



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 02:48 PM BST

PDB ID : 5UQQ  
Title : Crystal structure of 2-methylcitrate synthase from *Aspergillus fumigatus*  
Authors : Schlachter, C.; Chruszcz, M.  
Deposited on : 2017-02-08  
Resolution : 2.30 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

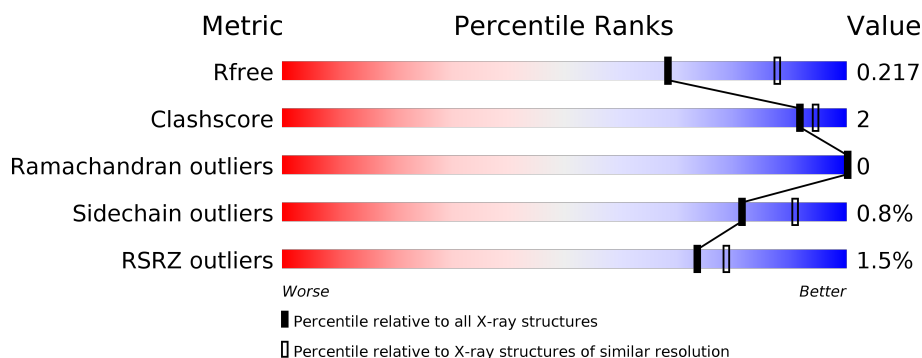
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 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	462	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>5%</div> <div>6%</div> </div> </div>
1	B	462	<div> <div></div> <div>91%</div> <div>6%</div> </div>
1	C	462	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>6%</div> <div>5%</div> </div> </div>
1	D	462	<div> <div></div> <div>87%</div> <div>7%</div> <div>6%</div> </div>
1	E	462	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>5%</div> <div>6%</div> </div> </div>
1	F	462	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>6%</div> <div>6%</div> </div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 21794 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 2-methylcitrate synthase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	436	Total	C	N	O	S	0	1	0
			3402	2179	589	625	9			
1	C	437	Total	C	N	O	S	11	2	0
			3421	2193	592	627	9			
1	A	435	Total	C	N	O	S	0	1	0
			3376	2162	583	622	9			
1	D	434	Total	C	N	O	S	0	2	0
			3391	2172	585	624	10			
1	E	434	Total	C	N	O	S	0	1	0
			3380	2167	584	620	9			
1	F	435	Total	C	N	O	S	0	0	0
			3365	2156	579	621	9			

There are 150 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	4	MET	-	initiating methionine	UNP Q50I20
B	5	HIS	-	expression tag	UNP Q50I20
B	6	HIS	-	expression tag	UNP Q50I20
B	7	HIS	-	expression tag	UNP Q50I20
B	8	HIS	-	expression tag	UNP Q50I20
B	9	HIS	-	expression tag	UNP Q50I20
B	10	HIS	-	expression tag	UNP Q50I20
B	11	SER	-	expression tag	UNP Q50I20
B	12	SER	-	expression tag	UNP Q50I20
B	13	GLY	-	expression tag	UNP Q50I20
B	14	VAL	-	expression tag	UNP Q50I20
B	15	ASP	-	expression tag	UNP Q50I20
B	16	LEU	-	expression tag	UNP Q50I20
B	17	GLY	-	expression tag	UNP Q50I20
B	18	THR	-	expression tag	UNP Q50I20
B	19	GLU	-	expression tag	UNP Q50I20
B	20	ASN	-	expression tag	UNP Q50I20

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Chain	Residue	Modelled	Actual	Comment	Reference
B	21	LEU	-	expression tag	UNP Q50I20
B	22	TYR	-	expression tag	UNP Q50I20
B	23	PHE	-	expression tag	UNP Q50I20
B	24	GLN	-	expression tag	UNP Q50I20
B	25	SER	-	expression tag	UNP Q50I20
B	26	GLY	-	expression tag	UNP Q50I20
B	27	SER	-	expression tag	UNP Q50I20
B	28	GLY	-	expression tag	UNP Q50I20
C	4	MET	-	initiating methionine	UNP Q50I20
C	5	HIS	-	expression tag	UNP Q50I20
C	6	HIS	-	expression tag	UNP Q50I20
C	7	HIS	-	expression tag	UNP Q50I20
C	8	HIS	-	expression tag	UNP Q50I20
C	9	HIS	-	expression tag	UNP Q50I20
C	10	HIS	-	expression tag	UNP Q50I20
C	11	SER	-	expression tag	UNP Q50I20
C	12	SER	-	expression tag	UNP Q50I20
C	13	GLY	-	expression tag	UNP Q50I20
C	14	VAL	-	expression tag	UNP Q50I20
C	15	ASP	-	expression tag	UNP Q50I20
C	16	LEU	-	expression tag	UNP Q50I20
C	17	GLY	-	expression tag	UNP Q50I20
C	18	THR	-	expression tag	UNP Q50I20
C	19	GLU	-	expression tag	UNP Q50I20
C	20	ASN	-	expression tag	UNP Q50I20
C	21	LEU	-	expression tag	UNP Q50I20
C	22	TYR	-	expression tag	UNP Q50I20
C	23	PHE	-	expression tag	UNP Q50I20
C	24	GLN	-	expression tag	UNP Q50I20
C	25	SER	-	expression tag	UNP Q50I20
C	26	GLY	-	expression tag	UNP Q50I20
C	27	SER	-	expression tag	UNP Q50I20
C	28	GLY	-	expression tag	UNP Q50I20
A	4	MET	-	initiating methionine	UNP Q50I20
A	5	HIS	-	expression tag	UNP Q50I20
A	6	HIS	-	expression tag	UNP Q50I20
A	7	HIS	-	expression tag	UNP Q50I20
A	8	HIS	-	expression tag	UNP Q50I20
A	9	HIS	-	expression tag	UNP Q50I20
A	10	HIS	-	expression tag	UNP Q50I20
A	11	SER	-	expression tag	UNP Q50I20
A	12	SER	-	expression tag	UNP Q50I20

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Chain	Residue	Modelled	Actual	Comment	Reference
A	13	GLY	-	expression tag	UNP Q50I20
A	14	VAL	-	expression tag	UNP Q50I20
A	15	ASP	-	expression tag	UNP Q50I20
A	16	LEU	-	expression tag	UNP Q50I20
A	17	GLY	-	expression tag	UNP Q50I20
A	18	THR	-	expression tag	UNP Q50I20
A	19	GLU	-	expression tag	UNP Q50I20
A	20	ASN	-	expression tag	UNP Q50I20
A	21	LEU	-	expression tag	UNP Q50I20
A	22	TYR	-	expression tag	UNP Q50I20
A	23	PHE	-	expression tag	UNP Q50I20
A	24	GLN	-	expression tag	UNP Q50I20
A	25	SER	-	expression tag	UNP Q50I20
A	26	GLY	-	expression tag	UNP Q50I20
A	27	SER	-	expression tag	UNP Q50I20
A	28	GLY	-	expression tag	UNP Q50I20
D	4	MET	-	initiating methionine	UNP Q50I20
D	5	HIS	-	expression tag	UNP Q50I20
D	6	HIS	-	expression tag	UNP Q50I20
D	7	HIS	-	expression tag	UNP Q50I20
D	8	HIS	-	expression tag	UNP Q50I20
D	9	HIS	-	expression tag	UNP Q50I20
D	10	HIS	-	expression tag	UNP Q50I20
D	11	SER	-	expression tag	UNP Q50I20
D	12	SER	-	expression tag	UNP Q50I20
D	13	GLY	-	expression tag	UNP Q50I20
D	14	VAL	-	expression tag	UNP Q50I20
D	15	ASP	-	expression tag	UNP Q50I20
D	16	LEU	-	expression tag	UNP Q50I20
D	17	GLY	-	expression tag	UNP Q50I20
D	18	THR	-	expression tag	UNP Q50I20
D	19	GLU	-	expression tag	UNP Q50I20
D	20	ASN	-	expression tag	UNP Q50I20
D	21	LEU	-	expression tag	UNP Q50I20
D	22	TYR	-	expression tag	UNP Q50I20
D	23	PHE	-	expression tag	UNP Q50I20
D	24	GLN	-	expression tag	UNP Q50I20
D	25	SER	-	expression tag	UNP Q50I20
D	26	GLY	-	expression tag	UNP Q50I20
D	27	SER	-	expression tag	UNP Q50I20
D	28	GLY	-	expression tag	UNP Q50I20
E	4	MET	-	initiating methionine	UNP Q50I20

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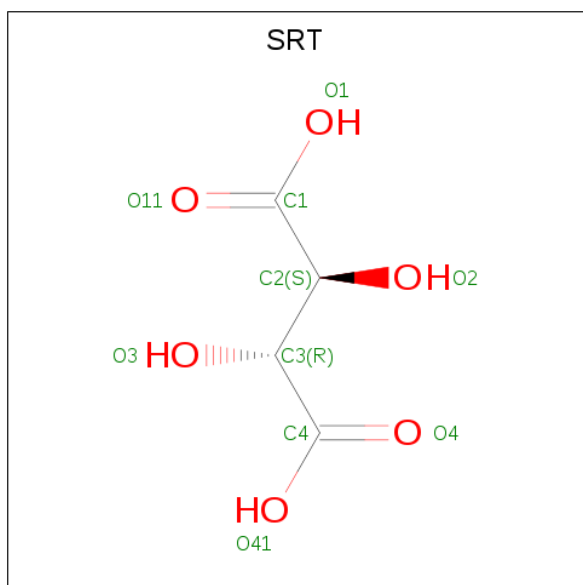
Chain	Residue	Modelled	Actual	Comment	Reference
E	5	HIS	-	expression tag	UNP Q50I20
E	6	HIS	-	expression tag	UNP Q50I20
E	7	HIS	-	expression tag	UNP Q50I20
E	8	HIS	-	expression tag	UNP Q50I20
E	9	HIS	-	expression tag	UNP Q50I20
E	10	HIS	-	expression tag	UNP Q50I20
E	11	SER	-	expression tag	UNP Q50I20
E	12	SER	-	expression tag	UNP Q50I20
E	13	GLY	-	expression tag	UNP Q50I20
E	14	VAL	-	expression tag	UNP Q50I20
E	15	ASP	-	expression tag	UNP Q50I20
E	16	LEU	-	expression tag	UNP Q50I20
E	17	GLY	-	expression tag	UNP Q50I20
E	18	THR	-	expression tag	UNP Q50I20
E	19	GLU	-	expression tag	UNP Q50I20
E	20	ASN	-	expression tag	UNP Q50I20
E	21	LEU	-	expression tag	UNP Q50I20
E	22	TYR	-	expression tag	UNP Q50I20
E	23	PHE	-	expression tag	UNP Q50I20
E	24	GLN	-	expression tag	UNP Q50I20
E	25	SER	-	expression tag	UNP Q50I20
E	26	GLY	-	expression tag	UNP Q50I20
E	27	SER	-	expression tag	UNP Q50I20
E	28	GLY	-	expression tag	UNP Q50I20
F	4	MET	-	initiating methionine	UNP Q50I20
F	5	HIS	-	expression tag	UNP Q50I20
F	6	HIS	-	expression tag	UNP Q50I20
F	7	HIS	-	expression tag	UNP Q50I20
F	8	HIS	-	expression tag	UNP Q50I20
F	9	HIS	-	expression tag	UNP Q50I20
F	10	HIS	-	expression tag	UNP Q50I20
F	11	SER	-	expression tag	UNP Q50I20
F	12	SER	-	expression tag	UNP Q50I20
F	13	GLY	-	expression tag	UNP Q50I20
F	14	VAL	-	expression tag	UNP Q50I20
F	15	ASP	-	expression tag	UNP Q50I20
F	16	LEU	-	expression tag	UNP Q50I20
F	17	GLY	-	expression tag	UNP Q50I20
F	18	THR	-	expression tag	UNP Q50I20
F	19	GLU	-	expression tag	UNP Q50I20
F	20	ASN	-	expression tag	UNP Q50I20
F	21	LEU	-	expression tag	UNP Q50I20

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Chain	Residue	Modelled	Actual	Comment	Reference
F	22	TYR	-	expression tag	UNP Q50I20
F	23	PHE	-	expression tag	UNP Q50I20
F	24	GLN	-	expression tag	UNP Q50I20
F	25	SER	-	expression tag	UNP Q50I20
F	26	GLY	-	expression tag	UNP Q50I20
F	27	SER	-	expression tag	UNP Q50I20
F	28	GLY	-	expression tag	UNP Q50I20

- Molecule 2 is S,R MESO-TARTARIC ACID (three-letter code: SRT) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			10	4	6		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	337	Total	O	0	0
			337	337		
3	C	286	Total	O	0	0
			286	286		
3	A	277	Total	O	0	0
			277	277		
3	D	300	Total	O	0	0
			300	300		
3	E	106	Total	O	0	0
			106	106		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	143	Total 143	O 143	0	0

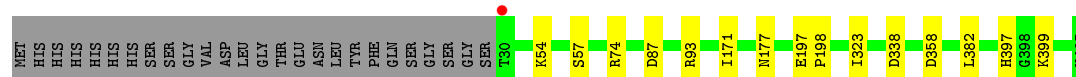


### 3 Residue-property plots [i](#)


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 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.

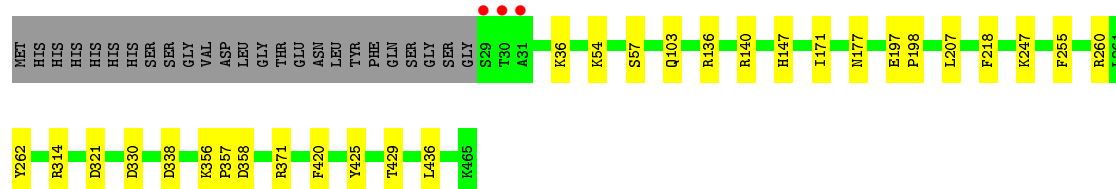
- Molecule 1: 2-methylcitrate synthase, mitochondrial

Chain B: 




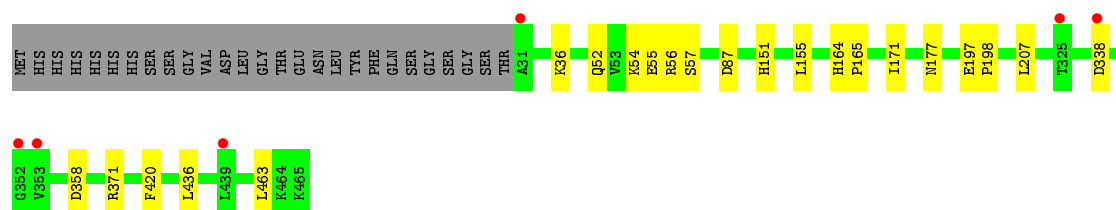
- Molecule 1: 2-methylcitrate synthase, mitochondrial

Chain C: 



- Molecule 1: 2-methylcitrate synthase, mitochondrial

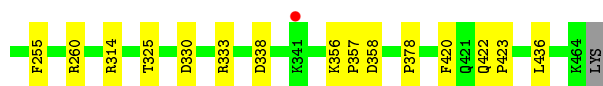
Chain A: 



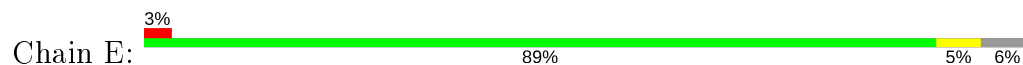
- Molecule 1: 2-methylcitrate synthase, mitochondrial

Chain D: 

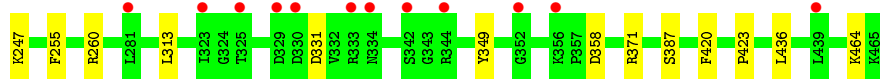
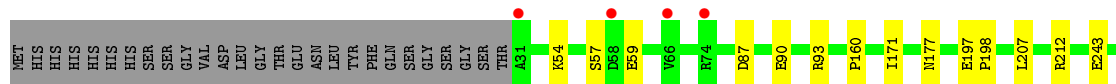
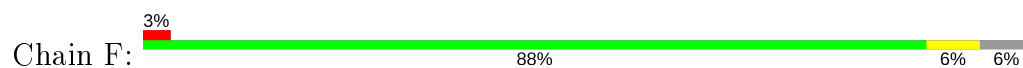




- Molecule 1: 2-methylcitrate synthase, mitochondrial



- Molecule 1: 2-methylcitrate synthase, mitochondrial



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.39Å 130.01Å 261.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.41 – 2.30 31.41 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (31.41-2.30) 99.7 (31.41-2.30)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.62 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.185 , 0.214 0.189 , 0.217	Depositor DCC
$R_{free}$ test set	6278 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.7	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 34.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	21794	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: SRT

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	0.62	0/3458	0.81	6/4697 (0.1%)
1	B	0.64	0/3484	0.81	5/4727 (0.1%)
1	C	0.62	0/3505	0.80	7/4755 (0.1%)
1	D	0.63	0/3473	0.85	11/4713 (0.2%)
1	E	0.57	1/3464 (0.0%)	0.77	3/4699 (0.1%)
1	F	0.60	0/3447	0.80	6/4683 (0.1%)
All	All	0.61	1/20831 (0.0%)	0.81	38/28274 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	128	GLN	CD-OE1	5.01	1.34	1.24

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	F	212	ARG	NE-CZ-NH2	-8.74	115.93	120.30
1	B	87	ASP	CB-CG-OD1	8.40	125.86	118.30
1	A	87	ASP	CB-CG-OD2	-7.90	111.19	118.30
1	F	331	ASP	CB-CG-OD1	7.43	124.99	118.30
1	A	87	ASP	CB-CG-OD1	7.36	124.92	118.30
1	B	87	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	D	58	ASP	CB-CG-OD1	-6.50	112.45	118.30
1	F	358	ASP	CB-CG-OD1	6.47	124.13	118.30
1	D	212	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	A	358	ASP	CB-CG-OD1	6.34	124.01	118.30
1	F	87	ASP	CB-CG-OD1	-6.32	112.61	118.30
1	C	314	ARG	NE-CZ-NH2	6.14	123.37	120.30
1	C	358	ASP	CB-CG-OD1	6.14	123.83	118.30
1	D	330	ASP	CB-CG-OD1	6.09	123.78	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	338	ASP	CB-CG-OD1	-6.05	112.86	118.30
1	D	358	ASP	CB-CG-OD1	6.00	123.70	118.30
1	B	358	ASP	CB-CG-OD1	5.99	123.69	118.30
1	D	136	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	B	338	ASP	CB-CG-OD1	5.94	123.65	118.30
1	C	260	ARG	NE-CZ-NH2	5.92	123.26	120.30
1	A	56	ARG	NE-CZ-NH1	-5.87	117.36	120.30
1	C	338	ASP	CB-CG-OD1	5.85	123.57	118.30
1	C	330	ASP	CB-CG-OD1	5.85	123.56	118.30
1	F	87	ASP	CB-CG-OD2	5.76	123.49	118.30
1	D	314	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	D	333	ARG	NE-CZ-NH2	5.66	123.13	120.30
1	C	136	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	D	87	ASP	CB-CG-OD1	5.54	123.28	118.30
1	A	338	ASP	CB-CG-OD1	5.53	123.28	118.30
1	B	93	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	E	87	ASP	CB-CG-OD1	-5.44	113.41	118.30
1	D	260	ARG	NE-CZ-NH2	5.30	122.95	120.30
1	F	260	ARG	NE-CZ-NH2	5.28	122.94	120.30
1	E	87	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	155	LEU	CA-CB-CG	5.17	127.19	115.30
1	D	58	ASP	CB-CG-OD2	5.11	122.89	118.30
1	C	140	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	E	136	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

## 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	3376	0	3359	9	0
1	B	3402	0	3414	7	0
1	C	3421	0	3428	14	0
1	D	3391	0	3391	15	0
1	E	3380	0	3391	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3365	0	3347	10	0
2	B	10	0	4	1	0
3	A	277	0	0	0	0
3	B	337	0	0	0	0
3	C	286	0	0	1	0
3	D	300	0	0	0	0
3	E	106	0	0	0	0
3	F	143	0	0	0	0
All	All	21794	0	20334	63	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 2.

All (63) 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:171:ILE:HG23	1:D:171:ILE:HG23	1.68	0.76
1:E:171:ILE:HG23	1:F:171:ILE:HG23	1.69	0.74
1:B:397:HIS:CE1	1:B:399:LYS:HG3	2.23	0.73
1:E:247:LYS:HD2	1:E:420:PHE:HE1	1.53	0.73
1:B:171:ILE:HG23	1:C:171:ILE:HG23	1.73	0.71
1:E:89:GLU:OE1	1:E:355:ARG:NH1	2.25	0.69
1:C:247:LYS:HD2	1:C:420:PHE:CE1	2.28	0.68
1:C:262:TYR:CE1	1:C:429:THR:HG22	2.35	0.62
1:E:322:LYS:HD2	1:E:322:LYS:O	2.00	0.62
1:C:218[B]:PHE:CZ	1:C:425:TYR:HB3	2.36	0.61
1:E:247:LYS:HD2	1:E:420:PHE:CE1	2.36	0.60
1:F:313:LEU:HD23	1:F:423:PRO:HG3	1.84	0.60
1:E:36:LYS:HE2	1:E:197:GLU:HG3	1.84	0.60
1:D:90:GLU:HG3	1:D:93:ARG:HH21	1.67	0.59
1:E:66:VAL:HG22	1:E:463:LEU:HD12	1.86	0.57
1:E:245:LEU:HD13	1:E:420:PHE:HZ	1.69	0.57
1:A:463:LEU:O	1:D:56:ARG:NH1	2.40	0.55
1:B:323:ILE:HD11	1:B:382:LEU:HD21	1.88	0.54
1:D:90:GLU:HG3	1:D:93:ARG:NH2	2.24	0.51
1:B:197:GLU:HB3	1:B:198:PRO:HD3	1.93	0.51
1:C:255:PHE:CZ	1:C:420:PHE:CE1	2.98	0.51
1:E:458:ILE:HG21	1:E:463:LEU:HD21	1.93	0.50
1:A:197:GLU:HB3	1:A:198:PRO:HD3	1.94	0.50
1:C:103:GLN:NE2	3:C:505:HOH:O	2.44	0.49
1:C:197:GLU:HB3	1:C:198:PRO:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:LYS:CD	1:C:420:PHE:CE1	2.94	0.49
1:E:197:GLU:HB3	1:E:198:PRO:HD3	1.95	0.49
1:D:89:GLU:O	1:D:356:LYS:HE2	2.12	0.48
1:C:356:LYS:HG3	1:C:357:PRO:O	2.14	0.48
1:E:56:ARG:NH1	1:F:464:LYS:O	2.46	0.48
1:A:151:HIS:CG	1:D:160:PRO:HG3	2.47	0.48
1:F:197:GLU:HB3	1:F:198:PRO:HD3	1.94	0.48
1:F:54:LYS:O	1:F:57:SER:HB2	2.14	0.47
1:C:247:LYS:HD2	1:C:420:PHE:CZ	2.48	0.47
1:A:54:LYS:O	1:A:57:SER:HB2	2.15	0.47
1:C:147[B]:HIS:CE1	1:E:150:GLN:HB2	2.50	0.47
1:D:197:GLU:HB3	1:D:198:PRO:HD3	1.97	0.46
1:B:74:ARG:NH2	2:B:501:SRT:O11	2.48	0.46
1:C:54:LYS:O	1:C:57:SER:HB2	2.15	0.46
1:D:325:THR:HG23	1:D:378:PRO:CG	2.46	0.46
1:F:207:LEU:HD11	1:F:436:LEU:HD23	1.98	0.46
1:C:36:LYS:HE2	1:C:197:GLU:HG3	1.99	0.45
1:B:54:LYS:O	1:B:57:SER:HB2	2.17	0.45
1:D:207:LEU:HD11	1:D:436:LEU:HD23	1.98	0.45
1:E:458:ILE:CG2	1:E:463:LEU:HD21	2.45	0.45
1:D:54:LYS:O	1:D:57:SER:HB2	2.16	0.45
1:E:54:LYS:O	1:E:57:SER:HB3	2.17	0.45
1:A:207:LEU:HD11	1:A:436:LEU:HD23	1.99	0.44
1:A:52:GLN:O	1:A:55:GLU:HG2	2.18	0.44
1:D:356:LYS:HB2	1:D:357:PRO:HD2	1.98	0.44
1:E:151:HIS:CG	1:F:160:PRO:HG3	2.52	0.44
1:B:397:HIS:CE1	1:B:399:LYS:CG	3.00	0.43
1:D:136:ARG:O	1:D:140:ARG:HG3	2.17	0.43
1:F:90:GLU:OE2	1:F:93:ARG:NH2	2.51	0.43
1:A:164:HIS:HA	1:A:165:PRO:HD3	1.94	0.42
1:C:207:LEU:HD11	1:C:436:LEU:HD23	2.01	0.41
1:D:356:LYS:HB2	1:D:357:PRO:CD	2.50	0.41
1:A:36:LYS:HE2	1:A:197:GLU:HG3	2.02	0.41
1:D:255:PHE:CZ	1:D:420:PHE:CE2	3.08	0.41
1:D:422:GLN:HA	1:D:423:PRO:HD2	1.95	0.41
1:E:245:LEU:HD13	1:E:420:PHE:CZ	2.53	0.41
1:F:255:PHE:CZ	1:F:420:PHE:CE2	3.09	0.41
1:F:349:TYR:OH	1:F:387:SER:HA	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	434/462 (94%)	431 (99%)	3 (1%)	0	100	100
1	B	435/462 (94%)	430 (99%)	5 (1%)	0	100	100
1	C	437/462 (95%)	432 (99%)	5 (1%)	0	100	100
1	D	434/462 (94%)	429 (99%)	5 (1%)	0	100	100
1	E	432/462 (94%)	428 (99%)	4 (1%)	0	100	100
1	F	433/462 (94%)	429 (99%)	4 (1%)	0	100	100
All	All	2605/2772 (94%)	2579 (99%)	26 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	356/384 (93%)	353 (99%)	3 (1%)	81	91
1	B	362/384 (94%)	361 (100%)	1 (0%)	92	97
1	C	364/384 (95%)	361 (99%)	3 (1%)	81	91
1	D	360/384 (94%)	357 (99%)	3 (1%)	81	91
1	E	359/384 (94%)	357 (99%)	2 (1%)	86	94
1	F	355/384 (92%)	350 (99%)	5 (1%)	67	81
All	All	2156/2304 (94%)	2139 (99%)	17 (1%)	81	91



All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	177	ASN
1	C	177	ASN
1	C	321	ASP
1	C	371	ARG
1	A	177	ASN
1	A	371	ARG
1	A	420	PHE
1	D	58	ASP
1	D	177	ASN
1	D	243	GLU
1	E	177	ASN
1	E	371	ARG
1	F	59	GLU
1	F	177	ASN
1	F	243	GLU
1	F	247	LYS
1	F	371	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	397	HIS
1	A	225	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

1 ligand is 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	SRT	B	501	-	3,9,9	0.18	0	6,12,12	0.82	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	SRT	B	501	-	-	4/4/12/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	SRT	C1-C2-C3-O3
2	B	501	SRT	C1-C2-C3-C4
2	B	501	SRT	O2-C2-C3-O3
2	B	501	SRT	O2-C2-C3-C4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	SRT	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	435/462 (94%)	-0.23	6 (1%) 75 80	19, 35, 69, 93	0
1	B	436/462 (94%)	-0.36	1 (0%) 95 96	21, 32, 55, 86	0
1	C	437/462 (94%)	-0.31	3 (0%) 87 91	22, 35, 60, 100	0
1	D	434/462 (93%)	-0.40	2 (0%) 91 94	19, 31, 57, 75	0
1	E	434/462 (93%)	0.12	12 (2%) 53 60	34, 57, 83, 105	0
1	F	435/462 (94%)	-0.03	16 (3%) 41 48	29, 50, 89, 126	0
All	All	2611/2772 (94%)	-0.20	40 (1%) 73 79	19, 39, 75, 126	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	30	THR	5.5
1	A	352	GLY	4.1
1	F	352	GLY	4.1
1	C	29	SER	3.8
1	C	30	THR	3.8
1	F	329	ASP	3.6
1	E	60	VAL	3.5
1	A	353	VAL	3.0
1	A	325	THR	3.0
1	E	249	GLY	2.9
1	F	330	ASP	2.9
1	E	189	GLY	2.9
1	E	297	LEU	2.8
1	A	31	ALA	2.8
1	E	31	ALA	2.8
1	D	31	ALA	2.7
1	F	31	ALA	2.7
1	F	325	THR	2.6
1	C	31	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	334	ASN	2.5
1	E	435	ALA	2.4
1	F	356	LYS	2.4
1	E	210	ILE	2.4
1	E	439	LEU	2.4
1	F	323	ILE	2.2
1	F	74	ARG	2.2
1	E	75	GLY	2.1
1	F	344	ARG	2.1
1	F	333	ARG	2.1
1	F	281	LEU	2.1
1	A	439	LEU	2.1
1	E	207	LEU	2.1
1	E	251	GLU	2.0
1	F	439	LEU	2.0
1	A	338	ASP	2.0
1	E	274	VAL	2.0
1	F	66	VAL	2.0
1	F	342	SER	2.0
1	F	58	ASP	2.0
1	D	341	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	SRT	B	501	10/10	0.87	0.17	61,68,71,73	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.