



wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 03:42 pm BST

PDB ID : 2QFW
Title : Crystal structure of *Saccharomyces cerevesiae* mitochondrial NADP(+)-dependent isocitrate dehydrogenase in complex with isocitrate
Authors : Peng, Y.J.; Ding, J.P.
Deposited on : 2007-06-28
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

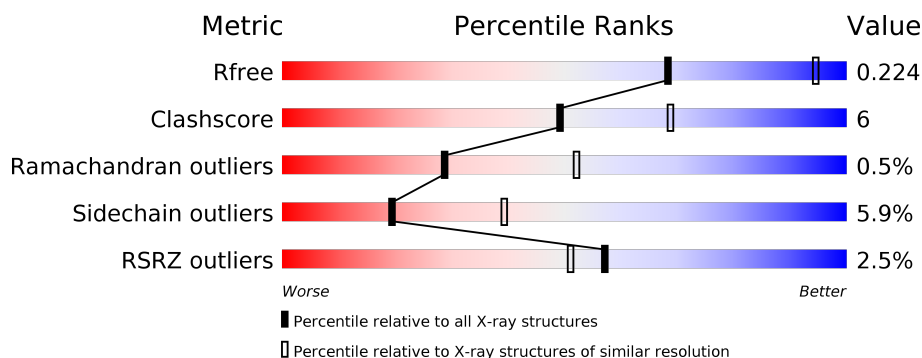
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	427	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 15%, green 79%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> % 79% 15% • 5% </div> </div>
1	B	427	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 15%, green 79%, grey 4%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> % 79% 15% • • </div> </div>
1	C	427	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 20%, green 75%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> 3% 75% 20% • • </div> </div>
1	D	427	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 17%, green 77%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> 3% 77% 17% • • </div> </div>
1	E	427	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 4%, orange 1%, yellow 17%, green 77%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> 4% 77% 17% • • </div> </div>
1	F	427	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 17%, green 78%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> 3% 78% 17% • • </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ICT	D	2104	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20688 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 Isocitrate dehydrogenase [NADP].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	0	0
			3222	2052	546	612	12			
1	B	408	Total	C	N	O	S	0	0	0
			3231	2058	548	613	12			
1	C	410	Total	C	N	O	S	0	0	0
			3245	2067	550	616	12			
1	D	412	Total	C	N	O	S	0	0	0
			3261	2079	552	618	12			
1	E	409	Total	C	N	O	S	0	0	0
			3237	2061	549	615	12			
1	F	411	Total	C	N	O	S	0	0	0
			3256	2076	551	617	12			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	EXPRESSION TAG	UNP P21954
A	-12	HIS	-	EXPRESSION TAG	UNP P21954
A	-11	HIS	-	EXPRESSION TAG	UNP P21954
A	-10	HIS	-	EXPRESSION TAG	UNP P21954
A	-9	HIS	-	EXPRESSION TAG	UNP P21954
A	-8	HIS	-	EXPRESSION TAG	UNP P21954
A	-7	HIS	-	EXPRESSION TAG	UNP P21954
A	-6	ALA	-	EXPRESSION TAG	UNP P21954
A	-5	MET	-	EXPRESSION TAG	UNP P21954
A	-4	GLY	-	EXPRESSION TAG	UNP P21954
A	-3	ILE	-	EXPRESSION TAG	UNP P21954
A	-2	PRO	-	EXPRESSION TAG	UNP P21954
A	-1	GLY	-	EXPRESSION TAG	UNP P21954
A	0	HIS	-	EXPRESSION TAG	UNP P21954
B	-13	MET	-	EXPRESSION TAG	UNP P21954
B	-12	HIS	-	EXPRESSION TAG	UNP P21954
B	-11	HIS	-	EXPRESSION TAG	UNP P21954

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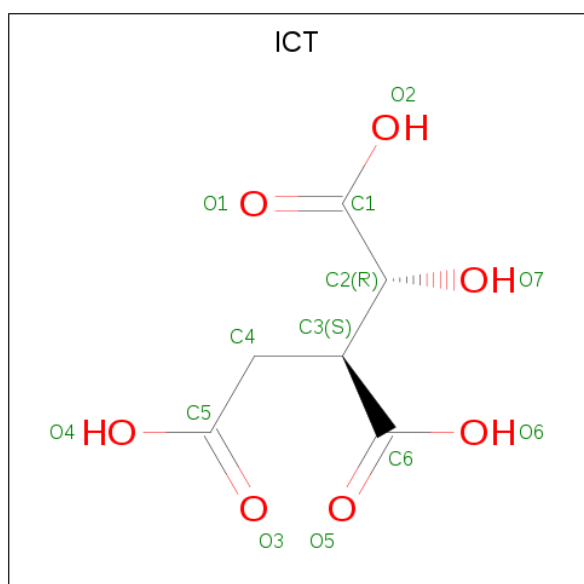
Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	HIS	-	EXPRESSION TAG	UNP P21954
B	-9	HIS	-	EXPRESSION TAG	UNP P21954
B	-8	HIS	-	EXPRESSION TAG	UNP P21954
B	-7	HIS	-	EXPRESSION TAG	UNP P21954
B	-6	ALA	-	EXPRESSION TAG	UNP P21954
B	-5	MET	-	EXPRESSION TAG	UNP P21954
B	-4	GLY	-	EXPRESSION TAG	UNP P21954
B	-3	ILE	-	EXPRESSION TAG	UNP P21954
B	-2	PRO	-	EXPRESSION TAG	UNP P21954
B	-1	GLY	-	EXPRESSION TAG	UNP P21954
B	0	HIS	-	EXPRESSION TAG	UNP P21954
C	-13	MET	-	EXPRESSION TAG	UNP P21954
C	-12	HIS	-	EXPRESSION TAG	UNP P21954
C	-11	HIS	-	EXPRESSION TAG	UNP P21954
C	-10	HIS	-	EXPRESSION TAG	UNP P21954
C	-9	HIS	-	EXPRESSION TAG	UNP P21954
C	-8	HIS	-	EXPRESSION TAG	UNP P21954
C	-7	HIS	-	EXPRESSION TAG	UNP P21954
C	-6	ALA	-	EXPRESSION TAG	UNP P21954
C	-5	MET	-	EXPRESSION TAG	UNP P21954
C	-4	GLY	-	EXPRESSION TAG	UNP P21954
C	-3	ILE	-	EXPRESSION TAG	UNP P21954
C	-2	PRO	-	EXPRESSION TAG	UNP P21954
C	-1	GLY	-	EXPRESSION TAG	UNP P21954
C	0	HIS	-	EXPRESSION TAG	UNP P21954
D	-13	MET	-	EXPRESSION TAG	UNP P21954
D	-12	HIS	-	EXPRESSION TAG	UNP P21954
D	-11	HIS	-	EXPRESSION TAG	UNP P21954
D	-10	HIS	-	EXPRESSION TAG	UNP P21954
D	-9	HIS	-	EXPRESSION TAG	UNP P21954
D	-8	HIS	-	EXPRESSION TAG	UNP P21954
D	-7	HIS	-	EXPRESSION TAG	UNP P21954
D	-6	ALA	-	EXPRESSION TAG	UNP P21954
D	-5	MET	-	EXPRESSION TAG	UNP P21954
D	-4	GLY	-	EXPRESSION TAG	UNP P21954
D	-3	ILE	-	EXPRESSION TAG	UNP P21954
D	-2	PRO	-	EXPRESSION TAG	UNP P21954
D	-1	GLY	-	EXPRESSION TAG	UNP P21954
D	0	HIS	-	EXPRESSION TAG	UNP P21954
E	-13	MET	-	EXPRESSION TAG	UNP P21954
E	-12	HIS	-	EXPRESSION TAG	UNP P21954
E	-11	HIS	-	EXPRESSION TAG	UNP P21954

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-10	HIS	-	EXPRESSION TAG	UNP P21954
E	-9	HIS	-	EXPRESSION TAG	UNP P21954
E	-8	HIS	-	EXPRESSION TAG	UNP P21954
E	-7	HIS	-	EXPRESSION TAG	UNP P21954
E	-6	ALA	-	EXPRESSION TAG	UNP P21954
E	-5	MET	-	EXPRESSION TAG	UNP P21954
E	-4	GLY	-	EXPRESSION TAG	UNP P21954
E	-3	ILE	-	EXPRESSION TAG	UNP P21954
E	-2	PRO	-	EXPRESSION TAG	UNP P21954
E	-1	GLY	-	EXPRESSION TAG	UNP P21954
E	0	HIS	-	EXPRESSION TAG	UNP P21954
F	-13	MET	-	EXPRESSION TAG	UNP P21954
F	-12	HIS	-	EXPRESSION TAG	UNP P21954
F	-11	HIS	-	EXPRESSION TAG	UNP P21954
F	-10	HIS	-	EXPRESSION TAG	UNP P21954
F	-9	HIS	-	EXPRESSION TAG	UNP P21954
F	-8	HIS	-	EXPRESSION TAG	UNP P21954
F	-7	HIS	-	EXPRESSION TAG	UNP P21954
F	-6	ALA	-	EXPRESSION TAG	UNP P21954
F	-5	MET	-	EXPRESSION TAG	UNP P21954
F	-4	GLY	-	EXPRESSION TAG	UNP P21954
F	-3	ILE	-	EXPRESSION TAG	UNP P21954
F	-2	PRO	-	EXPRESSION TAG	UNP P21954
F	-1	GLY	-	EXPRESSION TAG	UNP P21954
F	0	HIS	-	EXPRESSION TAG	UNP P21954

- Molecule 2 is ISOCITRIC ACID (three-letter code: ICT) (formula: C₆H₈O₇).

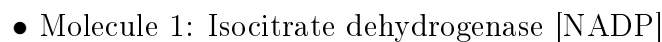
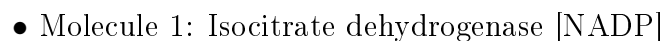


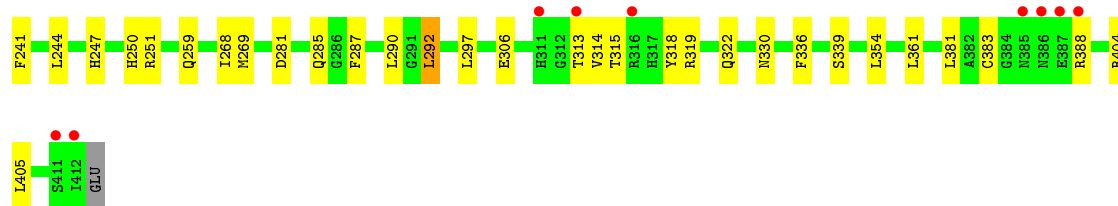
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 13 6 7	0	0
2	B	1	Total C O 13 6 7	0	0
2	C	1	Total C O 13 6 7	0	0
2	D	1	Total C O 13 6 7	0	0
2	E	1	Total C O 13 6 7	0	0
2	F	1	Total C O 13 6 7	0	0

- Molecule 3 is water.

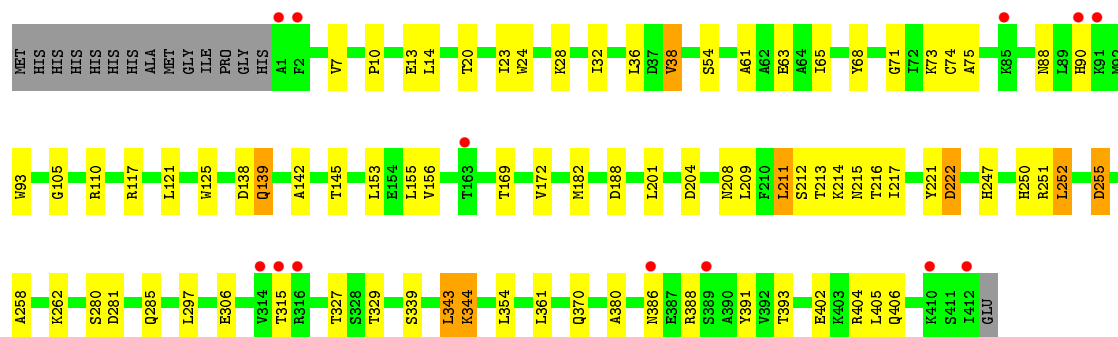
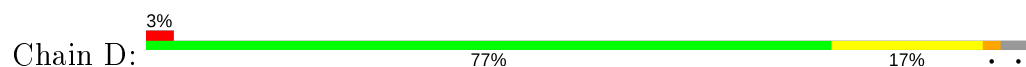
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	217	Total O 217 217	0	0
3	B	252	Total O 252 252	0	0
3	C	161	Total O 161 161	0	0
3	D	185	Total O 185 185	0	0
3	E	163	Total O 163 163	0	0
3	F	180	Total O 180 180	0	0

- Molecule 1: Isocitrate dehydrogenase [NADP]

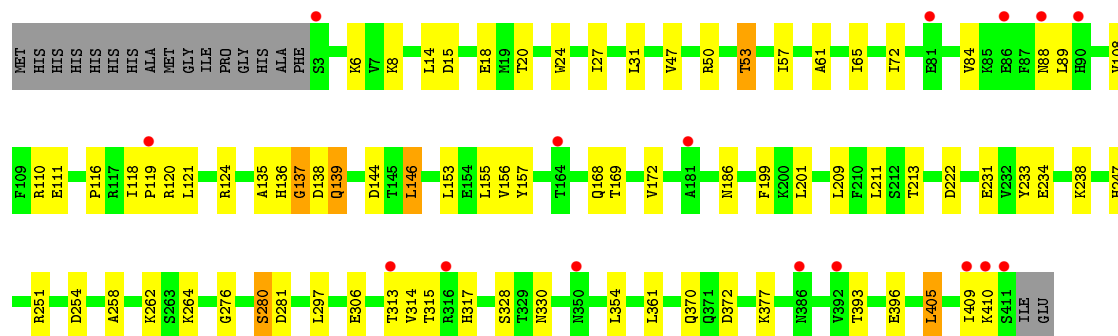
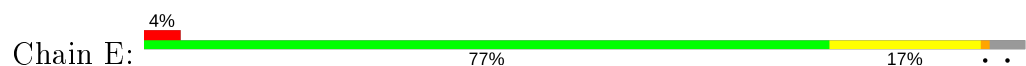




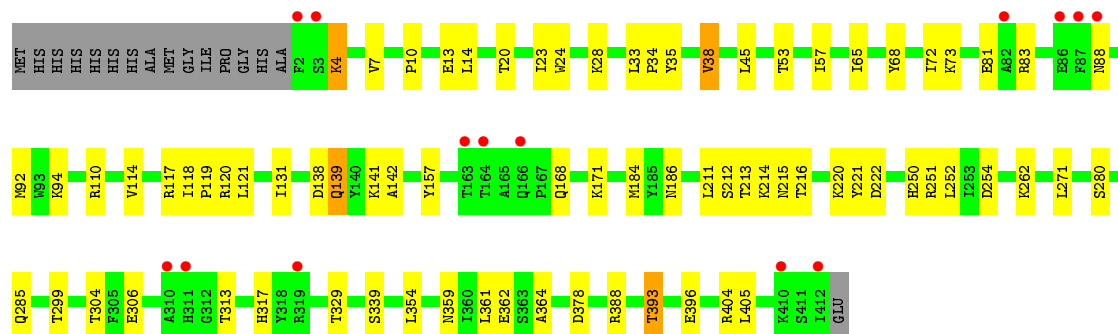
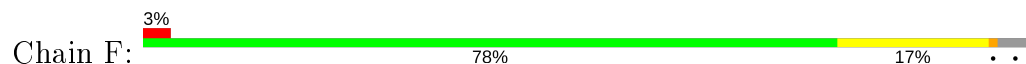
• Molecule 1: Isocitrate dehydrogenase [NADP]



• Molecule 1: Isocitrate dehydrogenase [NADP]



• Molecule 1: Isocitrate dehydrogenase [NADP]



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.70Å 97.89Å 190.65Å 90.00° 98.95° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 19.79 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.4 (20.00-2.60) 98.4 (19.79-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.59Å)	Xtriage
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.232 , 0.292 0.224 , 0.224	Depositor DCC
R_{free} test set	4114 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	44.4	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	20688	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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

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	0.29	0/3284	0.64	0/4431
1	B	0.29	0/3293	0.63	1/4442 (0.0%)
1	C	0.29	0/3307	0.64	2/4461 (0.0%)
1	D	0.29	0/3324	0.64	3/4484 (0.1%)
1	E	0.29	0/3299	0.64	1/4450 (0.0%)
1	F	0.29	0/3319	0.64	0/4477
All	All	0.29	0/19826	0.64	7/26745 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	188	ASP	CB-CG-OD2	5.62	123.36	118.30
1	C	37	ASP	CB-CG-OD2	5.51	123.25	118.30
1	D	281	ASP	CB-CG-OD2	5.49	123.24	118.30
1	C	188	ASP	CB-CG-OD2	5.24	123.01	118.30
1	D	222	ASP	CB-CG-OD2	5.23	123.01	118.30

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	3222	0	3264	33	0
1	B	3231	0	3277	34	0
1	C	3245	0	3293	49	0
1	D	3261	0	3310	50	0
1	E	3237	0	3282	39	0
1	F	3256	0	3302	44	0
2	A	13	0	5	1	0
2	B	13	0	5	0	0
2	C	13	0	5	0	0
2	D	13	0	5	0	0
2	E	13	0	5	0	0
2	F	13	0	5	0	0
3	A	217	0	0	1	0
3	B	252	0	0	1	0
3	C	161	0	0	1	0
3	D	185	0	0	2	0
3	E	163	0	0	4	0
3	F	180	0	0	2	0
All	All	20688	0	19758	233	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 6.

The worst 5 of 233 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:C:18:GLU:HB2	1:C:313:THR:HG21	1.19	1.15
1:C:238:LYS:HD2	1:C:239:SER:H	1.31	0.92
1:C:180:VAL:HG21	1:D:221:TYR:HA	1.59	0.85
1:A:117:ARG:H	1:A:370:GLN:HE22	1.25	0.84
1:D:214:LYS:HE3	1:D:217:ILE:HD13	1.60	0.83

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	405/427 (95%)	388 (96%)	14 (4%)	3 (1%)	22	43
1	B	406/427 (95%)	390 (96%)	15 (4%)	1 (0%)	47	71
1	C	408/427 (96%)	385 (94%)	21 (5%)	2 (0%)	29	52
1	D	410/427 (96%)	393 (96%)	15 (4%)	2 (0%)	29	52
1	E	407/427 (95%)	379 (93%)	25 (6%)	3 (1%)	22	43
1	F	409/427 (96%)	390 (95%)	17 (4%)	2 (0%)	29	52
All	All	2445/2562 (95%)	2325 (95%)	107 (4%)	13 (0%)	29	52

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	314	VAL
1	A	136	HIS
1	C	292	LEU
1	D	90	HIS

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	351/367 (96%)	328 (93%)	23 (7%)	16	33
1	B	352/367 (96%)	331 (94%)	21 (6%)	19	39
1	C	354/367 (96%)	335 (95%)	19 (5%)	22	44
1	D	355/367 (97%)	333 (94%)	22 (6%)	18	37
1	E	353/367 (96%)	329 (93%)	24 (7%)	16	32
1	F	355/367 (97%)	339 (96%)	16 (4%)	27	52
All	All	2120/2202 (96%)	1995 (94%)	125 (6%)	19	39

5 of 125 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	330	ASN
1	D	201	LEU
1	F	171	LYS
1	C	361	LEU
1	D	38	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	285	GLN
1	C	330	ASN
1	F	259	GLN
1	C	322	GLN
1	D	208	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](#)

6 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	ICT	A	2101	-	2,12,12	0.39	0	5,16,16	0.96	0
2	ICT	E	2105	-	2,12,12	0.40	0	5,16,16	0.89	0
2	ICT	D	2104	-	2,12,12	0.40	0	5,16,16	0.89	0
2	ICT	F	2106	-	2,12,12	0.39	0	5,16,16	0.50	0
2	ICT	C	2103	-	2,12,12	0.36	0	5,16,16	1.37	1 (20%)
2	ICT	B	2102	-	2,12,12	0.44	0	5,16,16	0.57	0

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	ICT	A	2101	-	-	3/6/16/16	-
2	ICT	E	2105	-	-	0/6/16/16	-
2	ICT	D	2104	-	-	0/6/16/16	-
2	ICT	F	2106	-	-	4/6/16/16	-
2	ICT	C	2103	-	-	0/6/16/16	-
2	ICT	B	2102	-	-	4/6/16/16	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2103	ICT	C1-C2-C3	-2.97	108.91	112.25

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2102	ICT	O7-C2-C3-C4
2	A	2101	ICT	C1-C2-C3-C6
2	F	2106	ICT	C1-C2-C3-C6
2	B	2102	ICT	C1-C2-C3-C6
2	A	2101	ICT	O7-C2-C3-C4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2101	ICT	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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	407/427 (95%)	-0.09	4 (0%) 82 80	34, 43, 72, 81	0
1	B	408/427 (95%)	-0.15	3 (0%) 87 86	29, 42, 70, 90	0
1	C	410/427 (96%)	0.12	12 (2%) 51 45	36, 50, 80, 116	0
1	D	412/427 (96%)	0.12	13 (3%) 47 40	34, 50, 83, 97	0
1	E	409/427 (95%)	0.22	16 (3%) 39 32	39, 52, 86, 116	0
1	F	411/427 (96%)	0.06	14 (3%) 45 38	33, 48, 79, 101	0
All	All	2457/2562 (95%)	0.05	62 (2%) 57 51	29, 47, 80, 116	0

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	ALA	6.6
1	D	2	PHE	4.5
1	E	3	SER	4.4
1	F	2	PHE	4.4
1	A	314	VAL	4.3

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ICT	D	2104	13/13	0.50	0.47	96,100,101,101	0
2	ICT	F	2106	13/13	0.69	0.26	81,82,84,84	0
2	ICT	B	2102	13/13	0.76	0.28	76,80,81,81	0
2	ICT	E	2105	13/13	0.82	0.26	75,76,77,77	0
2	ICT	C	2103	13/13	0.88	0.20	54,55,56,58	0
2	ICT	A	2101	13/13	0.90	0.18	43,48,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.