



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:28 PM GMT

PDB ID : 1B0J  
Title : CRYSTAL STRUCTURE OF ACONITASE WITH ISOCITRATE  
Authors : Lloyd, S.J.; Lauble, H.; Prasad, G.S.; Stout, C.D.  
Deposited on : 1998-11-10  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

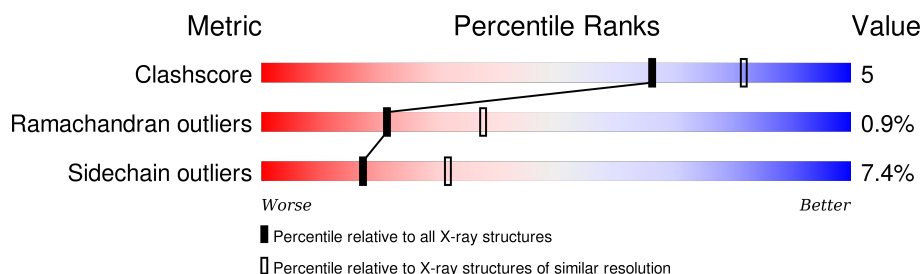
# 1 Overall quality at a glance

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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (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. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	754	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6153 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.

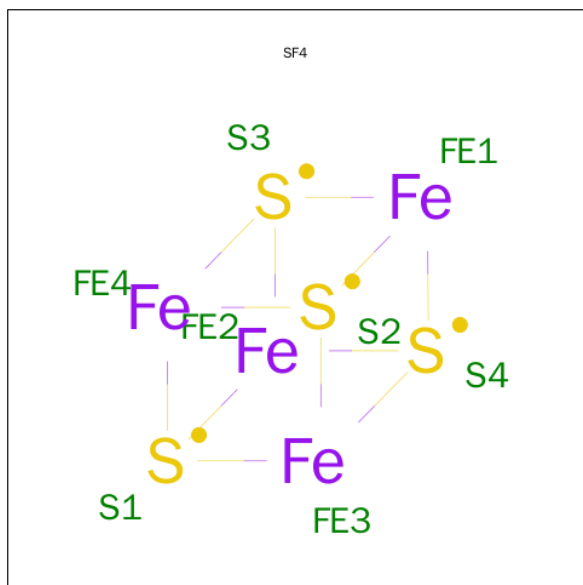
- Molecule 1 is a protein called ACONITATE HYDRATASE.

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:

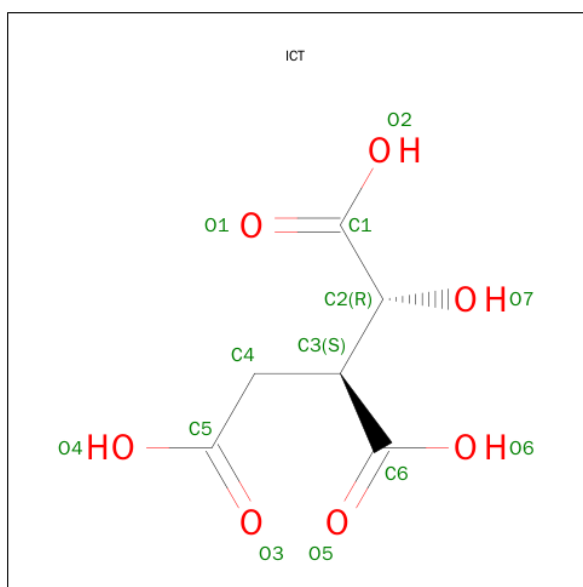
Chain	Residue	Modelled	Actual	Comment	Reference
A	642	ALA	SER	ENGINEERED	UNP P16276
A	648	ALA	ARG	CONFLICT	UNP P16276

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).



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

- Molecule 4 is water.

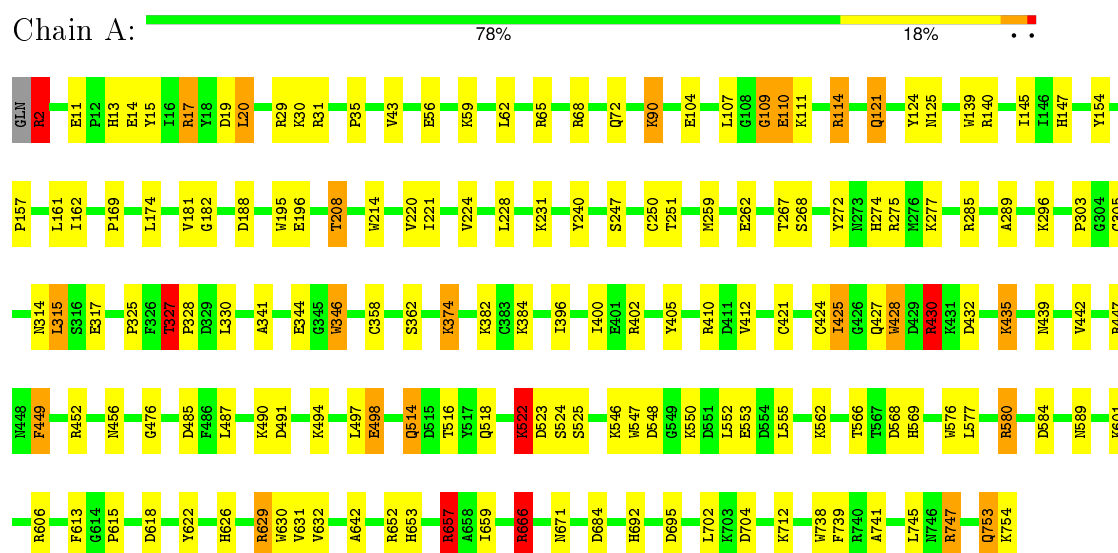
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	318	Total	O	0	0
			318	318		

### 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: ACONITATE HYDRATASE



## 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, $\alpha$ , $\beta$ , $\gamma$	187.40 Å   72.10 Å   73.90 Å 90.00°   90.00°   77.70°	Depositor
Resolution (Å)	20.00 – 2.50	Depositor
% Data completeness (in resolution range)	88.1 (20.00-2.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.162 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6153	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	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, ICT

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	0.88	0/5941	1.62	89/8049 (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	1

There are no bond length outliers.

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	580	ARG	NE-CZ-NH1	22.36	131.48	120.30
1	A	430	ARG	NE-CZ-NH2	-19.18	110.71	120.30
1	A	447	ARG	NE-CZ-NH2	-14.16	113.22	120.30
1	A	580	ARG	NE-CZ-NH2	-13.39	113.61	120.30
1	A	325	PRO	CA-C-N	10.44	140.17	117.20
1	A	410	ARG	NE-CZ-NH1	10.08	125.34	120.30
1	A	195	TRP	CD1-CG-CD2	9.99	114.29	106.30
1	A	402	ARG	NE-CZ-NH1	9.56	125.08	120.30
1	A	657	ARG	NE-CZ-NH2	-9.40	115.60	120.30
1	A	124	TYR	CB-CG-CD2	-9.12	115.53	121.00
1	A	31	ARG	NE-CZ-NH1	8.93	124.77	120.30
1	A	547	TRP	CD1-CG-CD2	8.80	113.34	106.30
1	A	31	ARG	NE-CZ-NH2	-8.73	115.94	120.30
1	A	17	ARG	NE-CZ-NH2	-8.64	115.98	120.30
1	A	240	TYR	CB-CG-CD2	-8.55	115.87	121.00
1	A	747	ARG	NE-CZ-NH2	-8.29	116.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	TRP	CE2-CD2-CG	-8.27	100.68	107.30
1	A	522	LYS	CA-C-N	-8.27	99.00	117.20
1	A	139	TRP	CD1-CG-CD2	8.23	112.88	106.30
1	A	430	ARG	NE-CZ-NH1	8.21	124.41	120.30
1	A	428	TRP	CD1-CG-CD2	8.20	112.86	106.30
1	A	666	ARG	NE-CZ-NH1	8.07	124.33	120.30
1	A	402	ARG	NE-CZ-NH2	-8.05	116.28	120.30
1	A	346	TRP	CD1-CG-CD2	7.98	112.69	106.30
1	A	410	ARG	NE-CZ-NH2	-7.95	116.33	120.30
1	A	738	TRP	CD1-CG-CD2	7.88	112.60	106.30
1	A	139	TRP	CE2-CD2-CG	-7.82	101.04	107.30
1	A	547	TRP	CE2-CD2-CG	-7.68	101.16	107.30
1	A	325	PRO	N-CA-C	7.46	131.50	112.10
1	A	154	TYR	CB-CG-CD1	-7.37	116.58	121.00
1	A	214	TRP	CE2-CD2-CG	-7.17	101.57	107.30
1	A	346	TRP	CE2-CD2-CG	-7.08	101.64	107.30
1	A	195	TRP	CG-CD1-NE1	-6.90	103.20	110.10
1	A	738	TRP	CE2-CD2-CG	-6.89	101.79	107.30
1	A	452	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	A	630	TRP	CD1-CG-CD2	6.83	111.76	106.30
1	A	15	TYR	CB-CG-CD2	-6.80	116.92	121.00
1	A	214	TRP	CD1-CG-CD2	6.78	111.72	106.30
1	A	747	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	A	124	TYR	CB-CG-CD1	6.68	125.01	121.00
1	A	325	PRO	CA-C-O	-6.54	104.51	120.20
1	A	428	TRP	CE2-CD2-CG	-6.51	102.09	107.30
1	A	285	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	A	547	TRP	CG-CD2-CE3	6.39	139.65	133.90
1	A	275	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	A	547	TRP	CG-CD1-NE1	-6.30	103.80	110.10
1	A	630	TRP	CE2-CD2-CG	-6.29	102.27	107.30
1	A	576	TRP	CD1-CG-CD2	6.23	111.28	106.30
1	A	498	GLU	CA-CB-CG	6.18	127.00	113.40
1	A	522	LYS	O-C-N	6.13	132.51	122.70
1	A	65	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	A	576	TRP	CE2-CD2-CG	-5.97	102.52	107.30
1	A	753	GLN	N-CA-C	5.81	126.69	111.00
1	A	188	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	A	327	THR	N-CA-CB	5.77	121.26	110.30
1	A	738	TRP	CG-CD1-NE1	-5.76	104.34	110.10
1	A	449	PHE	CB-CG-CD2	-5.74	116.78	120.80
1	A	2	ARG	NE-CZ-NH2	5.71	123.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2	ARG	N-CA-C	-5.71	95.58	111.00
1	A	90	LYS	CA-CB-CG	5.71	125.96	113.40
1	A	251	THR	CA-CB-CG2	-5.56	104.61	112.40
1	A	374	LYS	CA-CB-CG	5.56	125.63	113.40
1	A	447	ARG	CG-CD-NE	-5.46	100.33	111.80
1	A	428	TRP	CG-CD1-NE1	-5.46	104.64	110.10
1	A	139	TRP	CG-CD2-CE3	5.44	138.80	133.90
1	A	491	ASP	CB-CG-OD1	5.43	123.18	118.30
1	A	424	CYS	CA-C-N	5.39	129.07	117.20
1	A	514	GLN	CA-CB-CG	5.39	125.26	113.40
1	A	272	TYR	CB-CG-CD2	-5.36	117.78	121.00
1	A	275	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	43	VAL	CG1-CB-CG2	-5.34	102.36	110.90
1	A	738	TRP	CG-CD2-CE3	5.27	138.65	133.90
1	A	68	ARG	CA-CB-CG	5.27	125.00	113.40
1	A	695	ASP	CB-CG-OD1	5.26	123.03	118.30
1	A	447	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	485	ASP	CA-C-N	-5.22	105.71	117.20
1	A	114	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	A	59	LYS	CB-CG-CD	-5.18	98.12	111.60
1	A	231	LYS	CA-CB-CG	5.17	124.77	113.40
1	A	666	ARG	CA-CB-CG	5.16	124.76	113.40
1	A	548	ASP	CB-CG-OD1	5.14	122.93	118.30
1	A	161	LEU	CA-CB-CG	5.13	127.09	115.30
1	A	109	GLY	N-CA-C	5.09	125.83	113.10
1	A	684	ASP	CB-CG-OD1	5.07	122.86	118.30
1	A	29	ARG	CG-CD-NE	5.05	122.41	111.80
1	A	630	TRP	CG-CD2-CE3	5.03	138.42	133.90
1	A	139	TRP	CB-CG-CD1	-5.02	120.47	127.00
1	A	442	VAL	CG1-CB-CG2	-5.01	102.88	110.90
1	A	747	ARG	CA-CB-CG	5.00	124.40	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	666	ARG	Sidechain

## 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	5814	0	5804	57	0
2	A	8	0	0	1	0
3	A	13	0	5	2	0
4	A	318	0	0	6	0
All	All	6153	0	5809	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	1.30	0.79
1:A:430:ARG:HD2	1:A:432:ASP:OD1	1.96	0.66
1:A:566:THR:HG22	1:A:568:ASP:H	1.61	0.64
1:A:629:ARG:HG2	1:A:657:ARG:HD3	1.80	0.64
1:A:449:PHE:CD2	1:A:566:THR:HG21	2.36	0.60
1:A:642:ALA:HB1	3:A:756:ICT:H3	1.83	0.60
1:A:13:HIS:HB3	4:A:884:HOH:O	2.03	0.58
1:A:182:GLY:HA3	1:A:671:ASN:HD21	1.69	0.56
1:A:384:LYS:HD3	1:A:476:GLY:HA3	1.89	0.54
1:A:552:LEU:HB3	1:A:555:LEU:HD21	1.90	0.52
1:A:435:LYS:HD2	1:A:456:ASN:HB2	1.91	0.52
1:A:121:GLN:O	1:A:125:ASN:HB2	2.11	0.51
1:A:652:ARG:HD2	4:A:813:HOH:O	2.09	0.50
1:A:632:VAL:HB	1:A:659:ILE:HG23	1.92	0.50
1:A:622:TYR:O	1:A:626:HIS:HD2	1.95	0.49
1:A:208:THR:O	1:A:315:LEU:HB2	2.14	0.48
1:A:104:GLU:HA	1:A:427:GLN:HB3	1.95	0.48
1:A:147:HIS:HD2	1:A:358:CYS:SG	2.36	0.48
1:A:580:ARG:HH22	3:A:756:ICT:C5	2.27	0.48
1:A:174:LEU:HD13	1:A:250:CYS:SG	2.54	0.48
1:A:566:THR:HB	1:A:569:HIS:ND1	2.30	0.47
1:A:400:ILE:HB	1:A:405:TYR:HB2	1.97	0.47
1:A:430:ARG:NH2	1:A:439:ASN:HD21	2.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:THR:HG22	1:A:314:ASN:HA	1.96	0.46
1:A:17:ARG:HB3	1:A:20:LEU:HB2	1.96	0.46
1:A:384:LYS:O	1:A:384:LYS:HE2	2.15	0.46
1:A:274:HIS:HB3	4:A:1014:HOH:O	2.15	0.46
1:A:739:PHE:HB2	4:A:853:HOH:O	2.15	0.46
1:A:277:LYS:HG3	1:A:289:ALA:HB1	1.98	0.45
1:A:162:ILE:HD12	1:A:181:VAL:HG21	1.97	0.45
1:A:327:THR:HG22	1:A:328:PRO:HD2	1.99	0.45
1:A:546:LYS:HD3	1:A:741:ALA:O	2.17	0.45
1:A:145:ILE:HG21	1:A:358:CYS:HB3	2.00	0.44
1:A:425:ILE:H	1:A:425:ILE:HG13	1.63	0.44
1:A:341:ALA:HA	1:A:346:TRP:CE3	2.53	0.44
1:A:140:ARG:NH1	1:A:518:GLN:HB2	2.31	0.44
1:A:62:LEU:O	1:A:196:GLU:HA	2.18	0.44
1:A:35:PRO:HB2	1:A:305:CYS:HA	2.00	0.43
1:A:425:ILE:HG12	2:A:755:SF4:S4	2.59	0.43
1:A:303:PRO:HD2	4:A:821:HOH:O	2.18	0.43
1:A:221:ILE:HG12	1:A:259:MET:HB3	2.01	0.43
1:A:362:SER:HA	1:A:396:ILE:HD13	2.01	0.42
1:A:2:ARG:HD3	1:A:19:ASP:HB3	2.02	0.42
1:A:107:LEU:HD23	1:A:111:LYS:HD3	2.01	0.42
1:A:428:TRP:CZ2	1:A:430:ARG:HD3	2.55	0.42
1:A:421:CYS:HB2	1:A:425:ILE:HD11	2.01	0.42
1:A:220:VAL:O	1:A:224:VAL:HG23	2.20	0.42
1:A:615:PRO:HB2	1:A:618:ASP:OD1	2.20	0.41
1:A:110:GLU:O	1:A:114:ARG:HG3	2.20	0.41
1:A:745:LEU:HB2	4:A:1034:HOH:O	2.20	0.41
1:A:267:THR:OG1	1:A:268:SER:N	2.53	0.41
1:A:427:GLN:HE21	1:A:577:LEU:HD12	1.85	0.41
1:A:11:GLU:HB3	1:A:14:GLU:HG2	2.03	0.41
1:A:606:ARG:HB2	1:A:613:PHE:CZ	2.56	0.41
1:A:90:LYS:HE2	1:A:522:LYS:HD2	2.01	0.41
1:A:584:ASP:OD1	1:A:653:HIS:HE1	2.04	0.41
1:A:427:GLN:NE2	1:A:577:LEU:HD12	2.36	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%)	703 (94%)	41 (6%)	7 (1%)	21	37

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	524	SER
1	A	753	GLN
1	A	109	GLY
1	A	296	LYS
1	A	523	ASP
1	A	525	SER
1	A	157	PRO

### 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	621/622 (100%)	575 (93%)	46 (7%)	17	31

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	20	LEU
1	A	30	LYS
1	A	56	GLU

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Mol	Chain	Res	Type
1	A	72	GLN
1	A	110	GLU
1	A	121	GLN
1	A	169	PRO
1	A	208	THR
1	A	228	LEU
1	A	247	SER
1	A	262	GLU
1	A	315	LEU
1	A	317	GLU
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	487	LEU
1	A	490	LYS
1	A	494	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	589	ASN
1	A	601	LYS
1	A	629	ARG
1	A	631	VAL
1	A	657	ARG
1	A	666	ARG
1	A	692	HIS
1	A	702	LEU
1	A	704	ASP
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 (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	53	GLN
1	A	147	HIS
1	A	148	GLN
1	A	321	HIS
1	A	427	GLN
1	A	439	ASN
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

### 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
2	SF4	A	755	1,3,4	0,12,12	0.00	-	0,24,24	0.00	-
3	ICT	A	756	2	2,12,12	0.54	0	2,16,16	1.64	1 (50%)

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	755	1,3,4	-	0/0/48/48	2/6/5/5
3	ICT	A	756	2	-	0/6/16/16	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	A	756	ICT	O7-C2-C1	-2.16	105.77	111.21

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	755	SF4	FE1-FE2-S3-S4
2	A	755	SF4	FE3-FE4-S1-S2

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	755	SF4	1	0
3	A	756	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 ⓘ

### 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.