54
1:A:422:GLY:O	1:A:425:ILE:HG13	2.08	0.54
1:A:230:VAL:HA	1:A:263:ILE:HA	1.89	0.52
1:A:103:ILE:HD11	1:A:141:PRO:HB3	1.91	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:388:THR:HG22	1:A:415:ILE:CG2	2.42	0.50
1:A:115:ARG:HG2	1:A:119:ILE:HD12	1.94	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:647:SER:HB2	4:A:1056:HOH:O	2.12	0.49
1:A:546:LYS:HD2	4:A:1092:HOH:O	2.11	0.49
1:A:661:THR:O	1:A:681:THR:HA	2.11	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:330:LEU:HD22	1:A:332:HIS:CE1	2.48	0.48
1:A:181:VAL:HB	1:A:185:ASP:HB2	1.95	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:642:SER:HA	2:A:756:FLC:OA1	2.15	0.46
1:A:455:ALA:O	1:A:457:PRO:HD3	2.16	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:HA	1:A:675:GLN:HE21	1.81	0.45
1:A:430:ARG:NH2	1:A:439:ASN:HD21	2.14	0.45
1:A:123:VAL:O	1:A:126:PHE:HB3	2.17	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:351:ARG:HG3	1:A:439:ASN:HB2	2.00	0.44
1:A:65:ARG:NH2	1:A:194:PRO:HG3	2.32	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:129:THR:HG22	1:A:529:VAL:HG22	2.00	0.43
1:A:120:ASN:HB2	1:A:124:TYR:CE2	2.54	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:719:ASN:OD1	1:A:721:THR:HB	2.19	0.42
1:A:41:LYS:HE2	1:A:298:HIS:HA	2.01	0.42
1:A:113:LEU:HG	1:A:117:LYS:HE3	2.01	0.42
1:A:430:ARG:NH2	1:A:439:ASN:ND2	2.66	0.42
1:A:384:LYS:CD	1:A:476:GLY:HA3	2.49	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:671:ASN:O	1:A:675:GLN:HG2	2.20	0.42
1:A:325:PRO:HG2	1:A:326:PHE:CD2	2.55	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:439:ASN:ND2	1:A:459:THR:HG23	2.35	0.41
1:A:249:SER:HB2	1:A:504:GLU:HG3	2.02	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:561:VAL:HG11	1:A:565:CYS:HB2	2.02	0.40
1:A:110:GLU:OE2	1:A:111:LYS:HG3	2.22	0.40
1:A:713:CYS:HB2	1:A:727:LEU:HD11	2.03	0.40
1:A:490:LYS:HD3	4:A:957:HOH: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%)	697 (93%)	46 (6%)	8 (1%)	21	34

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
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%)	13	23

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
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

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Mol	Chain	Res	Type
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

Some 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
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 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 ⓘ

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	SF4	A	755	1,2,4	12,12,12	11.04	10 (83%)	0,24,24	0.00	-
2	FLC	A	756	3	5,12,12	2.71	3 (60%)	7,17,17	7.17	6 (85%)

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 (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	755	SF4	S4-FE2	25.81	2.50	2.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	755	SF4	S2-FE4	16.43	2.44	2.33
3	A	755	SF4	S4-FE3	15.45	2.43	2.33
3	A	755	SF4	S1-FE4	-8.82	2.27	2.33
3	A	755	SF4	S1-FE3	8.43	2.38	2.33
3	A	755	SF4	S2-FE1	7.27	2.38	2.33
3	A	755	SF4	S1-FE2	5.94	2.37	2.33
3	A	755	SF4	S2-FE3	5.55	2.37	2.33
2	A	756	FLC	CA-CB	-4.15	1.48	1.54
2	A	756	FLC	CG-CGC	2.92	1.51	1.49
3	A	755	SF4	S3-FE4	-2.92	2.31	2.33
3	A	755	SF4	S4-FE1	2.68	2.35	2.33
2	A	756	FLC	CG-CB	2.65	1.59	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	756	FLC	CB-CG-CGC	12.13	133.13	115.01
2	A	756	FLC	CB-CA-CAC	10.42	130.58	115.01
2	A	756	FLC	CA-CB-CBC	6.67	124.71	111.21
2	A	756	FLC	CG-CB-CA	-5.51	96.41	109.61
2	A	756	FLC	OHB-CB-CG	4.75	119.61	108.51
2	A	756	FLC	CG-CB-CBC	-2.30	106.57	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.