Full wwPDB X-ray Structure Validation Report (i)

Feb 24, 2024 – 02:05 PM EST

PDB ID	:	7ACN
Title	:	CRYSTAL STRUCTURES OF ACONITASE WITH ISOCITRATE AND NITROISOCITRATE BOUND
Authors	:	Lauble, H.; Kennedy, M.C.; Beinert, H.; Stout, C.D.
Deposited on	:	1991-05-15
Resolution	:	2.00 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

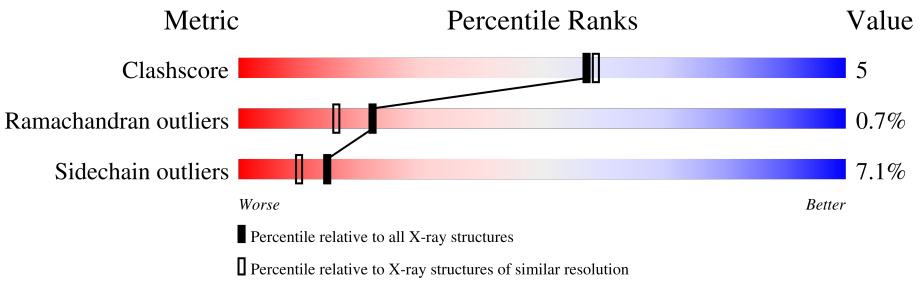
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	754	80% 15%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6174 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.

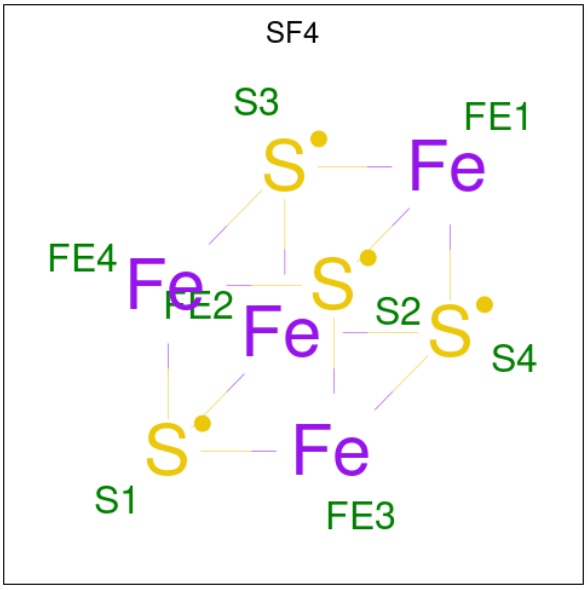
- Molecule 1 is a protein called ACONITASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	753	5815	3666	1034	1093	22	0	0	0

There is a discrepancy between the modelled and reference sequences:

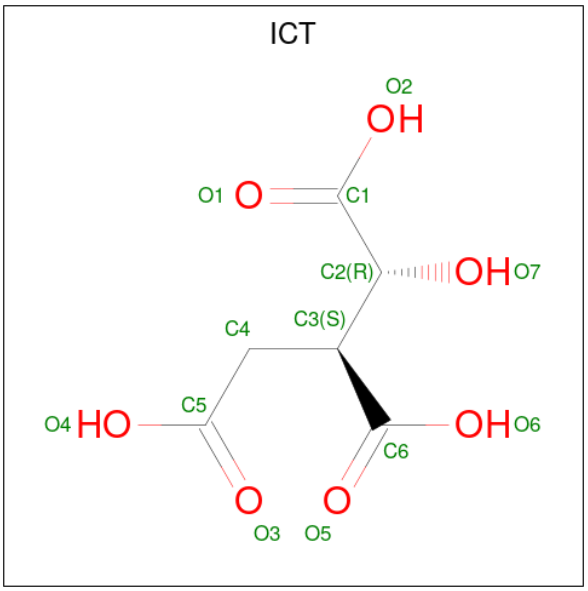
Chain	Residue	Modelled	Actual	Comment	Reference
A	647	SER	ARG	conflict	UNP P16276

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 3 is ISOCITRIC ACID (three-letter code: ICT) (formula: $C_6H_8O_7$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	338	338	338	0	0

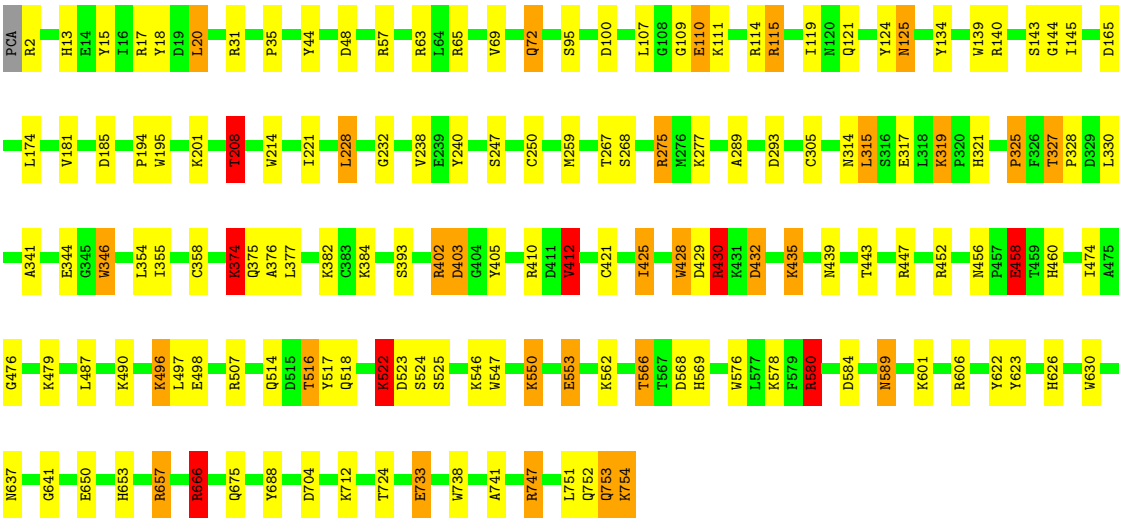
3 Residue-property plots (i)

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: ACONITASE

Chain A:



4 Data and refinement statistics (i)

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	185.50Å 72.00Å 73.00Å 90.00° 90.00° 77.70°	Depositor
Resolution (Å)	(Not available) – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.179 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6174	wwPDB-VP
Average B, all atoms ($Å^2$)	22.0	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: ICT, SF4

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	0.85	0/5942	1.61	89/8050 (1.1%)

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	2

There are no bond length outliers.

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	580	ARG	NE-CZ-NH1	27.17	133.89	120.30
1	A	580	ARG	NE-CZ-NH2	-22.54	109.03	120.30
1	A	402	ARG	NE-CZ-NH2	-18.78	110.91	120.30
1	A	430	ARG	NE-CZ-NH2	-18.33	111.13	120.30
1	A	430	ARG	NE-CZ-NH1	14.14	127.37	120.30
1	A	447	ARG	NE-CZ-NH2	-13.73	113.44	120.30
1	A	410	ARG	NE-CZ-NH1	12.39	126.50	120.30
1	A	666	ARG	NE-CZ-NH2	-11.93	114.34	120.30
1	A	402	ARG	NE-CZ-NH1	11.88	126.24	120.30
1	A	410	ARG	NE-CZ-NH2	-11.55	114.53	120.30
1	A	666	ARG	NE-CZ-NH1	10.70	125.65	120.30
1	A	346	TRP	CD1-CG-CD2	9.51	113.91	106.30
1	A	405	TYR	CB-CG-CD2	-9.37	115.38	121.00
1	A	195	TRP	CD1-CG-CD2	9.34	113.78	106.30
1	A	63	ARG	NE-CZ-NH2	-9.12	115.74	120.30
1	A	139	TRP	CD1-CG-CD2	9.02	113.51	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	325	PRO	CA-C-N	8.83	136.62	117.20
1	A	576	TRP	CD1-CG-CD2	8.64	113.21	106.30
1	A	452	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	A	630	TRP	CD1-CG-CD2	7.88	112.60	106.30
1	A	195	TRP	CE2-CD2-CG	-7.86	101.01	107.30
1	A	165	ASP	CB-CG-OD2	7.82	125.34	118.30
1	A	115	ARG	NE-CZ-NH2	-7.79	116.41	120.30
1	A	606	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	A	275	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	A	428	TRP	CD1-CG-CD2	7.70	112.46	106.30
1	A	606	ARG	NE-CZ-NH2	-7.65	116.47	120.30
1	A	346	TRP	CE2-CD2-CG	-7.57	101.25	107.30
1	A	738	TRP	CD1-CG-CD2	7.33	112.16	106.30
1	A	214	TRP	CD1-CG-CD2	7.27	112.12	106.30
1	A	576	TRP	CE2-CD2-CG	-7.25	101.50	107.30
1	A	522	LYS	CA-C-N	-7.22	101.32	117.20
1	A	139	TRP	CE2-CD2-CG	-7.20	101.54	107.30
1	A	630	TRP	CE2-CD2-CG	-7.19	101.55	107.30
1	A	458	GLU	OE1-CD-OE2	-7.14	114.73	123.30
1	A	747	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	A	428	TRP	CE2-CD2-CG	-6.87	101.80	107.30
1	A	44	TYR	CB-CG-CD2	-6.77	116.94	121.00
1	A	214	TRP	CE2-CD2-CG	-6.66	101.97	107.30
1	A	240	TYR	CB-CG-CD2	-6.65	117.01	121.00
1	A	195	TRP	CG-CD1-NE1	-6.63	103.47	110.10
1	A	517	TYR	CB-CG-CD1	-6.58	117.05	121.00
1	A	18	TYR	CB-CG-CD2	-6.53	117.08	121.00
1	A	738	TRP	CE2-CD2-CG	-6.53	102.08	107.30
1	A	57	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	A	403	ASP	CB-CG-OD2	6.49	124.14	118.30
1	A	566	THR	N-CA-CB	-6.40	98.14	110.30
1	A	63	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	A	547	TRP	CE2-CD2-CG	-6.28	102.28	107.30
1	A	547	TRP	CD1-CG-CD2	6.11	111.19	106.30
1	A	124	TYR	CB-CG-CD2	-5.99	117.41	121.00
1	A	507	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	A	346	TRP	CG-CD1-NE1	-5.97	104.13	110.10
1	A	630	TRP	CB-CG-CD1	-5.91	119.32	127.00
1	A	31	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	A	325	PRO	O-C-N	-5.87	113.31	122.70
1	A	31	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	733	GLU	OE1-CD-OE2	-5.83	116.31	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	139	TRP	CB-CG-CD1	-5.77	119.49	127.00
1	A	111	LYS	CD-CE-NZ	-5.76	98.45	111.70
1	A	134	TYR	CB-CG-CD1	-5.72	117.57	121.00
1	A	208	THR	N-CA-CB	-5.71	99.44	110.30
1	A	623	TYR	CB-CG-CD2	-5.71	117.57	121.00
1	A	325	PRO	N-CA-C	5.70	126.92	112.10
1	A	267	THR	CA-CB-CG2	5.63	120.28	112.40
1	A	57	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	A	452	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	100	ASP	CB-CG-OD1	5.58	123.32	118.30
1	A	115	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	374	LYS	CA-CB-CG	5.53	125.57	113.40
1	A	753	GLN	N-CA-C	5.45	125.72	111.00
1	A	688	TYR	CB-CG-CD1	-5.43	117.74	121.00
1	A	48	ASP	CB-CG-OD1	5.37	123.14	118.30
1	A	412	VAL	CB-CA-C	-5.34	101.25	111.40
1	A	630	TRP	CG-CD2-CE3	5.34	138.71	133.90
1	A	139	TRP	CG-CD1-NE1	-5.34	104.76	110.10
1	A	195	TRP	CG-CD2-CE3	5.32	138.69	133.90
1	A	657	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	A	576	TRP	CG-CD1-NE1	-5.20	104.90	110.10
1	A	432	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	630	TRP	CG-CD1-NE1	-5.17	104.93	110.10
1	A	2	ARG	N-CA-C	-5.17	97.05	111.00
1	A	429	ASP	CB-CG-OD1	5.15	122.94	118.30
1	A	738	TRP	CG-CD1-NE1	-5.11	104.99	110.10
1	A	553	GLU	CA-CB-CG	5.09	124.60	113.40
1	A	15	TYR	CB-CG-CD2	-5.09	117.95	121.00
1	A	293	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	641	GLY	CA-C-N	-5.09	106.00	117.20
1	A	410	ARG	CG-CD-NE	-5.03	101.25	111.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	580	ARG	Sidechain
1	A	666	ARG	Sidechain

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	5815	0	5804	57	0
2	A	8	0	0	0	0
3	A	13	0	4	2	0
4	A	338	0	0	1	0
All	All	6174	0	5808	57	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 5.

All (57) 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	1.31	0.77
1:A:430:ARG:HD2	1:A:432:ASP:OD1	1.88	0.73
1:A:566:THR:HG22	1:A:568:ASP:H	1.55	0.70
1:A:13:HIS:HB3	4:A:1202:HOH:O	1.95	0.65
1:A:622:TYR:O	1:A:626:HIS:HD2	1.83	0.62
1:A:221:ILE:HG12	1:A:259:MET:HB3	1.84	0.59
1:A:566:THR:HB	1:A:569:HIS:ND1	2.17	0.59
1:A:584:ASP:OD1	1:A:653:HIS:HE1	1.87	0.57
1:A:277:LYS:HG3	1:A:289:ALA:HB1	1.87	0.56
1:A:546:LYS:HD3	1:A:741:ALA:O	2.06	0.55
1:A:566:THR:HG22	1:A:568:ASP:N	2.22	0.55
1:A:430:ARG:HH22	1:A:439:ASN:ND2	2.01	0.54
1:A:712:LYS:HE2	1:A:724:THR:HG21	1.90	0.53
1:A:327:THR:HG22	1:A:328:PRO:HD2	1.90	0.52
1:A:402:ARG:HD2	1:A:403:ASP:OD1	2.09	0.52
1:A:580:ARG:HH22	3:A:755:ICT:C5	2.25	0.50
1:A:208:THR:O	1:A:315:LEU:HB2	2.12	0.50
1:A:17:ARG:HB3	1:A:20:LEU:HB2	1.94	0.50
1:A:208:THR:HG22	1:A:314:ASN:HA	1.93	0.50
1:A:319:LYS:O	1:A:321:HIS:HD2	1.96	0.48
1:A:341:ALA:HA	1:A:346:TRP:CE3	2.49	0.47
1:A:675:GLN:NE2	1:A:675:GLN:HA	2.28	0.47
1:A:522:LYS:HE3	1:A:522:LYS:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:LYS:HD2	1:A:456:ASN:HA	1.97	0.47
1:A:143:SER:HB3	1:A:516:THR:HB	1.98	0.46
1:A:376:ALA:HB2	1:A:474:ILE:HD13	1.98	0.45
1:A:374:LYS:HD2	1:A:375:GLN:HG3	1.98	0.45
1:A:69:VAL:O	1:A:95:SER:HA	2.16	0.45
1:A:752:GLN:O	1:A:754:LYS:HG3	2.17	0.45
1:A:589:ASN:ND2	1:A:650:GLU:OE1	2.50	0.45
1:A:145:ILE:HG21	1:A:358:CYS:HB3	1.99	0.44
1:A:174:LEU:HD13	1:A:250:CYS:SG	2.56	0.44
1:A:13:HIS:CD2	1:A:13:HIS:H	2.34	0.44
1:A:35:PRO:HB2	1:A:305:CYS:HA	1.99	0.43
1:A:458:GLU:OE1	1:A:460:HIS:HE1	2.01	0.43
1:A:435:LYS:HD3	1:A:435:LYS:HA	1.73	0.43
1:A:181:VAL:HB	1:A:185:ASP:HB2	1.99	0.43
1:A:384:LYS:HD3	1:A:476:GLY:HA3	2.00	0.43
1:A:144:GLY:HA3	1:A:393:SER:HA	2.01	0.43
1:A:428:TRP:CZ2	1:A:430:ARG:HD3	2.54	0.43
1:A:479:LYS:HE3	1:A:479:LYS:HB3	1.90	0.42
1:A:275:ARG:HA	1:A:275:ARG:HD2	1.92	0.42
1:A:550:LYS:HB2	1:A:550:LYS:NZ	2.34	0.42
1:A:110:GLU:O	1:A:114:ARG:HG3	2.19	0.42
1:A:140:ARG:HD3	1:A:518:GLN:OE1	2.20	0.42
1:A:72:GLN:NE2	3:A:755:ICT:H41	2.35	0.42
1:A:496:LYS:HE3	1:A:496:LYS:HB3	1.94	0.42
1:A:121:GLN:O	1:A:125:ASN:HB2	2.21	0.41
1:A:65:ARG:NH2	1:A:194:PRO:HG3	2.35	0.41
1:A:355:ILE:HD13	1:A:355:ILE:HG21	1.82	0.41
1:A:377:LEU:HG	1:A:412:VAL:HG13	2.02	0.41
1:A:421:CYS:HB2	1:A:425:ILE:HD11	2.01	0.41
1:A:115:ARG:HG2	1:A:119:ILE:HD12	2.03	0.40
1:A:228:LEU:O	1:A:232:GLY:HA3	2.20	0.40
1:A:238:VAL:O	1:A:268:SER:HA	2.21	0.40
1:A:354:LEU:HD13	1:A:443:THR:HG22	2.02	0.40
1:A:751:LEU:HD23	1:A:751:LEU:HA	1.90	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	751/754 (100%)	717 (96%)	29 (4%)	5 (1%)	22 16

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	524	SER
1	A	753	GLN
1	A	109	GLY
1	A	523	ASP
1	A	525	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%)	578 (93%)	44 (7%)	14 10

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	72	GLN
1	A	107	LEU
1	A	110	GLU
1	A	125	ASN
1	A	201	LYS

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Mol	Chain	Res	Type
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	325	PRO
1	A	327	THR
1	A	330	LEU
1	A	344	GLU
1	A	374	LYS
1	A	382	LYS
1	A	412	VAL
1	A	425	ILE
1	A	430	ARG
1	A	435	LYS
1	A	458	GLU
1	A	487	LEU
1	A	490	LYS
1	A	496	LYS
1	A	497	LEU
1	A	498	GLU
1	A	514	GLN
1	A	516	THR
1	A	522	LYS
1	A	550	LYS
1	A	553	GLU
1	A	562	LYS
1	A	578	LYS
1	A	589	ASN
1	A	601	LYS
1	A	637	ASN
1	A	657	ARG
1	A	666	ARG
1	A	704	ASP
1	A	733	GLU
1	A	747	ARG
1	A	754	LYS

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

Mol	Chain	Res	Type
1	A	13	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	626	HIS
1	A	637	ASN
1	A	653	HIS
1	A	671	ASN
1	A	675	GLN

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 monosaccharides 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	$\#\|Z\| > 2$
2	SF4	A	999	1,4,3	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ICT	A	755	2	12,12,12	1.46	3 (25%)	13,16,16	2.20	4 (30%)

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	SF4	A	999	1,4,3	-	-	0/6/5/5
3	ICT	A	755	2	-	5/16/16/16	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	755	ICT	C2-C1	-2.25	1.49	1.52
3	A	755	ICT	O6-C6	-2.16	1.23	1.30
3	A	755	ICT	O1-C1	2.08	1.28	1.22

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	755	ICT	O6-C6-O5	-4.00	115.02	124.09
3	A	755	ICT	O6-C6-C3	3.77	124.41	114.03
3	A	755	ICT	O3-C5-C4	-3.48	111.64	122.80
3	A	755	ICT	O4-C5-C4	3.42	125.02	114.07

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	755	ICT	C1-C2-C3-C4
3	A	755	ICT	O7-C2-C3-C4
3	A	755	ICT	C4-C3-C6-O6
3	A	755	ICT	C6-C3-C4-C5
3	A	755	ICT	C4-C3-C6-O5

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	755	ICT	2	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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.