



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 6, 2020 – 11:48 pm BST

PDB ID : 3KWC
Title : Oxidized, active structure of the beta-carboxysomal gamma-Carbonic Anhydrase, CcmM
Authors : Kimber, M.S.; Castel, S.E.; Pena, K.L.
Deposited on : 2009-12-01
Resolution : 2.00 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 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

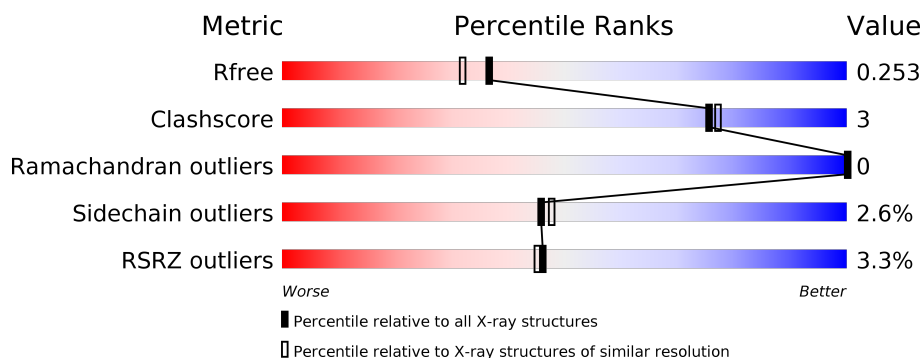
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	229	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>8%</div> <div>10%</div> </div> </div>
1	B	229	<div> <div>4%</div> <div> <div></div> <div>83%</div> <div>6%</div> <div>11%</div> </div> </div>
1	C	229	<div> <div>0%</div> <div> <div></div> <div>79%</div> <div>9%</div> <div>10%</div> </div> </div>
1	D	229	<div> <div>4%</div> <div> <div></div> <div>86%</div> <div>10%</div> </div> </div>
1	E	229	<div> <div></div> <div> <div></div> <div>83%</div> <div>6%</div> <div>10%</div> </div> </div>
1	F	229	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>6%</div> <div>11%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10237 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 Carbon dioxide concentrating mechanism protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	2	0
			1574	993	275	298	8			
1	B	204	Total	C	N	O	S	0	0	0
			1554	979	272	295	8			
1	C	205	Total	C	N	O	S	0	3	0
			1580	997	276	299	8			
1	D	205	Total	C	N	O	S	0	1	0
			1566	988	273	297	8			
1	E	205	Total	C	N	O	S	0	0	0
			1562	985	273	296	8			
1	F	204	Total	C	N	O	S	0	0	0
			1554	979	272	295	8			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP Q8DKB5
A	-18	GLY	-	EXPRESSION TAG	UNP Q8DKB5
A	-17	SER	-	EXPRESSION TAG	UNP Q8DKB5
A	-16	SER	-	EXPRESSION TAG	UNP Q8DKB5
A	-15	HIS	-	EXPRESSION TAG	UNP Q8DKB5
A	-14	HIS	-	EXPRESSION TAG	UNP Q8DKB5
A	-13	HIS	-	EXPRESSION TAG	UNP Q8DKB5
A	-12	HIS	-	EXPRESSION TAG	UNP Q8DKB5
A	-11	HIS	-	EXPRESSION TAG	UNP Q8DKB5
A	-10	HIS	-	EXPRESSION TAG	UNP Q8DKB5
A	-9	SER	-	EXPRESSION TAG	UNP Q8DKB5
A	-8	SER	-	EXPRESSION TAG	UNP Q8DKB5
A	-7	GLY	-	EXPRESSION TAG	UNP Q8DKB5
A	-6	LEU	-	EXPRESSION TAG	UNP Q8DKB5
A	-5	VAL	-	EXPRESSION TAG	UNP Q8DKB5
A	-4	PRO	-	EXPRESSION TAG	UNP Q8DKB5
A	-3	ARG	-	EXPRESSION TAG	UNP Q8DKB5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP Q8DKB5
A	-1	SER	-	EXPRESSION TAG	UNP Q8DKB5
A	0	HIS	-	EXPRESSION TAG	UNP Q8DKB5
B	-19	MET	-	EXPRESSION TAG	UNP Q8DKB5
B	-18	GLY	-	EXPRESSION TAG	UNP Q8DKB5
B	-17	SER	-	EXPRESSION TAG	UNP Q8DKB5
B	-16	SER	-	EXPRESSION TAG	UNP Q8DKB5
B	-15	HIS	-	EXPRESSION TAG	UNP Q8DKB5
B	-14	HIS	-	EXPRESSION TAG	UNP Q8DKB5
B	-13	HIS	-	EXPRESSION TAG	UNP Q8DKB5
B	-12	HIS	-	EXPRESSION TAG	UNP Q8DKB5
B	-11	HIS	-	EXPRESSION TAG	UNP Q8DKB5
B	-10	HIS	-	EXPRESSION TAG	UNP Q8DKB5
B	-9	SER	-	EXPRESSION TAG	UNP Q8DKB5
B	-8	SER	-	EXPRESSION TAG	UNP Q8DKB5
B	-7	GLY	-	EXPRESSION TAG	UNP Q8DKB5
B	-6	LEU	-	EXPRESSION TAG	UNP Q8DKB5
B	-5	VAL	-	EXPRESSION TAG	UNP Q8DKB5
B	-4	PRO	-	EXPRESSION TAG	UNP Q8DKB5
B	-3	ARG	-	EXPRESSION TAG	UNP Q8DKB5
B	-2	GLY	-	EXPRESSION TAG	UNP Q8DKB5
B	-1	SER	-	EXPRESSION TAG	UNP Q8DKB5
B	0	HIS	-	EXPRESSION TAG	UNP Q8DKB5
C	-19	MET	-	EXPRESSION TAG	UNP Q8DKB5
C	-18	GLY	-	EXPRESSION TAG	UNP Q8DKB5
C	-17	SER	-	EXPRESSION TAG	UNP Q8DKB5
C	-16	SER	-	EXPRESSION TAG	UNP Q8DKB5
C	-15	HIS	-	EXPRESSION TAG	UNP Q8DKB5
C	-14	HIS	-	EXPRESSION TAG	UNP Q8DKB5
C	-13	HIS	-	EXPRESSION TAG	UNP Q8DKB5
C	-12	HIS	-	EXPRESSION TAG	UNP Q8DKB5
C	-11	HIS	-	EXPRESSION TAG	UNP Q8DKB5
C	-10	HIS	-	EXPRESSION TAG	UNP Q8DKB5
C	-9	SER	-	EXPRESSION TAG	UNP Q8DKB5
C	-8	SER	-	EXPRESSION TAG	UNP Q8DKB5
C	-7	GLY	-	EXPRESSION TAG	UNP Q8DKB5
C	-6	LEU	-	EXPRESSION TAG	UNP Q8DKB5
C	-5	VAL	-	EXPRESSION TAG	UNP Q8DKB5
C	-4	PRO	-	EXPRESSION TAG	UNP Q8DKB5
C	-3	ARG	-	EXPRESSION TAG	UNP Q8DKB5
C	-2	GLY	-	EXPRESSION TAG	UNP Q8DKB5
C	-1	SER	-	EXPRESSION TAG	UNP Q8DKB5

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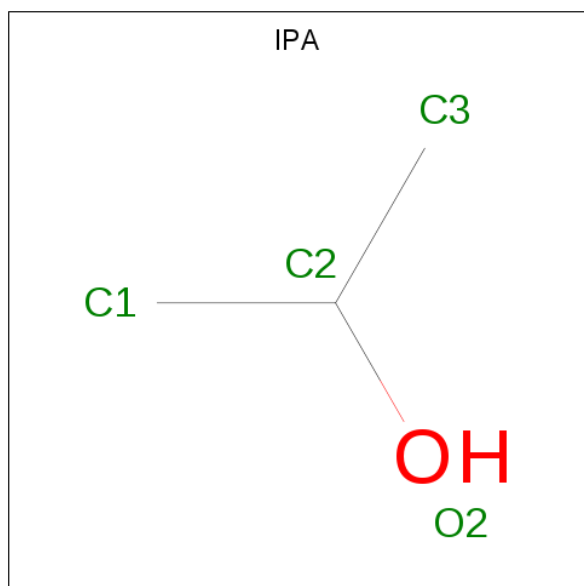
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	EXPRESSION TAG	UNP Q8DKB5
D	-19	MET	-	EXPRESSION TAG	UNP Q8DKB5
D	-18	GLY	-	EXPRESSION TAG	UNP Q8DKB5
D	-17	SER	-	EXPRESSION TAG	UNP Q8DKB5
D	-16	SER	-	EXPRESSION TAG	UNP Q8DKB5
D	-15	HIS	-	EXPRESSION TAG	UNP Q8DKB5
D	-14	HIS	-	EXPRESSION TAG	UNP Q8DKB5
D	-13	HIS	-	EXPRESSION TAG	UNP Q8DKB5
D	-12	HIS	-	EXPRESSION TAG	UNP Q8DKB5
D	-11	HIS	-	EXPRESSION TAG	UNP Q8DKB5
D	-10	HIS	-	EXPRESSION TAG	UNP Q8DKB5
D	-9	SER	-	EXPRESSION TAG	UNP Q8DKB5
D	-8	SER	-	EXPRESSION TAG	UNP Q8DKB5
D	-7	GLY	-	EXPRESSION TAG	UNP Q8DKB5
D	-6	LEU	-	EXPRESSION TAG	UNP Q8DKB5
D	-5	VAL	-	EXPRESSION TAG	UNP Q8DKB5
D	-4	PRO	-	EXPRESSION TAG	UNP Q8DKB5
D	-3	ARG	-	EXPRESSION TAG	UNP Q8DKB5
D	-2	GLY	-	EXPRESSION TAG	UNP Q8DKB5
D	-1	SER	-	EXPRESSION TAG	UNP Q8DKB5
D	0	HIS	-	EXPRESSION TAG	UNP Q8DKB5
E	-19	MET	-	EXPRESSION TAG	UNP Q8DKB5
E	-18	GLY	-	EXPRESSION TAG	UNP Q8DKB5
E	-17	SER	-	EXPRESSION TAG	UNP Q8DKB5
E	-16	SER	-	EXPRESSION TAG	UNP Q8DKB5
E	-15	HIS	-	EXPRESSION TAG	UNP Q8DKB5
E	-14	HIS	-	EXPRESSION TAG	UNP Q8DKB5
E	-13	HIS	-	EXPRESSION TAG	UNP Q8DKB5
E	-12	HIS	-	EXPRESSION TAG	UNP Q8DKB5
E	-11	HIS	-	EXPRESSION TAG	UNP Q8DKB5
E	-10	HIS	-	EXPRESSION TAG	UNP Q8DKB5
E	-9	SER	-	EXPRESSION TAG	UNP Q8DKB5
E	-8	SER	-	EXPRESSION TAG	UNP Q8DKB5
E	-7	GLY	-	EXPRESSION TAG	UNP Q8DKB5
E	-6	LEU	-	EXPRESSION TAG	UNP Q8DKB5
E	-5	VAL	-	EXPRESSION TAG	UNP Q8DKB5
E	-4	PRO	-	EXPRESSION TAG	UNP Q8DKB5
E	-3	ARG	-	EXPRESSION TAG	UNP Q8DKB5
E	-2	GLY	-	EXPRESSION TAG	UNP Q8DKB5
E	-1	SER	-	EXPRESSION TAG	UNP Q8DKB5
E	0	HIS	-	EXPRESSION TAG	UNP Q8DKB5
F	-19	MET	-	EXPRESSION TAG	UNP Q8DKB5

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-18	GLY	-	EXPRESSION TAG	UNP Q8DKB5
F	-17	SER	-	EXPRESSION TAG	UNP Q8DKB5
F	-16	SER	-	EXPRESSION TAG	UNP Q8DKB5
F	-15	HIS	-	EXPRESSION TAG	UNP Q8DKB5
F	-14	HIS	-	EXPRESSION TAG	UNP Q8DKB5
F	-13	HIS	-	EXPRESSION TAG	UNP Q8DKB5
F	-12	HIS	-	EXPRESSION TAG	UNP Q8DKB5
F	-11	HIS	-	EXPRESSION TAG	UNP Q8DKB5
F	-10	HIS	-	EXPRESSION TAG	UNP Q8DKB5
F	-9	SER	-	EXPRESSION TAG	UNP Q8DKB5
F	-8	SER	-	EXPRESSION TAG	UNP Q8DKB5
F	-7	GLY	-	EXPRESSION TAG	UNP Q8DKB5
F	-6	LEU	-	EXPRESSION TAG	UNP Q8DKB5
F	-5	VAL	-	EXPRESSION TAG	UNP Q8DKB5
F	-4	PRO	-	EXPRESSION TAG	UNP Q8DKB5
F	-3	ARG	-	EXPRESSION TAG	UNP Q8DKB5
F	-2	GLY	-	EXPRESSION TAG	UNP Q8DKB5
F	-1	SER	-	EXPRESSION TAG	UNP Q8DKB5
F	0	HIS	-	EXPRESSION TAG	UNP Q8DKB5

- Molecule 2 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C₃H₈O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 3 1	0	0
2	A	1	Total C O 4 3 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	3	1		
2	C	1	Total	C	O	0	0
			4	3	1		
2	E	1	Total	C	O	0	0
			4	3	1		
2	E	1	Total	C	O	0	0
			4	3	1		
2	E	1	Total	C	O	0	0
			4	3	1		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	132	Total	O	0	0
			132	132		
5	B	133	Total	O	0	1
			134	134		

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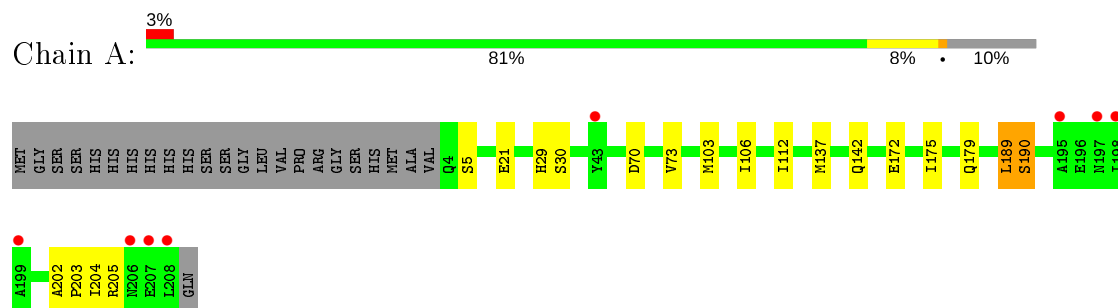
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	119	Total 121	O 121	0	2
5	D	130	Total 130	O 130	0	0
5	E	156	Total 157	O 157	0	1
5	F	137	Total 137	O 137	0	0

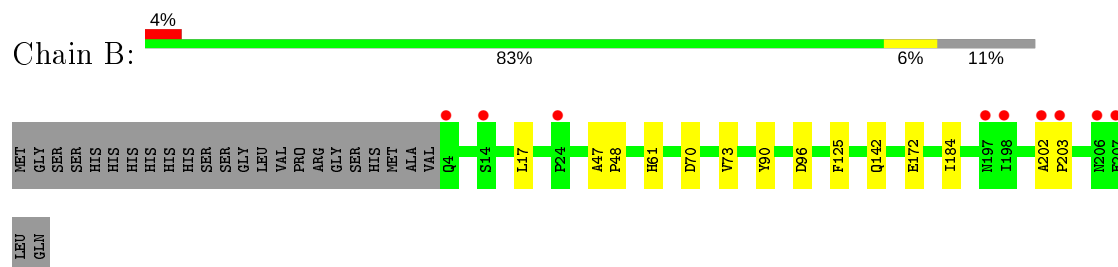
3 Residue-property plots [i](#)

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.

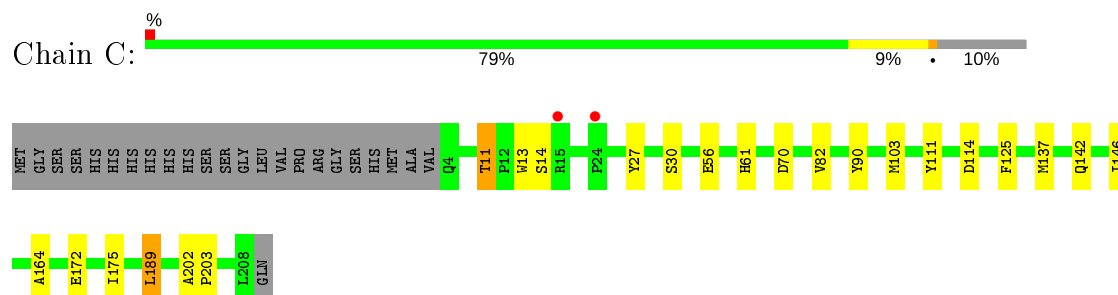
- Molecule 1: Carbon dioxide concentrating mechanism protein



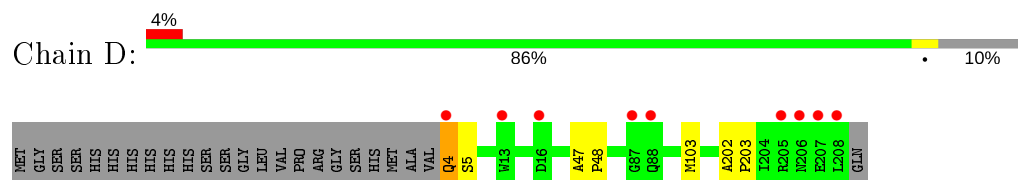
- Molecule 1: Carbon dioxide concentrating mechanism protein



- Molecule 1: Carbon dioxide concentrating mechanism protein



- Molecule 1: Carbon dioxide concentrating mechanism protein



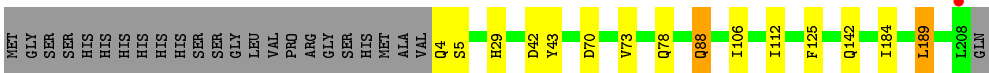
- Molecule 1: Carbon dioxide concentrating mechanism protein

Chain E:

83%

6%

10%



- Molecule 1: Carbon dioxide concentrating mechanism protein

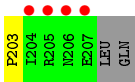
Chain F:

5%

83%

6%

11%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.90Å 105.04Å 196.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	16.88 – 2.00 16.88 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (16.88-2.00) 98.7 (16.88-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.200 , 0.247 0.204 , 0.253	Depositor DCC
R_{free} test set	5221 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	27.2	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10237	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.67 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6421e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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, IPA, 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	0.57	0/1618	0.65	0/2208
1	B	0.53	0/1592	0.65	1/2173 (0.0%)
1	C	0.57	0/1627	0.66	1/2220 (0.0%)
1	D	0.61	0/1607	0.64	0/2194
1	E	0.60	0/1600	0.67	0/2184
1	F	0.56	0/1592	0.64	0/2173
All	All	0.58	0/9636	0.65	2/13152 (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	C	114	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	96	ASP	CB-CG-OD2	5.01	122.81	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	1574	0	1527	11	0
1	B	1554	0	1500	8	0
1	C	1580	0	1537	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1566	0	1518	6	0
1	E	1562	0	1511	10	0
1	F	1554	0	1500	10	0
2	A	8	0	16	3	0
2	B	4	0	8	1	0
2	C	4	0	8	1	0
2	E	12	0	24	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
5	A	132	0	0	2	0
5	B	134	0	0	1	0
5	C	121	0	0	2	0
5	D	130	0	0	0	0
5	E	157	0	0	3	0
5	F	137	0	0	2	0
All	All	10237	0	9149	57	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (57) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:VAL:HG11	1:C:111:TYR:HB2	1.53	0.90
2:E:211:IPA:H32	5:E:875:HOH:O	1.75	0.86
1:E:29:HIS:ND1	2:E:211:IPA:H33	1.92	0.84
1:C:11:THR:HG21	1:C:13:TRP:CE2	2.25	0.72
1:E:4:GLN:N	5:E:550:HOH:O	2.30	0.65
2:E:301:IPA:H12	1:F:77:LEU:CD2	2.27	0.64
1:F:97:ASN:N	1:F:97:ASN:HD22	1.96	0.64
2:E:301:IPA:H12	1:F:77:LEU:HD23	1.82	0.61
1:C:11:THR:HG23	1:C:13:TRP:H	1.66	0.59
1:F:56:GLU:OE2	5:F:346:HOH:O	2.17	0.58
1:A:202:ALA:HB3	1:A:203:PRO:HD3	1.85	0.57
2:B:301:IPA:H12	5:C:616:HOH:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:TYR:CB	1:C:189:LEU:HD22	2.36	0.54
1:A:29:HIS:HB3	2:A:211:IPA:H33	1.88	0.54
1:A:205:ARG:HG3	1:B:17:LEU:HD13	1.91	0.53
1:A:204:ILE:HG22	1:B:17:LEU:HD11	1.92	0.52
1:D:103:MET:HE2	1:E:73:VAL:HG23	1.91	0.52
1:A:175:ILE:HD12	5:A:226:HOH:O	2.09	0.52
1:B:202:ALA:HB3	1:B:203:PRO:HD3	1.92	0.51
1:A:30:SER:HB3	2:A:211:IPA:H32	1.91	0.51
1:D:202:ALA:HB3	1:D:203:PRO:HD3	1.93	0.51
1:A:106:ILE:HD12	1:A:112:ILE:HD11	1.92	0.51
1:C:82:VAL:HG13	5:C:423:HOH:O	2.11	0.51
1:B:47:ALA:HB1	1:B:48:PRO:CD	2.41	0.50
1:F:97:ASN:ND2	1:F:97:ASN:N	2.60	0.49
1:B:61:HIS:HB2	1:B:90:TYR:CE2	2.48	0.49
1:C:11:THR:HG22	1:C:14:SER:H	1.76	0.49
1:A:73:VAL:HG23	1:C:103:MET:HE2	1.96	0.48
1:D:47:ALA:HB1	1:D:48:PRO:HD2	1.96	0.47
1:D:4:GLN:HE21	1:D:5:SER:H	1.61	0.47
1:E:106:ILE:HD12	1:E:112:ILE:HD11	1.97	0.47
1:D:103:MET:HE3	1:E:73:VAL:HB	1.96	0.47
1:A:189:LEU:HD12	1:A:190:SER:N	2.30	0.46
2:A:301:IPA:C1	5:B:874:HOH:O	2.62	0.46
1:C:172:GLU:HA	1:C:175:ILE:HD12	1.98	0.46
1:E:184:ILE:HG21	1:F:56:GLU:CD	2.36	0.46
1:C:27:TYR:HB3	1:C:189:LEU:HD22	1.97	0.45
1:F:202:ALA:HB3	1:F:203:PRO:HD3	1.99	0.45
1:F:47:ALA:HB1	1:F:48:PRO:CD	2.47	0.45
1:E:88:GLN:NE2	5:E:797:HOH:O	2.43	0.44
1:D:47:ALA:HB1	1:D:48:PRO:CD	2.47	0.44
1:E:125:PHE:O	1:E:142:GLN:HA	2.17	0.44
1:E:189:LEU:C	1:E:189:LEU:HD12	2.38	0.44
1:F:175:ILE:HD13	5:F:231:HOH:O	2.18	0.44
1:C:146:ILE:HD13	1:C:164:ALA:HB1	1.99	0.44
1:C:30:SER:H	2:C:210:IPA:H31	1.83	0.43
1:C:27:TYR:HB2	1:C:189:LEU:HD22	1.99	0.43
1:B:125:PHE:O	1:B:142:GLN:HA	2.19	0.43
1:C:61:HIS:HB2	1:C:90:TYR:CE2	2.54	0.42
1:B:184:ILE:HG21	1:C:56[A]:GLU:CD	2.40	0.42
1:A:103:MET:HE2	1:B:73:VAL:HG23	2.00	0.41
1:A:21:GLU:HG3	5:A:240:HOH:O	2.19	0.41
1:C:202:ALA:HB3	1:C:203:PRO:CD	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:PHE:HD2	1:C:142:GLN:HE21	1.68	0.41
1:C:11:THR:CG2	1:C:13:TRP:CE2	3.01	0.41
1:F:125:PHE:O	1:F:142:GLN:HA	2.21	0.41
1:E:42:ASP:HB3	1:E:43:TYR:CD2	2.55	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	205/229 (90%)	202 (98%)	3 (2%)	0	100	100
1	B	202/229 (88%)	198 (98%)	4 (2%)	0	100	100
1	C	206/229 (90%)	202 (98%)	4 (2%)	0	100	100
1	D	204/229 (89%)	200 (98%)	4 (2%)	0	100	100
1	E	203/229 (89%)	201 (99%)	2 (1%)	0	100	100
1	F	202/229 (88%)	198 (98%)	4 (2%)	0	100	100
All	All	1222/1374 (89%)	1201 (98%)	21 (2%)	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	170/188 (90%)	161 (95%)	9 (5%)	22	18
1	B	167/188 (89%)	165 (99%)	2 (1%)	71	76
1	C	171/188 (91%)	167 (98%)	4 (2%)	50	53
1	D	169/188 (90%)	168 (99%)	1 (1%)	86	90
1	E	168/188 (89%)	163 (97%)	5 (3%)	41	41
1	F	167/188 (89%)	161 (96%)	6 (4%)	35	34
All	All	1012/1128 (90%)	985 (97%)	27 (3%)	46	46

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	70	ASP
1	A	137	MET
1	A	142[A]	GLN
1	A	142[B]	GLN
1	A	172	GLU
1	A	179	GLN
1	A	189	LEU
1	A	190	SER
1	B	70	ASP
1	B	172	GLU
1	C	11	THR
1	C	70	ASP
1	C	137	MET
1	C	189	LEU
1	D	4	GLN
1	E	5	SER
1	E	70	ASP
1	E	78	GLN
1	E	88	GLN
1	E	189	LEU
1	F	4	GLN
1	F	70	ASP
1	F	97	ASN
1	F	137	MET
1	F	172	GLU
1	F	189	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	179	GLN
1	B	176	HIS
1	B	185	ASN
1	B	206	ASN
1	C	97	ASN
1	C	179	GLN
1	D	4	GLN
1	D	142	GLN
1	E	88	GLN
1	E	176	HIS
1	F	79	GLN
1	F	97	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](#)

Of 15 ligands modelled in this entry, 8 are monoatomic - leaving 7 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	$\# Z > 2$
2	IPA	A	211	-	3,3,3	0.79	0	3,3,3	0.14	0
2	IPA	E	211	-	3,3,3	0.61	0	3,3,3	0.22	0
2	IPA	C	210	-	3,3,3	0.72	0	3,3,3	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	IPA	E	301	-	3,3,3	0.54	0	3,3,3	0.20	0
2	IPA	A	301	-	3,3,3	0.54	0	3,3,3	0.29	0
2	IPA	E	210	-	3,3,3	0.56	0	3,3,3	0.19	0
2	IPA	B	301	-	3,3,3	0.55	0	3,3,3	0.22	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.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	211	IPA	2	0
2	E	211	IPA	2	0
2	C	210	IPA	1	0
2	E	301	IPA	2	0
2	A	301	IPA	1	0
2	B	301	IPA	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	205/229 (89%)	0.37	8 (3%)	39	38	23, 26, 27, 29	0
1	B	204/229 (89%)	0.50	9 (4%)	34	33	23, 26, 27, 29	0
1	C	205/229 (89%)	0.33	2 (0%)	82	81	23, 26, 28, 30	0
1	D	205/229 (89%)	0.43	9 (4%)	34	33	24, 26, 28, 30	0
1	E	205/229 (89%)	0.28	1 (0%)	91	90	23, 26, 28, 31	0
1	F	204/229 (89%)	0.50	12 (5%)	22	21	24, 26, 28, 30	0
All	All	1228/1374 (89%)	0.40	41 (3%)	46	45	23, 26, 28, 31	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	208	LEU	6.8
1	B	206	ASN	5.3
1	D	87	GLY	4.9
1	D	4	GLN	4.4
1	A	208	LEU	4.1
1	A	206	ASN	4.0
1	D	206	ASN	3.9
1	F	204	ILE	3.9
1	A	207	GLU	3.8
1	B	24	PRO	3.8
1	A	198	ILE	3.7
1	F	206	ASN	3.6
1	B	207	GLU	3.5
1	F	5	SER	3.2
1	F	4	GLN	3.2
1	B	202	ALA	3.0
1	F	207	GLU	3.0
1	D	13	TRP	2.9
1	E	208	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	199	ALA	2.6
1	B	14	SER	2.6
1	F	90	TYR	2.5
1	F	199	ALA	2.5
1	B	4	GLN	2.5
1	B	203	PRO	2.5
1	D	205	ARG	2.5
1	A	197	ASN	2.4
1	D	16	ASP	2.4
1	B	198	ILE	2.4
1	D	207	GLU	2.3
1	F	87	GLY	2.3
1	F	44	VAL	2.3
1	C	15	ARG	2.3
1	F	205	ARG	2.3
1	A	195	ALA	2.2
1	C	24	PRO	2.2
1	B	197	ASN	2.2
1	F	88	GLN	2.1
1	F	198	ILE	2.1
1	D	88	GLN	2.1
1	A	43	TYR	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 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(Å ²)	Q<0.9
2	IPA	C	210	4/4	0.70	0.28	24,24,24,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	IPA	A	211	4/4	0.77	0.20	19,20,20,20	0
2	IPA	E	211	4/4	0.80	0.19	25,26,26,27	0
2	IPA	E	301	4/4	0.86	0.20	30,30,30,30	0
2	IPA	B	301	4/4	0.92	0.13	35,35,35,35	0
2	IPA	E	210	4/4	0.93	0.12	41,41,41,41	0
2	IPA	A	301	4/4	0.93	0.14	33,34,34,34	0
3	ZN	C	300	1/1	0.97	0.21	35,35,35,35	0
3	ZN	B	300	1/1	0.98	0.21	38,38,38,38	0
3	ZN	E	300	1/1	0.99	0.18	29,29,29,29	0
4	CL	D	210	1/1	0.99	0.10	16,16,16,16	0
3	ZN	D	300	1/1	0.99	0.20	36,36,36,36	0
3	ZN	A	300	1/1	0.99	0.18	32,32,32,32	0
4	CL	A	210	1/1	0.99	0.05	20,20,20,20	0
3	ZN	F	300	1/1	0.99	0.21	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.