



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:03 PM UTC

PDB ID : 5SWC / pdb_00005swc
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

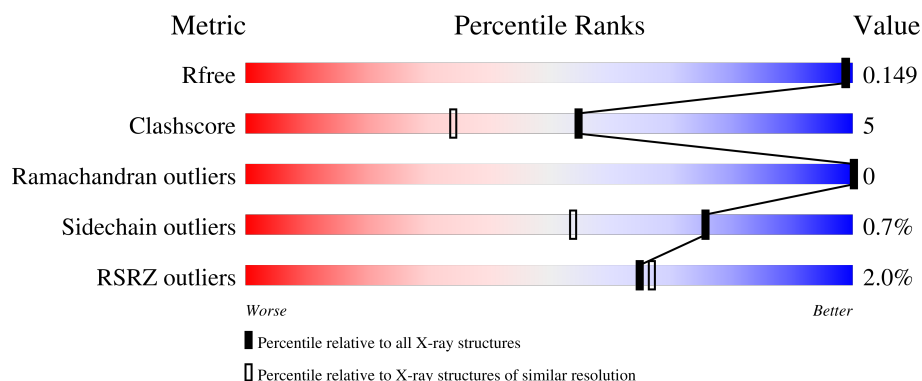
1 Overall quality at a glance

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}	180053	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	0% 85% 8% 7%
1	B	239	2% 87% 6% 7%
1	C	239	3% 79% 8% 13%
1	D	239	3% 79% 6% 14%
1	E	239	2% 85% 8% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	239	81% 8% 11%

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

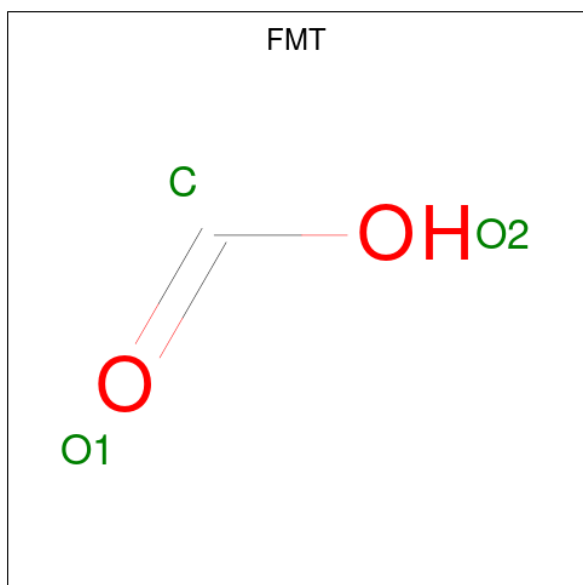
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Cl 2 2	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 4 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



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

Continued on next page...

Continued from previous page...

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

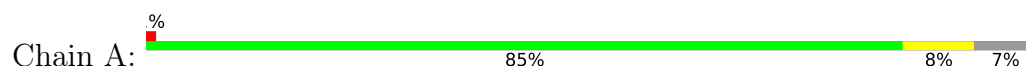
- Molecule 5 is water.

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

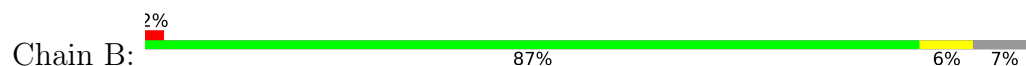
3 Residue-property plots [i](#)

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.

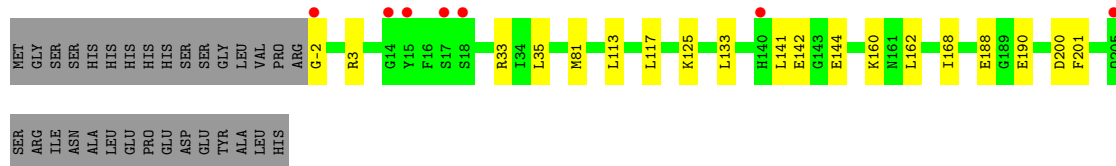
- Molecule 1: Carbonic anhydrase



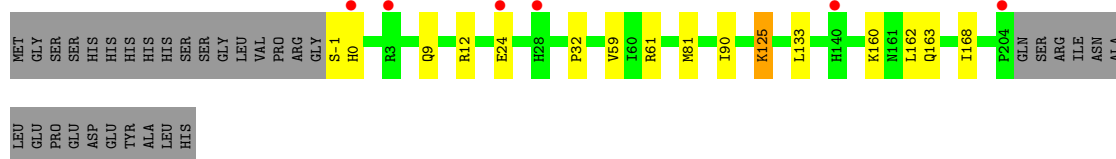
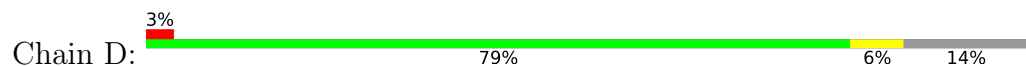
- Molecule 1: Carbonic anhydrase



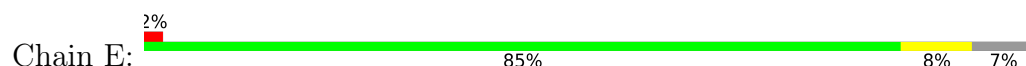
- Molecule 1: Carbonic anhydrase

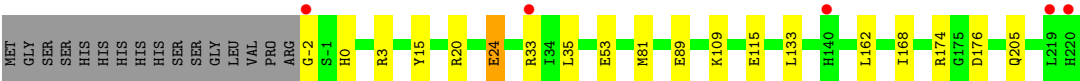


- Molecule 1: Carbonic anhydrase

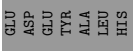
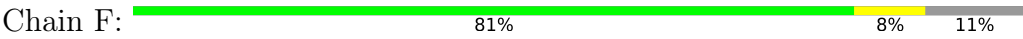


- Molecule 1: Carbonic anhydrase





● Molecule 1: Carbonic anhydrase



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	202.95Å 202.95Å 70.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.82 – 1.45 48.82 – 1.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.82-1.45) 99.9 (48.82-1.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 1.34Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.131 , 0.146 0.134 , 0.149	Depositor DCC
R_{free} test set	3099 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	14.3	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMT, CL, ZN

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	0.77	0/1877	0.81	0/2541
1	B	0.83	0/1862	0.86	0/2523
1	C	0.71	0/1711	0.80	0/2316
1	D	0.73	0/1749	0.77	0/2369
1	E	0.75	0/1858	0.81	0/2516
1	F	0.75	0/1788	0.84	2/2421 (0.1%)
All	All	0.76	0/10845	0.82	2/14686 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	176	ASP	N-CA-CB	-5.93	101.19	110.44
1	F	68	PRO	O-C-N	5.73	123.95	121.31

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	1814	1802	1804	19	0
1	B	1802	1775	1776	14	0
1	C	1665	1644	1646	17	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1685	1668	1669	21	0
1	E	1801	1788	1788	19	0
1	F	1723	1722	1711	18	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	6	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	100	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 (100) 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:B:13:GLU:OE2	5:B:401:HOH:O	1.81	0.99
1:C:-2:GLY:N	5:C:401:HOH:O	1.90	0.95
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
1:A:70:TYR:OH	5:A:402:HOH:O	2.03	0.75
1:F:81[B]:MET:HE1	1:F:162:LEU:HD22	1.69	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:81[B]:MET:HE1	1:D:168:ILE:HD11	1.77	0.66
1:D:81[B]:MET:HE1	1:D:162:LEU:HD22	1.76	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:D:24:GLU:CD	5:D:401:HOH:O	2.41	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:E:81[B]:MET:HE1	1:E:168:ILE:HD11	1.81	0.61
1:B:217:TYR:OH	5:B:402:HOH:O	2.16	0.60
1:D:81[B]:MET:SD	1:D:162:LEU:HD21	2.42	0.59
1:A:81[B]:MET:HE1	1:A:168:ILE:HD11	1.84	0.59
1:A:81[B]:MET:SD	1:A:162:LEU:HD21	2.42	0.58
1:A:217:TYR:HB2	1:F:160[B]:LYS:HE3	1.85	0.58
1:C:81[B]:MET:HE1	1:C:162:LEU:HD22	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:C:81[B]:MET:HE1	1:C:168:ILE:HD11	1.87	0.57
1:F:187:GLU:OE1	5:F:401:HOH:O	2.17	0.57
1:B:81[B]:MET:SD	1:B:162:LEU:CD2	2.93	0.56
1:D:125:LYS:NZ	5:D:403:HOH:O	2.26	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:E:81[B]:MET:HE1	1:E:162:LEU:HD22	1.90	0.53
1:D:125:LYS:CE	5:D:403:HOH:O	2.56	0.53
1:A:81[B]:MET:HE1	1:A:162:LEU:HD22	1.91	0.52
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:F:81[B]:MET:HE1	1:F:168:ILE:HD11	1.92	0.51
1:D:24:GLU:OE1	5:D:401:HOH:O	2.18	0.50
1:B:81[B]:MET:SD	1:B:162:LEU:HD21	2.52	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9[B]:GLN:OE1	1:D:12:ARG:NH2	2.44	0.49
1:B:187:GLU:H	1:B:187:GLU:CD	2.21	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:F:81[B]:MET:HE1	1:F:162:LEU:CD2	2.42	0.48
1:D:32:PRO:HG2	1:D:90:ILE:HD11	1.96	0.48
1:F:163:GLN:CD	5:F:410:HOH:O	2.57	0.47
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:C:81[B]:MET:HE2	1:C:81[B]:MET:HB3	1.79	0.46
1:D:125:LYS:N	1:D:125:LYS:HD2	2.30	0.46
1:E:35:LEU:CD2	1:E:81[B]:MET:HE3	2.46	0.45
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:A:133:LEU:HD23	1:A:133:LEU:C	2.43	0.44
1:C:188:GLU:HB2	1:C:190:GLU:HG2	1.99	0.44
1:E:133:LEU:C	1:E:133:LEU:HD23	2.42	0.44
1:C:125:LYS:HE3	5:C:418:HOH:O	2.17	0.44
1:E:33:ARG:HB2	5:E:407:HOH:O	2.17	0.44
1:A:35:LEU:CD2	1:A:81[B]:MET:HE3	2.47	0.44
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:E:81[B]:MET:HE2	1:E:81[B]:MET:HB3	1.77	0.43
1:B:114[A]:GLN:NE2	5:B:407:HOH:O	2.44	0.42
1:D:133:LEU:C	1:D:133:LEU:HD23	2.45	0.42
1:A:81[B]:MET:HB3	1:A:81[B]:MET:HE2	1.76	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:C:35:LEU:CD2	1:C:81[B]:MET:HE3	2.49	0.42
1:D:125:LYS:HE3	5:D:403:HOH:O	2.17	0.42
1:E:109[B]:LYS:HB2	1:E:109[B]:LYS:HE2	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:E:15:TYR:OH	1:E:53:GLU:OE2	2.39	0.41
1:C:81[B]:MET:CE	1:C:168:ILE:HD11	2.50	0.41
1:D:81[B]:MET:HE2	1:D:81[B]:MET:HB3	1.69	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81[B]:MET:CE	1:D:168:ILE:HD11	2.48	0.40
1:E:0:HIS:CE1	1:F:33:ARG:HG3	2.57	0.40
1:B:133:LEU:C	1:B:133:LEU:HD23	2.46	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:C:133:LEU:HD23	1:C:133:LEU:C	2.46	0.40
1:A:10[B]:LYS:HE3	1:B:51:GLN:OE1	2.21	0.40
1:F:81[B]:MET:HE2	1:F:81[B]:MET:HB3	1.73	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	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 [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	197/203 (97%)	196 (100%)	1 (0%)	81	64
1	B	196/203 (97%)	194 (99%)	2 (1%)	68	42
1	C	179/203 (88%)	178 (99%)	1 (1%)	78	58
1	D	183/203 (90%)	182 (100%)	1 (0%)	81	64
1	E	195/203 (96%)	192 (98%)	3 (2%)	57	25
1	F	188/203 (93%)	187 (100%)	1 (0%)	81	64
All	All	1138/1218 (93%)	1129 (99%)	9 (1%)	76	50

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	205	GLN
1	B	214[A]	GLU
1	B	214[B]	GLU
1	C	3	ARG
1	D	125	LYS
1	E	20	ARG
1	E	24	GLU
1	E	205	GLN
1	F	185	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	0	HIS
1	C	0	HIS
1	C	31	HIS
1	D	199	HIS
1	E	31	HIS
1	E	140	HIS

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	308	-	2,2,2	0.60	0	1,1,1	0.03	0
4	FMT	C	304	-	2,2,2	0.94	0	1,1,1	0.82	0
4	FMT	B	306	-	2,2,2	0.18	0	1,1,1	0.45	0
4	FMT	B	305	-	2,2,2	1.08	0	1,1,1	0.32	0
4	FMT	E	307	-	2,2,2	0.43	0	1,1,1	0.22	0
4	FMT	E	306	-	2,2,2	1.02	0	1,1,1	0.55	0
4	FMT	E	305	-	2,2,2	0.85	0	1,1,1	0.04	0
4	FMT	B	304	-	2,2,2	0.23	0	1,1,1	0.36	0
4	FMT	B	303	-	2,2,2	1.06	0	1,1,1	0.45	0
4	FMT	C	306	-	2,2,2	0.78	0	1,1,1	0.00	0
4	FMT	A	306	-	2,2,2	0.55	0	1,1,1	0.64	0
4	FMT	A	305	-	2,2,2	0.52	0	1,1,1	0.40	0
4	FMT	E	304	-	2,2,2	0.89	0	1,1,1	0.52	0
4	FMT	A	304	-	2,2,2	0.64	0	1,1,1	0.18	0
4	FMT	C	305	-	2,2,2	0.58	0	1,1,1	0.22	0
4	FMT	D	303	-	2,2,2	0.79	0	1,1,1	0.27	0
4	FMT	B	302	-	2,2,2	0.43	0	1,1,1	0.36	0
4	FMT	F	302	-	2,2,2	0.62	0	1,1,1	0.10	0
4	FMT	D	302	-	2,2,2	0.89	0	1,1,1	0.41	0
4	FMT	C	303	-	2,2,2	0.88	0	1,1,1	0.30	0
4	FMT	F	303	-	2,2,2	1.14	0	1,1,1	0.31	0

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, 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	223/239 (93%)	-0.47	2 (0%) 81 84	9, 20, 45, 54	8 (3%)
1	B	223/239 (93%)	-0.51	5 (2%) 62 65	8, 19, 41, 68	9 (4%)
1	C	208/239 (87%)	-0.12	7 (3%) 48 51	10, 26, 57, 66	3 (1%)
1	D	206/239 (86%)	-0.14	6 (2%) 53 56	9, 25, 57, 66	7 (3%)
1	E	223/239 (93%)	-0.28	5 (2%) 62 65	9, 21, 55, 70	6 (2%)
1	F	213/239 (89%)	-0.46	1 (0%) 87 90	10, 23, 42, 53	7 (3%)
All	All	1296/1434 (90%)	-0.33	26 (2%) 65 67	8, 22, 52, 70	40 (3%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	220	HIS	5.0
1	B	-2	GLY	4.7
1	C	140[A]	HIS	4.5
1	D	140[A]	HIS	4.4
1	B	220	HIS	3.9
1	B	-1	SER	3.4
1	B	219	LEU	3.2
1	D	3	ARG	3.0
1	D	28	HIS	2.9
1	C	15	TYR	2.8
1	E	-2	GLY	2.8
1	A	220	HIS	2.7
1	D	24	GLU	2.6
1	A	140	HIS	2.6
1	F	176	ASP	2.6
1	C	205	GLN	2.5
1	E	33	ARG	2.5
1	E	140	HIS	2.5
1	C	17	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	18	SER	2.3
1	D	204	PRO	2.3
1	E	219	LEU	2.3
1	D	0[A]	HIS	2.2
1	C	-2	GLY	2.2
1	B	140	HIS	2.2
1	C	14	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 oligosaccharides 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(Å ²)	Q<0.9
4	FMT	C	306	3/3	0.92	0.12	28,33,36,40	0
4	FMT	D	303	3/3	0.92	0.12	29,30,31,37	0
4	FMT	F	303	3/3	0.92	0.12	28,32,36,39	0
4	FMT	E	307	3/3	0.94	0.10	25,29,31,35	0
4	FMT	E	308	3/3	0.95	0.08	20,25,25,30	0
4	FMT	B	305	3/3	0.95	0.08	23,28,33,34	0
4	FMT	B	304	3/3	0.97	0.06	17,19,19,23	0
4	FMT	E	305	3/3	0.97	0.06	19,19,22,23	0
3	CL	E	303	1/1	0.97	0.11	25,25,25,25	0
4	FMT	C	305	3/3	0.97	0.09	19,22,25,27	0
4	FMT	B	303	3/3	0.97	0.07	19,19,20,23	0
4	FMT	B	306	3/3	0.98	0.05	22,22,22,27	0
4	FMT	C	303	3/3	0.98	0.05	20,20,22,24	0
4	FMT	C	304	3/3	0.98	0.06	21,22,23,26	0
4	FMT	A	304	3/3	0.98	0.05	20,20,21,24	0
4	FMT	A	305	3/3	0.98	0.06	16,20,21,24	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	FMT	D	302	3/3	0.98	0.06	18,21,21,26	0
4	FMT	A	306	3/3	0.98	0.05	16,19,20,24	0
4	FMT	E	304	3/3	0.98	0.05	19,21,21,25	0
4	FMT	B	302	3/3	0.98	0.06	19,22,23,26	0
4	FMT	E	306	3/3	0.98	0.07	19,20,22,25	0
3	CL	C	302	1/1	0.98	0.11	24,24,24,24	0
3	CL	E	302	1/1	0.98	0.11	26,26,26,26	0
4	FMT	F	302	3/3	0.98	0.06	18,20,21,24	0
3	CL	A	303	1/1	0.98	0.07	18,18,18,18	0
3	CL	A	302	1/1	0.99	0.14	26,26,26,26	0
2	ZN	C	301	1/1	1.00	0.01	17,17,17,17	0
2	ZN	D	301	1/1	1.00	0.01	15,15,15,15	0
2	ZN	E	301	1/1	1.00	0.01	14,14,14,14	0
2	ZN	F	301	1/1	1.00	0.01	14,14,14,14	0
2	ZN	A	301	1/1	1.00	0.01	11,11,11,11	0
2	ZN	B	301	1/1	1.00	0.01	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.