



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 12:33 pm BST

PDB ID : 5SWC  
Title : The structure of the beta-carbonic anhydrase CcaA  
Authors : Kimber, M.S.; McGurn, L.; White, S.A.  
Deposited on : 2016-08-08  
Resolution : 1.45 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 : 2.11  
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



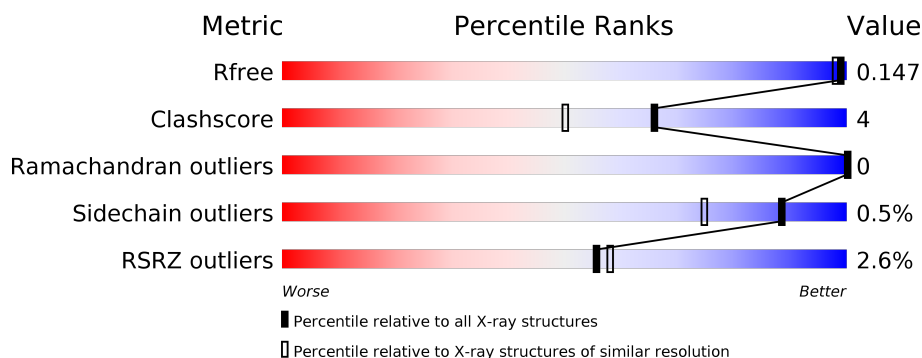
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.45 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	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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	239	<div> <div>86%</div> <div>7%</div> <div>7%</div> </div>
1	B	239	<div> <div>%</div> <div>87%</div> <div>6%</div> <div>7%</div> </div>
1	C	239	<div> <div>2%</div> <div>80%</div> <div>7%</div> <div>13%</div> </div>
1	D	239	<div> <div>3%</div> <div>80%</div> <div>6%</div> <div>14%</div> </div>
1	E	239	<div> <div>6%</div> <div>86%</div> <div>6%</div> <div>7%</div> </div>
1	F	239	<div> <div>%</div> <div>81%</div> <div>8%</div> <div>11%</div> </div>



## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22022 atoms, of which 10420 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 Carbonic anhydrase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	223	Total	C	H	N	O	S	0	8	0
			3616	1153	1802	318	335	8			
1	B	223	Total	C	H	N	O	S	0	7	0
			3577	1142	1775	315	337	8			
1	C	208	Total	C	H	N	O	S	0	3	0
			3309	1056	1644	297	304	8			
1	D	206	Total	C	H	N	O	S	0	7	0
			3353	1074	1668	298	305	8			
1	E	223	Total	C	H	N	O	S	0	6	0
			3589	1144	1788	317	332	8			
1	F	213	Total	C	H	N	O	S	0	9	0
			3445	1095	1722	306	314	8			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	expression tag	UNP Q54735
A	-17	GLY	-	expression tag	UNP Q54735
A	-16	SER	-	expression tag	UNP Q54735
A	-15	SER	-	expression tag	UNP Q54735
A	-14	HIS	-	expression tag	UNP Q54735
A	-13	HIS	-	expression tag	UNP Q54735
A	-12	HIS	-	expression tag	UNP Q54735
A	-11	HIS	-	expression tag	UNP Q54735
A	-10	HIS	-	expression tag	UNP Q54735
A	-9	SER	-	expression tag	UNP Q54735
A	-8	SER	-	expression tag	UNP Q54735
A	-7	GLY	-	expression tag	UNP Q54735
A	-6	LEU	-	expression tag	UNP Q54735
A	-5	VAL	-	expression tag	UNP Q54735
A	-4	PRO	-	expression tag	UNP Q54735
A	-3	ARG	-	expression tag	UNP Q54735
A	-2	GLY	-	expression tag	UNP Q54735

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP Q54735
A	0	HIS	-	expression tag	UNP Q54735
A	219	LEU	PRO	conflict	UNP Q54735
B	-18	MET	-	expression tag	UNP Q54735
B	-17	GLY	-	expression tag	UNP Q54735
B	-16	SER	-	expression tag	UNP Q54735
B	-15	SER	-	expression tag	UNP Q54735
B	-14	HIS	-	expression tag	UNP Q54735
B	-13	HIS	-	expression tag	UNP Q54735
B	-12	HIS	-	expression tag	UNP Q54735
B	-11	HIS	-	expression tag	UNP Q54735
B	-10	HIS	-	expression tag	UNP Q54735
B	-9	SER	-	expression tag	UNP Q54735
B	-8	SER	-	expression tag	UNP Q54735
B	-7	GLY	-	expression tag	UNP Q54735
B	-6	LEU	-	expression tag	UNP Q54735
B	-5	VAL	-	expression tag	UNP Q54735
B	-4	PRO	-	expression tag	UNP Q54735
B	-3	ARG	-	expression tag	UNP Q54735
B	-2	GLY	-	expression tag	UNP Q54735
B	-1	SER	-	expression tag	UNP Q54735
B	0	HIS	-	expression tag	UNP Q54735
B	219	LEU	PRO	conflict	UNP Q54735
C	-18	MET	-	expression tag	UNP Q54735
C	-17	GLY	-	expression tag	UNP Q54735
C	-16	SER	-	expression tag	UNP Q54735
C	-15	SER	-	expression tag	UNP Q54735
C	-14	HIS	-	expression tag	UNP Q54735
C	-13	HIS	-	expression tag	UNP Q54735
C	-12	HIS	-	expression tag	UNP Q54735
C	-11	HIS	-	expression tag	UNP Q54735
C	-10	HIS	-	expression tag	UNP Q54735
C	-9	SER	-	expression tag	UNP Q54735
C	-8	SER	-	expression tag	UNP Q54735
C	-7	GLY	-	expression tag	UNP Q54735
C	-6	LEU	-	expression tag	UNP Q54735
C	-5	VAL	-	expression tag	UNP Q54735
C	-4	PRO	-	expression tag	UNP Q54735
C	-3	ARG	-	expression tag	UNP Q54735
C	-2	GLY	-	expression tag	UNP Q54735
C	-1	SER	-	expression tag	UNP Q54735
C	0	HIS	-	expression tag	UNP Q54735

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Chain	Residue	Modelled	Actual	Comment	Reference
C	219	LEU	PRO	conflict	UNP Q54735
D	-18	MET	-	expression tag	UNP Q54735
D	-17	GLY	-	expression tag	UNP Q54735
D	-16	SER	-	expression tag	UNP Q54735
D	-15	SER	-	expression tag	UNP Q54735
D	-14	HIS	-	expression tag	UNP Q54735
D	-13	HIS	-	expression tag	UNP Q54735
D	-12	HIS	-	expression tag	UNP Q54735
D	-11	HIS	-	expression tag	UNP Q54735
D	-10	HIS	-	expression tag	UNP Q54735
D	-9	SER	-	expression tag	UNP Q54735
D	-8	SER	-	expression tag	UNP Q54735
D	-7	GLY	-	expression tag	UNP Q54735
D	-6	LEU	-	expression tag	UNP Q54735
D	-5	VAL	-	expression tag	UNP Q54735
D	-4	PRO	-	expression tag	UNP Q54735
D	-3	ARG	-	expression tag	UNP Q54735
D	-2	GLY	-	expression tag	UNP Q54735
D	-1	SER	-	expression tag	UNP Q54735
D	0	HIS	-	expression tag	UNP Q54735
D	219	LEU	PRO	conflict	UNP Q54735
E	-18	MET	-	expression tag	UNP Q54735
E	-17	GLY	-	expression tag	UNP Q54735
E	-16	SER	-	expression tag	UNP Q54735
E	-15	SER	-	expression tag	UNP Q54735
E	-14	HIS	-	expression tag	UNP Q54735
E	-13	HIS	-	expression tag	UNP Q54735
E	-12	HIS	-	expression tag	UNP Q54735
E	-11	HIS	-	expression tag	UNP Q54735
E	-10	HIS	-	expression tag	UNP Q54735
E	-9	SER	-	expression tag	UNP Q54735
E	-8	SER	-	expression tag	UNP Q54735
E	-7	GLY	-	expression tag	UNP Q54735
E	-6	LEU	-	expression tag	UNP Q54735
E	-5	VAL	-	expression tag	UNP Q54735
E	-4	PRO	-	expression tag	UNP Q54735
E	-3	ARG	-	expression tag	UNP Q54735
E	-2	GLY	-	expression tag	UNP Q54735
E	-1	SER	-	expression tag	UNP Q54735
E	0	HIS	-	expression tag	UNP Q54735
E	219	LEU	PRO	conflict	UNP Q54735
F	-18	MET	-	expression tag	UNP Q54735

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-17	GLY	-	expression tag	UNP Q54735
F	-16	SER	-	expression tag	UNP Q54735
F	-15	SER	-	expression tag	UNP Q54735
F	-14	HIS	-	expression tag	UNP Q54735
F	-13	HIS	-	expression tag	UNP Q54735
F	-12	HIS	-	expression tag	UNP Q54735
F	-11	HIS	-	expression tag	UNP Q54735
F	-10	HIS	-	expression tag	UNP Q54735
F	-9	SER	-	expression tag	UNP Q54735
F	-8	SER	-	expression tag	UNP Q54735
F	-7	GLY	-	expression tag	UNP Q54735
F	-6	LEU	-	expression tag	UNP Q54735
F	-5	VAL	-	expression tag	UNP Q54735
F	-4	PRO	-	expression tag	UNP Q54735
F	-3	ARG	-	expression tag	UNP Q54735
F	-2	GLY	-	expression tag	UNP Q54735
F	-1	SER	-	expression tag	UNP Q54735
F	0	HIS	-	expression tag	UNP Q54735
F	219	LEU	PRO	conflict	UNP Q54735

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Cl 2 2	0	0

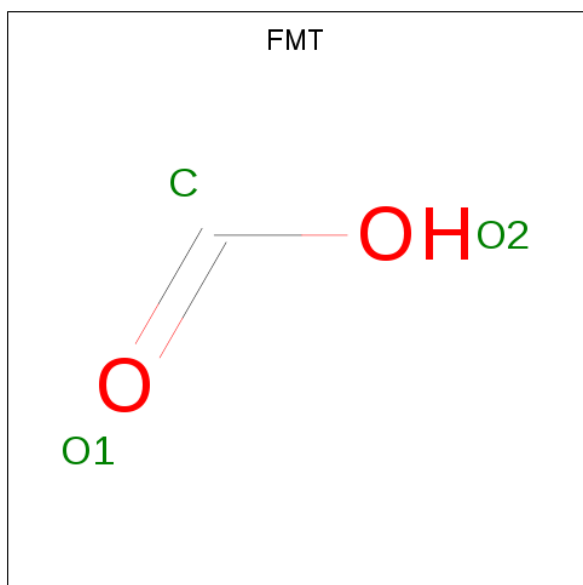
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Cl	0	0
			1	1		
3	E	2	Total	Cl	0	0
			2	2		

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			4	1	1	2		
4	A	1	Total	C	H	O	0	0
			4	1	1	2		
4	A	1	Total	C	H	O	0	0
			4	1	1	2		
4	B	1	Total	C	H	O	0	0
			4	1	1	2		
4	B	1	Total	C	H	O	0	0
			4	1	1	2		
4	B	1	Total	C	H	O	0	0
			4	1	1	2		
4	B	1	Total	C	H	O	0	0
			4	1	1	2		
4	C	1	Total	C	H	O	0	0
			4	1	1	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total 4	C 1	H 1	O 2	0	0
4	C	1	Total 4	C 1	H 1	O 2	0	0
4	C	1	Total 4	C 1	H 1	O 2	0	0
4	D	1	Total 4	C 1	H 1	O 2	0	0
4	D	1	Total 4	C 1	H 1	O 2	0	0
4	E	1	Total 4	C 1	H 1	O 2	0	0
4	E	1	Total 4	C 1	H 1	O 2	0	0
4	E	1	Total 4	C 1	H 1	O 2	0	0
4	E	1	Total 4	C 1	H 1	O 2	0	0
4	E	1	Total 4	C 1	H 1	O 2	0	0
4	F	1	Total 4	C 1	H 1	O 2	0	0
4	F	1	Total 4	C 1	H 1	O 2	0	0

- Molecule 5 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	200	Total 200	O 200	0	0
5	B	219	Total 219	O 219	0	0
5	C	130	Total 130	O 130	0	0
5	D	145	Total 145	O 145	0	0
5	E	165	Total 165	O 165	0	0
5	F	179	Total 179	O 179	0	0

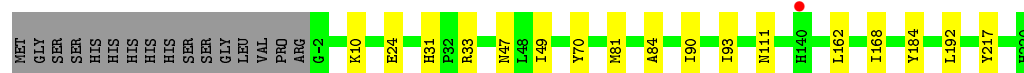


### 3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA and DNA 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: Carbonic anhydrase

Chain A: 




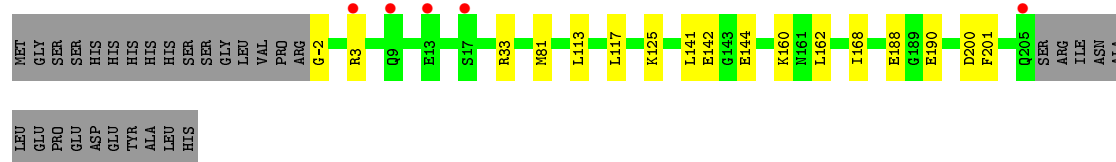
- Molecule 1: Carbonic anhydrase

Chain B: 




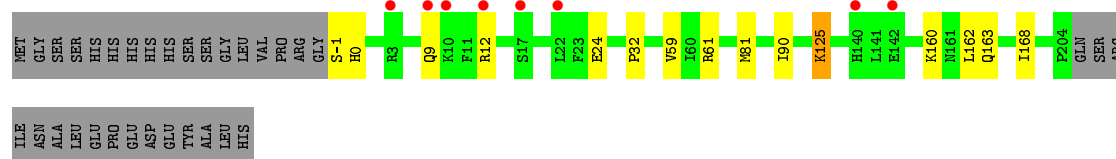
- Molecule 1: Carbonic anhydrase

Chain C: 




- Molecule 1: Carbonic anhydrase

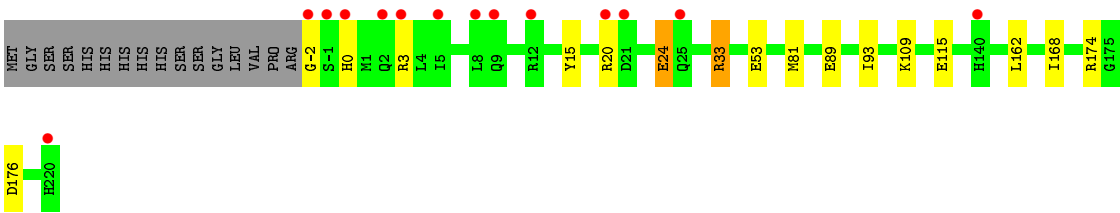
Chain D: 



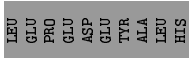
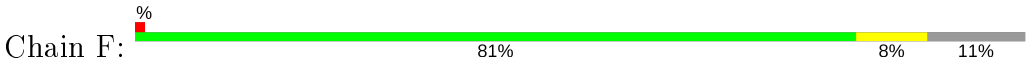
- Molecule 1: Carbonic anhydrase

Chain E: 





● Molecule 1: Carbonic anhydrase





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	202.95Å 202.95Å 70.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.82 – 1.45 48.82 – 1.34	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.82-1.45) 99.0 (48.82-1.34)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 1.34Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.131 , 0.146 0.133 , 0.147	Depositor DCC
$R_{free}$ test set	3099 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.3	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.44 , 45.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	22022	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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: ZN, FMT, CL

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	0.65	0/1877	0.72	0/2541
1	B	0.71	0/1862	0.77	2/2523 (0.1%)
1	C	0.58	0/1711	0.68	0/2316
1	D	0.58	0/1749	0.67	0/2369
1	E	0.59	0/1858	0.70	0/2516
1	F	0.61	0/1788	0.75	2/2421 (0.1%)
All	All	0.62	0/10845	0.72	4/14686 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	12	ARG	NE-CZ-NH2	5.23	122.92	120.30
1	F	176	ASP	N-CA-CB	-5.23	101.19	110.60
1	B	12	ARG	NE-CZ-NH2	5.22	122.91	120.30
1	B	131	ARG	NE-CZ-NH1	-5.13	117.73	120.30

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	1814	1802	1804	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1802	1775	1776	12	0
1	C	1665	1644	1646	12	0
1	D	1685	1668	1669	19	0
1	E	1801	1788	1788	16	0
1	F	1723	1722	1711	16	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	2	0	0	0	0
3	C	1	0	0	0	0
3	E	2	0	0	0	0
4	A	9	3	3	0	0
4	B	15	5	5	0	0
4	C	12	4	4	0	0
4	D	6	2	2	0	0
4	E	15	5	5	0	0
4	F	6	2	2	0	0
5	A	200	0	0	6	0
5	B	219	0	0	5	0
5	C	130	0	0	3	0
5	D	145	0	0	8	0
5	E	165	0	0	5	0
5	F	179	0	0	3	0
All	All	11602	10420	10415	83	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 4.

All (83) 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:-2:GLY:N	5:C:401:HOH:O	1.90	1.04
1:B:13:GLU:OE2	5:B:401:HOH:O	1.81	0.99
1:A:47[B]:ASN:ND2	5:A:401:HOH:O	1.99	0.93
1:E:24:GLU:OE2	5:E:401:HOH:O	1.86	0.93
1:E:-2:GLY:N	5:E:402:HOH:O	2.12	0.81
1:D:-1:SER:N	5:D:402:HOH:O	2.17	0.77
1:F:174:ARG:NH2	1:F:176:ASP:OD1	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:TYR:OH	5:A:402:HOH:O	2.03	0.75
1:C:81[B]:MET:HE2	1:C:168:ILE:HD11	1.70	0.72
1:D:24:GLU:OE2	5:D:401:HOH:O	2.09	0.69
1:A:24:GLU:OE1	5:A:403:HOH:O	2.12	0.66
1:F:81[B]:MET:HE2	1:F:168:ILE:HD11	1.77	0.66
1:D:125:LYS:NZ	5:D:403:HOH:O	2.26	0.66
1:E:81[B]:MET:SD	1:E:162:LEU:HD21	2.37	0.65
1:C:144:GLU:OE2	5:C:402:HOH:O	2.14	0.63
1:E:81[B]:MET:SD	1:E:162:LEU:CD2	2.87	0.63
1:E:33:ARG:NH2	1:E:89:GLU:O	2.33	0.62
1:E:3:ARG:NH1	1:F:50:THR:O	2.33	0.61
1:A:81[B]:MET:SD	1:A:162:LEU:CD2	2.88	0.61
1:A:49[B]:ILE:HD11	1:A:184:TYR:CE2	2.36	0.61
1:D:81[B]:MET:SD	1:D:162:LEU:HD21	2.42	0.59
1:A:81[B]:MET:SD	1:A:162:LEU:HD21	2.42	0.58
1:D:24:GLU:CD	5:D:401:HOH:O	2.41	0.58
1:A:217:TYR:HB2	1:F:160[B]:LYS:HE3	1.85	0.58
1:D:81[B]:MET:SD	1:D:162:LEU:CD2	2.91	0.58
1:B:54[A]:VAL:HG23	5:B:473:HOH:O	2.04	0.58
1:F:187:GLU:OE1	5:F:401:HOH:O	2.17	0.57
1:D:81[B]:MET:HE1	1:D:162:LEU:HD22	1.87	0.57
1:B:81[B]:MET:SD	1:B:162:LEU:CD2	2.93	0.56
1:A:111:ASN:OD1	5:A:404:HOH:O	2.17	0.56
1:C:81[B]:MET:SD	1:C:162:LEU:CD2	2.95	0.55
1:F:116:LYS:HG3	1:F:117:LEU:HG	1.89	0.55
1:E:33:ARG:HG3	1:F:0:HIS:CE1	2.41	0.55
1:F:81[B]:MET:SD	1:F:162:LEU:HD21	2.47	0.54
1:F:81[B]:MET:SD	1:F:162:LEU:CD2	2.96	0.54
1:D:163:GLN:NE2	5:D:406:HOH:O	2.39	0.54
1:D:125:LYS:CE	5:D:403:HOH:O	2.56	0.53
1:A:81[B]:MET:HE2	1:A:168:ILE:HD11	1.90	0.53
1:C:81[B]:MET:SD	1:C:162:LEU:HD21	2.50	0.52
1:F:9[A]:GLN:HG2	5:F:479:HOH:O	2.09	0.51
1:A:49[B]:ILE:HD11	1:A:184:TYR:CZ	2.46	0.51
1:D:24:GLU:OE1	5:D:401:HOH:O	2.18	0.50
1:E:81[B]:MET:HE2	1:E:168:ILE:HD11	1.93	0.50
1:B:81[B]:MET:SD	1:B:162:LEU:HD21	2.52	0.50
1:D:9[B]:GLN:OE1	1:D:12:ARG:NH2	2.44	0.49
1:D:160:LYS:HD3	5:E:417:HOH:O	2.13	0.49
1:E:174[B]:ARG:NE	1:E:176[B]:ASP:OD2	2.42	0.48
1:D:32:PRO:HG2	1:D:90:ILE:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:LEU:HD23	5:A:465:HOH:O	2.13	0.47
1:C:200:ASP:OD1	1:C:201:PHE:N	2.49	0.46
1:B:217:TYR:HB2	1:C:160:LYS:HE2	1.97	0.46
1:D:125:LYS:HD2	1:D:125:LYS:N	2.30	0.46
1:B:3:ARG:HG2	5:B:577:HOH:O	2.17	0.45
1:E:115:GLU:HG3	5:E:478:HOH:O	2.15	0.45
1:C:113:LEU:HD22	1:C:117:LEU:HD12	1.99	0.45
1:C:188:GLU:HB2	1:C:190:GLU:HG2	1.99	0.44
1:B:187:GLU:H	1:B:187:GLU:CD	2.21	0.44
1:C:125:LYS:HE3	5:C:418:HOH:O	2.17	0.44
1:E:81[B]:MET:HE1	1:E:93:ILE:HD13	2.00	0.44
1:E:33:ARG:HB2	5:E:407:HOH:O	2.17	0.44
1:D:81[B]:MET:CE	1:D:168:ILE:HD11	2.48	0.43
1:C:33[A]:ARG:HG3	1:D:0[A]:HIS:CE1	2.53	0.43
1:A:84:ALA:HB1	1:A:90[A]:ILE:HD12	2.00	0.43
1:F:163:GLN:CD	5:F:410:HOH:O	2.57	0.43
1:B:114[A]:GLN:NE2	5:B:407:HOH:O	2.44	0.42
1:D:81[B]:MET:HE2	1:D:168:ILE:HD11	2.02	0.42
1:D:59:VAL:HG12	1:D:61:ARG:HG3	2.01	0.42
1:F:3:ARG:HD2	1:F:3:ARG:O	2.20	0.42
1:B:187:GLU:HG2	1:B:188:GLU:HG3	2.02	0.42
1:D:125:LYS:HE3	5:D:403:HOH:O	2.17	0.42
1:E:109[B]:LYS:HE2	1:E:109[B]:LYS:HB2	1.75	0.41
1:B:24:GLU:OE2	1:B:28:HIS:NE2	2.52	0.41
1:B:47[B]:ASN:ND2	5:B:415:HOH:O	2.53	0.41
1:F:59:VAL:HG12	1:F:61:ARG:HG3	2.02	0.41
1:A:31:HIS:HD2	5:A:567:HOH:O	2.02	0.41
1:A:81[B]:MET:HE1	1:A:93:ILE:HD13	2.03	0.41
1:E:15:TYR:OH	1:E:53:GLU:OE2	2.39	0.41
1:E:0:HIS:CE1	1:F:33:ARG:HG3	2.57	0.40
1:C:141:LEU:O	1:C:142:GLU:HG3	2.21	0.40
1:E:176[A]:ASP:HA	1:F:-3:ARG:NH1	2.35	0.40
1:A:10[B]:LYS:HE3	1:B:51:GLN:OE1	2.21	0.40
1:F:81[B]:MET:HE1	1:F:162:LEU:HD22	2.04	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	229/239 (96%)	228 (100%)	1 (0%)	0	100	100
1	B	228/239 (95%)	225 (99%)	3 (1%)	0	100	100
1	C	209/239 (87%)	208 (100%)	1 (0%)	0	100	100
1	D	212/239 (89%)	211 (100%)	1 (0%)	0	100	100
1	E	227/239 (95%)	225 (99%)	2 (1%)	0	100	100
1	F	220/239 (92%)	220 (100%)	0	0	100	100
All	All	1325/1434 (92%)	1317 (99%)	8 (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	197/203 (97%)	197 (100%)	0	100	100
1	B	196/203 (97%)	196 (100%)	0	100	100
1	C	179/203 (88%)	178 (99%)	1 (1%)	86	69
1	D	183/203 (90%)	182 (100%)	1 (0%)	88	75
1	E	195/203 (96%)	192 (98%)	3 (2%)	65	35
1	F	188/203 (93%)	187 (100%)	1 (0%)	88	75
All	All	1138/1218 (93%)	1132 (100%)	6 (0%)	88	75



All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	3	ARG
1	D	125	LYS
1	E	20	ARG
1	E	24	GLU
1	E	33	ARG
1	F	185	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

Of 32 ligands modelled in this entry, 11 are monoatomic - leaving 21 for Mogul analysis.

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	$\# Z  > 2$
4	FMT	E	304	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	C	303	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	E	308	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	E	307	-	0,2,2	0.00	-	0,1,1	0.00	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	FMT	C	304	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	B	306	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	B	304	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	D	302	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	B	302	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	A	304	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	B	305	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	A	305	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	C	305	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	E	305	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	A	306	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	F	302	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	B	303	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	F	303	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	E	306	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	C	306	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	D	303	-	0,2,2	0.00	-	0,1,1	0.00	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	223/239 (93%)	-0.42	1 (0%)	92 94	11, 18, 40, 51	0
1	B	223/239 (93%)	-0.60	3 (1%)	77 78	11, 17, 40, 64	2 (0%)
1	C	208/239 (87%)	-0.37	5 (2%)	59 61	12, 24, 52, 62	0
1	D	206/239 (86%)	-0.32	8 (3%)	39 42	12, 23, 52, 59	0
1	E	223/239 (93%)	-0.10	14 (6%)	20 22	12, 20, 50, 64	0
1	F	213/239 (89%)	-0.43	3 (1%)	75 76	12, 21, 38, 48	0
All	All	1296/1434 (90%)	-0.37	34 (2%)	56 58	11, 20, 48, 64	2 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	220	HIS	6.0
1	B	220	HIS	5.6
1	E	140	HIS	4.5
1	A	140	HIS	4.3
1	B	140	HIS	3.7
1	E	5	ILE	3.6
1	E	9	GLN	3.5
1	C	13	GLU	3.5
1	D	9[A]	GLN	3.5
1	C	205	GLN	3.5
1	D	12	ARG	3.3
1	E	20	ARG	3.2
1	C	3	ARG	3.0
1	E	-1	SER	3.0
1	D	142	GLU	3.0
1	C	17	SER	2.8
1	D	3	ARG	2.8
1	E	2	GLN	2.8
1	E	12	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	3	ARG	2.7
1	E	-2	GLY	2.7
1	D	140[A]	HIS	2.6
1	E	8	LEU	2.5
1	E	21	ASP	2.5
1	F	203	ALA	2.3
1	E	25	GLN	2.3
1	C	9	GLN	2.3
1	F	176	ASP	2.3
1	D	17	SER	2.2
1	E	0	HIS	2.2
1	F	197	VAL	2.2
1	D	22	LEU	2.1
1	D	10	LYS	2.1
1	B	-2	GLY	2.1

## 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 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, 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(Å <sup>2</sup> )	Q<0.9
4	FMT	F	303	3/3	0.83	0.19	28,32,36,39	0
4	FMT	E	307	3/3	0.86	0.12	25,29,31,35	0
4	FMT	C	306	3/3	0.88	0.13	28,33,36,40	0
4	FMT	D	303	3/3	0.89	0.14	29,30,31,37	0
4	FMT	B	305	3/3	0.90	0.11	23,28,33,34	0
4	FMT	E	308	3/3	0.92	0.07	20,25,25,30	0
4	FMT	B	304	3/3	0.97	0.06	17,19,19,23	0
4	FMT	B	306	3/3	0.97	0.05	22,22,22,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	FMT	E	305	3/3	0.97	0.05	19,19,22,23	0
4	FMT	C	305	3/3	0.97	0.05	19,22,25,27	0
4	FMT	B	303	3/3	0.97	0.05	19,19,20,23	0
4	FMT	C	303	3/3	0.98	0.04	20,20,22,24	0
4	FMT	B	302	3/3	0.98	0.06	19,22,23,26	0
4	FMT	A	304	3/3	0.98	0.05	20,20,21,24	0
4	FMT	E	306	3/3	0.98	0.04	19,20,22,25	0
4	FMT	A	306	3/3	0.98	0.05	16,19,20,24	0
3	CL	E	303	1/1	0.98	0.05	25,25,25,25	0
4	FMT	E	304	3/3	0.98	0.10	19,21,21,25	0
4	FMT	D	302	3/3	0.98	0.04	18,21,21,26	0
4	FMT	F	302	3/3	0.98	0.04	18,20,21,24	0
3	CL	E	302	1/1	0.99	0.03	26,26,26,26	0
4	FMT	C	304	3/3	0.99	0.04	21,22,23,26	0
4	FMT	A	305	3/3	0.99	0.06	16,20,21,24	0
3	CL	C	302	1/1	0.99	0.03	24,24,24,24	0
3	CL	A	302	1/1	0.99	0.04	26,26,26,26	0
3	CL	A	303	1/1	0.99	0.05	18,18,18,18	0
2	ZN	D	301	1/1	1.00	0.06	15,15,15,15	0
2	ZN	A	301	1/1	1.00	0.06	11,11,11,11	0
2	ZN	F	301	1/1	1.00	0.05	14,14,14,14	0
2	ZN	E	301	1/1	1.00	0.06	14,14,14,14	0
2	ZN	C	301	1/1	1.00	0.06	17,17,17,17	0
2	ZN	B	301	1/1	1.00	0.06	12,12,12,12	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.