



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:15 PM UTC

PDB ID : 5O3M / pdb_00005o3m
Title : Crystal structure of apo *Klebsiella pneumoniae* 3,4-dihydroxybenzoic acid decarboxylase (AroY)
Authors : Marshall, S.A.; Leys, D.
Deposited on : 2017-05-24
Resolution : 2.23 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

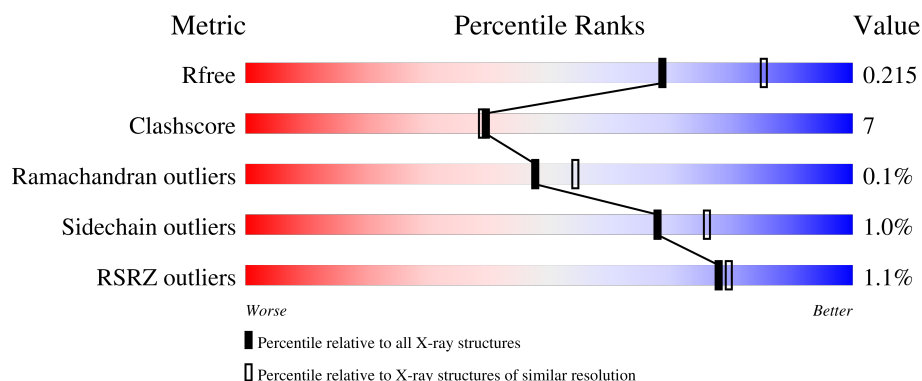
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.23 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	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

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	522	% 84% 11% 6%
1	B	522	3% 75% 18% 6%
1	C	522	% 81% 12% 6%
1	D	522	85% 9% 6%
1	E	522	83% 11% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	522	2% 74% 19% • 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23577 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 Protocatechuate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	493	Total	C	N	O	S	0	0	0
			3734	2366	653	698	17			
1	B	490	Total	C	N	O	S	0	0	0
			3706	2349	647	693	17			
1	C	489	Total	C	N	O	S	0	0	0
			3701	2346	646	692	17			
1	D	491	Total	C	N	O	S	0	0	0
			3711	2352	648	694	17			
1	E	491	Total	C	N	O	S	0	0	0
			3720	2358	651	694	17			
1	F	488	Total	C	N	O	S	0	0	0
			3689	2338	643	691	17			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP B9A9M6
A	-18	GLY	-	expression tag	UNP B9A9M6
A	-17	SER	-	expression tag	UNP B9A9M6
A	-16	SER	-	expression tag	UNP B9A9M6
A	-15	HIS	-	expression tag	UNP B9A9M6
A	-14	HIS	-	expression tag	UNP B9A9M6
A	-13	HIS	-	expression tag	UNP B9A9M6
A	-12	HIS	-	expression tag	UNP B9A9M6
A	-11	HIS	-	expression tag	UNP B9A9M6
A	-10	HIS	-	expression tag	UNP B9A9M6
A	-9	SER	-	expression tag	UNP B9A9M6
A	-8	SER	-	expression tag	UNP B9A9M6
A	-7	GLY	-	expression tag	UNP B9A9M6
A	-6	LEU	-	expression tag	UNP B9A9M6
A	-5	VAL	-	expression tag	UNP B9A9M6
A	-4	PRO	-	expression tag	UNP B9A9M6
A	-3	ARG	-	expression tag	UNP B9A9M6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP B9A9M6
A	-1	SER	-	expression tag	UNP B9A9M6
A	0	HIS	-	expression tag	UNP B9A9M6
B	-19	MET	-	initiating methionine	UNP B9A9M6
B	-18	GLY	-	expression tag	UNP B9A9M6
B	-17	SER	-	expression tag	UNP B9A9M6
B	-16	SER	-	expression tag	UNP B9A9M6
B	-15	HIS	-	expression tag	UNP B9A9M6
B	-14	HIS	-	expression tag	UNP B9A9M6
B	-13	HIS	-	expression tag	UNP B9A9M6
B	-12	HIS	-	expression tag	UNP B9A9M6
B	-11	HIS	-	expression tag	UNP B9A9M6
B	-10	HIS	-	expression tag	UNP B9A9M6
B	-9	SER	-	expression tag	UNP B9A9M6
B	-8	SER	-	expression tag	UNP B9A9M6
B	-7	GLY	-	expression tag	UNP B9A9M6
B	-6	LEU	-	expression tag	UNP B9A9M6
B	-5	VAL	-	expression tag	UNP B9A9M6
B	-4	PRO	-	expression tag	UNP B9A9M6
B	-3	ARG	-	expression tag	UNP B9A9M6
B	-2	GLY	-	expression tag	UNP B9A9M6
B	-1	SER	-	expression tag	UNP B9A9M6
B	0	HIS	-	expression tag	UNP B9A9M6
C	-19	MET	-	initiating methionine	UNP B9A9M6
C	-18	GLY	-	expression tag	UNP B9A9M6
C	-17	SER	-	expression tag	UNP B9A9M6
C	-16	SER	-	expression tag	UNP B9A9M6
C	-15	HIS	-	expression tag	UNP B9A9M6
C	-14	HIS	-	expression tag	UNP B9A9M6
C	-13	HIS	-	expression tag	UNP B9A9M6
C	-12	HIS	-	expression tag	UNP B9A9M6
C	-11	HIS	-	expression tag	UNP B9A9M6
C	-10	HIS	-	expression tag	UNP B9A9M6
C	-9	SER	-	expression tag	UNP B9A9M6
C	-8	SER	-	expression tag	UNP B9A9M6
C	-7	GLY	-	expression tag	UNP B9A9M6
C	-6	LEU	-	expression tag	UNP B9A9M6
C	-5	VAL	-	expression tag	UNP B9A9M6
C	-4	PRO	-	expression tag	UNP B9A9M6
C	-3	ARG	-	expression tag	UNP B9A9M6
C	-2	GLY	-	expression tag	UNP B9A9M6
C	-1	SER	-	expression tag	UNP B9A9M6

Continued on next page...

Continued from previous page...

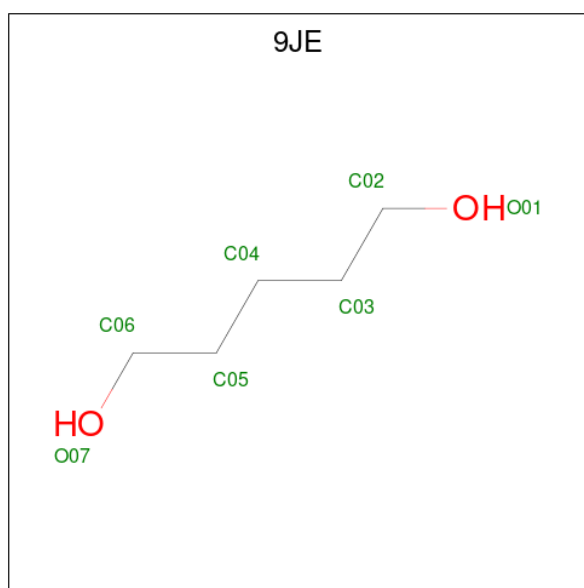
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	expression tag	UNP B9A9M6
D	-19	MET	-	initiating methionine	UNP B9A9M6
D	-18	GLY	-	expression tag	UNP B9A9M6
D	-17	SER	-	expression tag	UNP B9A9M6
D	-16	SER	-	expression tag	UNP B9A9M6
D	-15	HIS	-	expression tag	UNP B9A9M6
D	-14	HIS	-	expression tag	UNP B9A9M6
D	-13	HIS	-	expression tag	UNP B9A9M6
D	-12	HIS	-	expression tag	UNP B9A9M6
D	-11	HIS	-	expression tag	UNP B9A9M6
D	-10	HIS	-	expression tag	UNP B9A9M6
D	-9	SER	-	expression tag	UNP B9A9M6
D	-8	SER	-	expression tag	UNP B9A9M6
D	-7	GLY	-	expression tag	UNP B9A9M6
D	-6	LEU	-	expression tag	UNP B9A9M6
D	-5	VAL	-	expression tag	UNP B9A9M6
D	-4	PRO	-	expression tag	UNP B9A9M6
D	-3	ARG	-	expression tag	UNP B9A9M6
D	-2	GLY	-	expression tag	UNP B9A9M6
D	-1	SER	-	expression tag	UNP B9A9M6
D	0	HIS	-	expression tag	UNP B9A9M6
E	-19	MET	-	initiating methionine	UNP B9A9M6
E	-18	GLY	-	expression tag	UNP B9A9M6
E	-17	SER	-	expression tag	UNP B9A9M6
E	-16	SER	-	expression tag	UNP B9A9M6
E	-15	HIS	-	expression tag	UNP B9A9M6
E	-14	HIS	-	expression tag	UNP B9A9M6
E	-13	HIS	-	expression tag	UNP B9A9M6
E	-12	HIS	-	expression tag	UNP B9A9M6
E	-11	HIS	-	expression tag	UNP B9A9M6
E	-10	HIS	-	expression tag	UNP B9A9M6
E	-9	SER	-	expression tag	UNP B9A9M6
E	-8	SER	-	expression tag	UNP B9A9M6
E	-7	GLY	-	expression tag	UNP B9A9M6
E	-6	LEU	-	expression tag	UNP B9A9M6
E	-5	VAL	-	expression tag	UNP B9A9M6
E	-4	PRO	-	expression tag	UNP B9A9M6
E	-3	ARG	-	expression tag	UNP B9A9M6
E	-2	GLY	-	expression tag	UNP B9A9M6
E	-1	SER	-	expression tag	UNP B9A9M6
E	0	HIS	-	expression tag	UNP B9A9M6
F	-19	MET	-	initiating methionine	UNP B9A9M6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	-18	GLY	-	expression tag	UNP B9A9M6
F	-17	SER	-	expression tag	UNP B9A9M6
F	-16	SER	-	expression tag	UNP B9A9M6
F	-15	HIS	-	expression tag	UNP B9A9M6
F	-14	HIS	-	expression tag	UNP B9A9M6
F	-13	HIS	-	expression tag	UNP B9A9M6
F	-12	HIS	-	expression tag	UNP B9A9M6
F	-11	HIS	-	expression tag	UNP B9A9M6
F	-10	HIS	-	expression tag	UNP B9A9M6
F	-9	SER	-	expression tag	UNP B9A9M6
F	-8	SER	-	expression tag	UNP B9A9M6
F	-7	GLY	-	expression tag	UNP B9A9M6
F	-6	LEU	-	expression tag	UNP B9A9M6
F	-5	VAL	-	expression tag	UNP B9A9M6
F	-4	PRO	-	expression tag	UNP B9A9M6
F	-3	ARG	-	expression tag	UNP B9A9M6
F	-2	GLY	-	expression tag	UNP B9A9M6
F	-1	SER	-	expression tag	UNP B9A9M6
F	0	HIS	-	expression tag	UNP B9A9M6

- Molecule 2 is pentane-1,5-diol (CCD ID: 9JE) (formula: C₅H₁₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	5	2		
2	A	1	Total	C	O	0	0
			7	5	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 7 5 2	0	0
2	C	1	Total C O 7 5 2	0	0
2	C	1	Total C O 7 5 2	0	0
2	C	1	Total C O 7 5 2	0	0
2	D	1	Total C O 7 5 2	0	0
2	D	1	Total C O 7 5 2	0	0
2	E	1	Total C O 7 5 2	0	0
2	F	1	Total C O 7 5 2	0	0

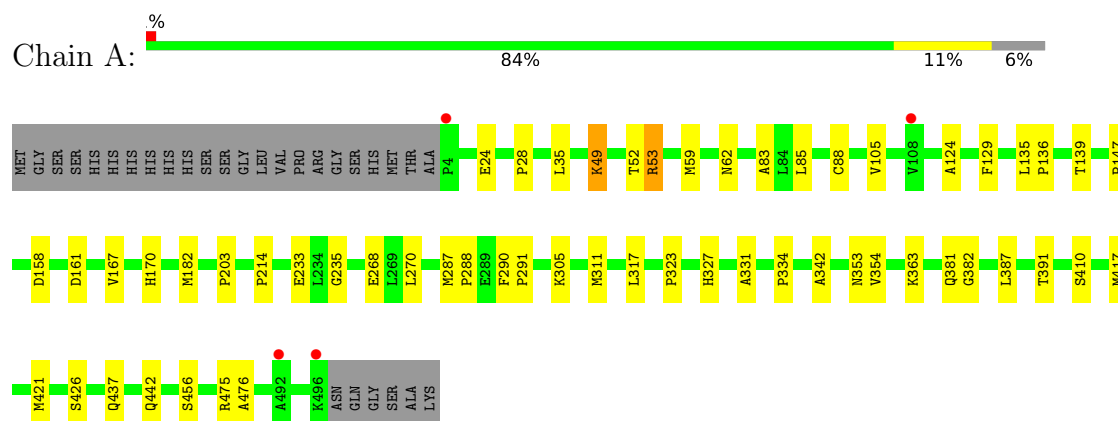
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	235	Total O 235 235	0	0
3	B	176	Total O 176 176	0	0
3	C	178	Total O 178 178	0	0
3	D	311	Total O 311 311	0	0
3	E	217	Total O 217 217	0	0
3	F	129	Total O 129 129	0	0

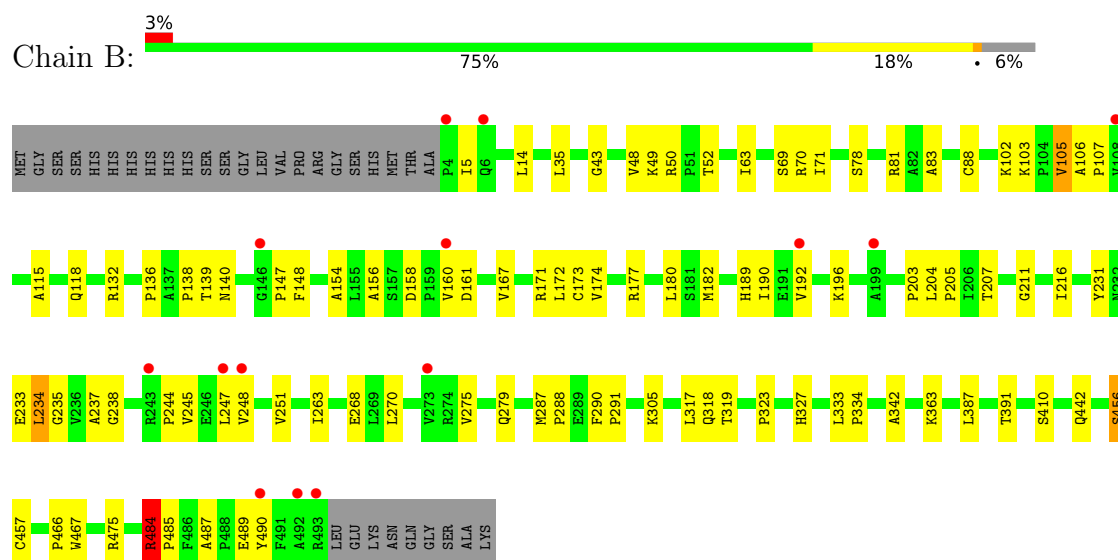
3 Residue-property plots

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.

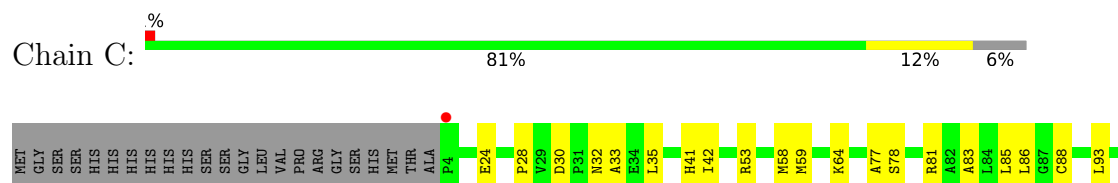
• Molecule 1: Protocatechuate decarboxylase

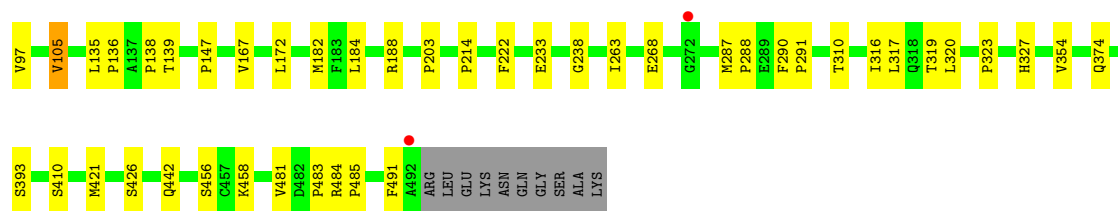


• Molecule 1: Protocatechuate decarboxylase



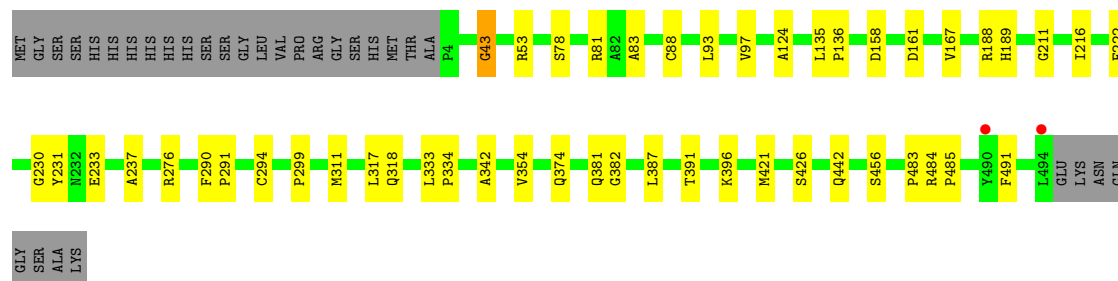
• Molecule 1: Protocatechuate decarboxylase





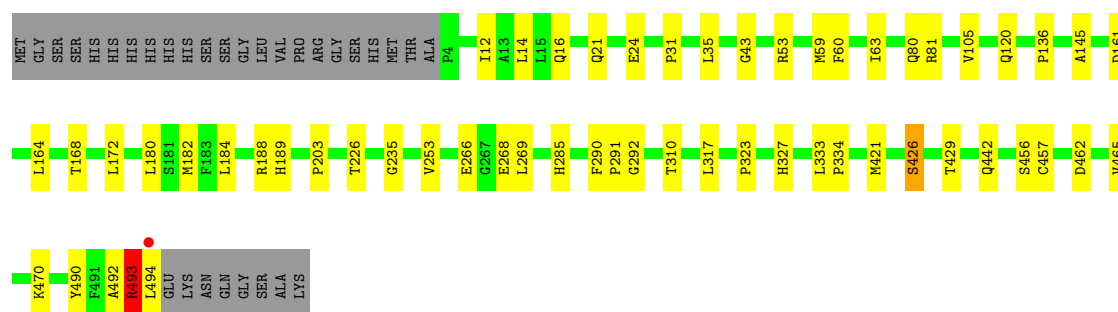
• Molecule 1: Protocatechuate decarboxylase

Chain D: 85% 9% 6%



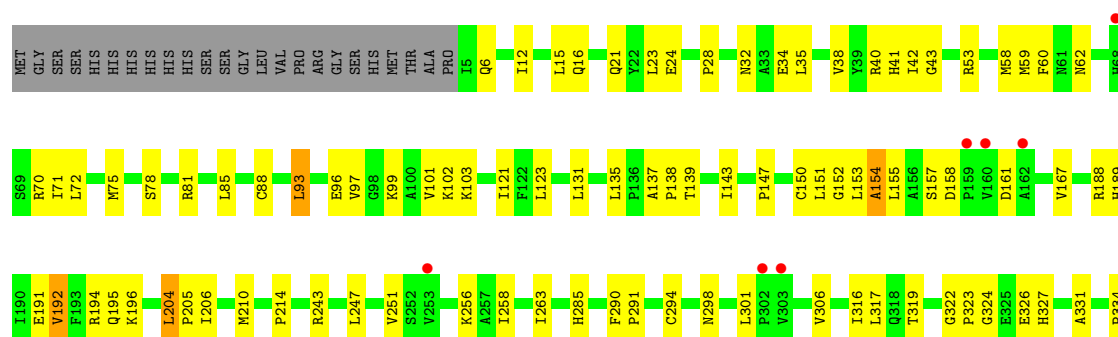
• Molecule 1: Protocatechuate decarboxylase

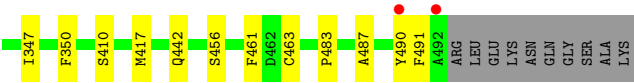
Chain E: 83% 11% 6%



• Molecule 1: Protocatechuate decarboxylase

Chain F: 2% 74% 19% 7%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.88Å 209.70Å 116.02Å 90.00° 107.63° 90.00°	Depositor
Resolution (Å)	38.08 – 2.23 38.08 – 2.23	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.08-2.23) 99.8 (38.08-2.23)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.22Å)	Xtriage
Refinement program	PHENIX (dev_2689)	Depositor
R, R_{free}	0.163 , 0.209 0.175 , 0.215	Depositor DCC
R_{free} test set	8848 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.468	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	23577	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 9JE

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	0.45	3/3821 (0.1%)	0.56	4/5209 (0.1%)
1	B	0.43	1/3793 (0.0%)	0.53	2/5172 (0.0%)
1	C	0.30	1/3788 (0.0%)	0.53	3/5165 (0.1%)
1	D	0.38	0/3798	0.54	2/5179 (0.0%)
1	E	0.38	1/3807 (0.0%)	0.49	0/5190
1	F	0.31	0/3774	0.47	1/5146 (0.0%)
All	All	0.38	6/22781 (0.0%)	0.52	12/31061 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	52	THR	C-N	-10.05	1.20	1.33
1	B	484	ARG	C-O	-7.02	1.17	1.24
1	C	77	ALA	C-N	-6.30	1.24	1.33
1	E	80	GLN	C-O	-5.97	1.17	1.24
1	A	354	VAL	C-O	-5.82	1.18	1.24
1	A	353	ASN	C-O	-5.15	1.18	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	77	ALA	CA-C-N	11.48	143.46	121.54
1	C	77	ALA	C-N-CA	11.48	143.46	121.54
1	A	53	ARG	O-C-N	-9.00	114.29	123.29
1	C	77	ALA	O-C-N	-8.72	109.17	121.72
1	A	53	ARG	CA-C-N	7.92	131.92	120.91
1	A	53	ARG	C-N-CA	7.92	131.92	120.91
1	D	124	ALA	CA-C-N	6.64	129.47	120.38
1	D	124	ALA	C-N-CA	6.64	129.47	120.38
1	A	52	THR	O-C-N	-6.43	116.51	123.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	154	ALA	N-CA-C	5.99	118.72	109.07
1	B	457	CYS	N-CA-C	-5.19	101.24	109.96
1	B	456	SER	N-CA-C	5.05	116.66	109.14

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	3734	0	3724	38	0
1	B	3706	0	3694	77	0
1	C	3701	0	3691	45	0
1	D	3711	0	3696	25	0
1	E	3720	0	3716	33	0
1	F	3689	0	3679	87	0
2	A	14	0	0	0	0
2	B	7	0	0	0	0
2	C	21	0	0	0	0
2	D	14	0	0	0	0
2	E	7	0	0	0	0
2	F	7	0	0	0	0
3	A	235	0	0	3	0
3	B	176	0	0	4	0
3	C	178	0	0	1	0
3	D	311	0	0	1	0
3	E	217	0	0	2	0
3	F	129	0	0	1	0
All	All	23577	0	22200	297	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 7.

All (297) 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:42:ILE:HD13	1:C:58:MET:HE1	1.30	1.12
1:B:115:ALA:HB2	1:B:248:VAL:HG21	1.41	0.98
1:C:53:ARG:NH1	1:F:490:TYR:OH	1.97	0.97
1:F:42:ILE:HD13	1:F:58:MET:HE1	1.48	0.95
1:F:72:LEU:HD21	1:F:75:MET:HE3	1.50	0.91
1:B:387:LEU:O	1:B:391:THR:HG23	1.77	0.83
1:F:32:ASN:HA	1:F:139:THR:HG22	1.60	0.83
1:F:23:LEU:HD23	1:F:58:MET:HE2	1.63	0.81
1:B:50:ARG:HD3	1:B:52:THR:HG22	1.64	0.80
1:E:168:THR:HG22	1:E:188:ARG:HH21	1.46	0.79
1:F:42:ILE:HG21	1:F:58:MET:CE	2.13	0.79
1:C:53:ARG:HH12	1:F:490:TYR:HH	1.33	0.77
1:C:136:PRO:O	1:C:317:LEU:HD22	1.86	0.76
1:B:234:LEU:HB3	1:B:245:VAL:HG11	1.68	0.75
1:F:42:ILE:HG21	1:F:58:MET:HE1	1.69	0.74
1:C:30:ASP:OD2	3:C:701:HOH:O	2.05	0.74
1:F:35:LEU:HD21	1:F:60:PHE:CD2	2.23	0.73
1:A:170:HIS:CG	1:A:182:MET:HE2	2.24	0.73
1:F:59:MET:HE1	1:F:316:ILE:HG23	1.68	0.73
1:E:188:ARG:HD2	1:E:189:HIS:H	1.53	0.72
1:F:6:GLN:HG3	1:F:243:ARG:HE	1.53	0.72
1:B:167:VAL:HG21	1:B:234:LEU:HD22	1.70	0.72
1:F:15:LEU:HD21	1:F:85:LEU:HD21	1.74	0.70
1:C:42:ILE:HD13	1:C:58:MET:CE	2.18	0.69
1:F:155:LEU:O	1:F:206:ILE:HD12	1.93	0.69
1:F:6:GLN:HG3	1:F:243:ARG:HH21	1.58	0.67
1:F:85:LEU:HD13	1:F:214:PRO:HG3	1.77	0.66
1:F:23:LEU:HD23	1:F:58:MET:CE	2.27	0.65
1:C:42:ILE:HG21	1:C:58:MET:CE	2.27	0.65
1:B:204:LEU:HD12	1:B:205:PRO:HD2	1.78	0.64
1:F:99:LYS:HA	1:F:102:LYS:HD2	1.78	0.64
1:F:290:PHE:CG	1:F:291:PRO:HD3	2.33	0.64
1:B:189:HIS:HA	1:B:192:VAL:HG12	1.79	0.64
1:F:6:GLN:CG	1:F:243:ARG:HE	2.11	0.64
1:F:42:ILE:HD13	1:F:58:MET:CE	2.27	0.63
1:B:102:LYS:O	1:B:103:LYS:HD2	1.99	0.63
1:E:168:THR:CG2	1:E:188:ARG:HH21	2.11	0.63
1:B:139:THR:HG22	1:B:147:PRO:HA	1.81	0.62
1:A:387:LEU:O	1:A:391:THR:HG23	1.98	0.62
1:A:53:ARG:NH1	1:B:490:TYR:OH	2.33	0.62
1:F:72:LEU:HD21	1:F:75:MET:CE	2.25	0.62
1:C:42:ILE:HG21	1:C:58:MET:HE3	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:158:ASP:HB3	1:F:161:ASP:O	2.00	0.61
1:F:442:GLN:CD	1:F:456:SER:HB2	2.26	0.61
1:B:172:LEU:HD21	1:B:182:MET:HE3	1.82	0.61
1:B:167:VAL:HG21	1:B:234:LEU:CD2	2.30	0.61
1:E:168:THR:HG21	1:E:188:ARG:HE	1.66	0.61
1:A:342:ALA:CB	1:A:391:THR:HG21	2.32	0.60
1:F:42:ILE:HG21	1:F:58:MET:HE3	1.83	0.60
1:F:24:GLU:HG2	1:F:59:MET:HB3	1.84	0.59
1:C:290:PHE:CG	1:C:291:PRO:HD3	2.38	0.59
1:B:342:ALA:CB	1:B:391:THR:HG21	2.34	0.58
1:D:484:ARG:HB2	1:D:485:PRO:HD3	1.86	0.58
1:B:107:PRO:HB2	1:B:247:LEU:HD11	1.84	0.58
1:B:275:VAL:HB	1:B:279:GLN:NE2	2.19	0.58
1:F:121:ILE:HD12	1:F:251:VAL:HG11	1.85	0.58
1:C:97:VAL:HG11	1:C:222:PHE:CE1	2.38	0.58
1:D:211:GLY:HA2	1:D:318:GLN:OE1	2.03	0.58
1:E:60:PHE:O	1:E:63:ILE:HD11	2.04	0.58
1:E:290:PHE:CG	1:E:291:PRO:HD3	2.40	0.57
1:B:139:THR:HG23	3:B:731:HOH:O	2.03	0.57
1:E:182:MET:HE3	1:E:184:LEU:HD21	1.86	0.57
1:D:135:LEU:HD21	1:D:311:MET:HE1	1.86	0.57
1:B:275:VAL:HB	1:B:279:GLN:HE22	1.70	0.56
1:E:421:MET:HG2	1:E:426:SER:HB2	1.87	0.56
1:B:136:PRO:O	1:B:317:LEU:HD22	2.05	0.56
1:B:107:PRO:HB2	1:B:247:LEU:CD1	2.35	0.56
1:C:135:LEU:HD21	1:C:263:ILE:HG21	1.87	0.56
1:F:154:ALA:HB1	1:F:206:ILE:HD11	1.86	0.56
1:B:231:TYR:HB3	1:B:234:LEU:HD23	1.87	0.56
1:A:437:GLN:NE2	3:A:703:HOH:O	2.39	0.56
1:C:85:LEU:HD13	1:C:214:PRO:HG3	1.88	0.55
1:F:152:GLY:HA2	1:F:210:MET:HG2	1.88	0.55
1:B:102:LYS:C	1:B:103:LYS:HD2	2.31	0.55
1:F:194:ARG:HA	1:F:204:LEU:HD12	1.89	0.55
1:F:263:ILE:HD12	1:F:317:LEU:HD13	1.88	0.55
1:F:6:GLN:HG3	1:F:243:ARG:NE	2.22	0.55
1:B:156:ALA:HB3	1:B:190:ILE:CD1	2.37	0.55
1:B:484:ARG:CB	1:B:485:PRO:HD3	2.37	0.55
1:D:342:ALA:CB	1:D:391:THR:HG21	2.37	0.55
1:E:442:GLN:CD	1:E:456:SER:HB2	2.32	0.55
1:F:191:GLU:O	1:F:195:GLN:HG3	2.06	0.54
1:A:49:LYS:HG3	1:B:475:ARG:HD3	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:PRO:HB2	1:B:174:VAL:HG22	1.89	0.54
1:F:32:ASN:OD1	1:F:139:THR:HG21	2.07	0.54
1:D:158:ASP:HB3	1:D:161:ASP:O	2.08	0.54
1:F:323:PRO:HB2	1:F:327:HIS:HB2	1.90	0.54
1:B:83:ALA:HB1	1:B:88:CYS:O	2.07	0.54
1:F:15:LEU:CD2	1:F:85:LEU:HD21	2.37	0.54
1:B:270:LEU:HD11	1:B:305:LYS:HB2	1.90	0.53
1:F:81:ARG:O	1:F:85:LEU:HG	2.07	0.53
1:C:78:SER:HB3	1:C:81:ARG:HB3	1.91	0.53
1:B:107:PRO:HB3	1:B:245:VAL:HG13	1.89	0.53
1:F:6:GLN:HG3	1:F:243:ARG:NH2	2.24	0.53
1:A:136:PRO:O	1:A:317:LEU:HD22	2.09	0.53
1:C:167:VAL:HB	1:C:233:GLU:HB2	1.91	0.53
1:F:97:VAL:O	1:F:101:VAL:HG23	2.09	0.52
1:B:442:GLN:CD	1:B:456:SER:HB2	2.35	0.52
1:B:158:ASP:OD1	1:B:160:VAL:HG22	2.10	0.52
1:C:320:LEU:HD12	1:C:320:LEU:C	2.34	0.52
1:B:156:ALA:HB3	1:B:190:ILE:HD11	1.92	0.52
1:B:234:LEU:HB3	1:B:245:VAL:CG1	2.40	0.52
1:E:182:MET:HE2	1:E:269:LEU:HD21	1.90	0.52
1:A:290:PHE:CG	1:A:291:PRO:HD3	2.45	0.52
1:B:333:LEU:HB2	1:B:334:PRO:HD3	1.92	0.52
1:A:421:MET:HG2	1:A:426:SER:HB2	1.92	0.51
1:B:106:ALA:O	1:B:244:PRO:HB3	2.10	0.51
1:A:170:HIS:CB	1:A:182:MET:HE2	2.39	0.51
1:A:287:MET:HB2	1:A:288:PRO:HD2	1.92	0.51
1:F:78:SER:HB3	1:F:81:ARG:HB3	1.92	0.51
1:F:15:LEU:HD22	1:F:21:GLN:HB3	1.92	0.51
1:B:5:ILE:HD11	1:B:14:LEU:HD22	1.93	0.51
1:C:32:ASN:O	1:C:33:ALA:HB3	2.11	0.51
1:E:292:GLY:HA2	3:E:839:HOH:O	2.10	0.51
1:E:24:GLU:HG2	1:E:59:MET:HB3	1.93	0.51
1:B:105:VAL:HG22	1:B:238:GLY:HA3	1.93	0.51
1:F:247:LEU:HD23	1:F:256:LYS:HB3	1.93	0.51
1:C:139:THR:HG22	1:C:147:PRO:HA	1.93	0.50
1:D:136:PRO:O	1:D:317:LEU:HD22	2.11	0.50
1:A:287:MET:HB2	1:A:288:PRO:CD	2.41	0.50
1:A:203:PRO:HB2	1:A:268:GLU:HB2	1.92	0.50
1:A:290:PHE:CZ	1:A:363:LYS:HD3	2.47	0.49
1:B:275:VAL:CG1	1:B:279:GLN:HE22	2.25	0.49
1:A:35:LEU:C	1:A:35:LEU:HD23	2.37	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:VAL:HB	1:B:233:GLU:HB2	1.94	0.49
1:F:204:LEU:HD23	1:F:205:PRO:HD2	1.93	0.49
1:A:85:LEU:HD13	1:A:214:PRO:HG3	1.94	0.49
1:C:135:LEU:HD23	1:C:263:ILE:HD13	1.95	0.49
1:E:136:PRO:O	1:E:317:LEU:HD22	2.12	0.49
1:B:484:ARG:N	1:B:485:PRO:CD	2.75	0.49
1:C:323:PRO:HB2	1:C:327:HIS:HB2	1.92	0.49
1:E:31:PRO:HD3	1:E:63:ILE:HG23	1.95	0.49
1:C:105:VAL:HG22	1:C:238:GLY:HA3	1.94	0.49
1:E:323:PRO:HB2	1:E:327:HIS:HB2	1.94	0.49
1:F:155:LEU:HD11	1:F:258:ILE:HD12	1.94	0.49
1:C:42:ILE:HG21	1:C:58:MET:HE1	1.95	0.49
1:B:132:ARG:NH2	1:B:177:ARG:HB3	2.27	0.48
1:B:189:HIS:HA	1:B:192:VAL:CG1	2.43	0.48
1:F:192:VAL:O	1:F:196:LYS:HG3	2.13	0.48
1:F:103:LYS:HB2	1:F:103:LYS:HE2	1.61	0.48
1:B:118:GLN:NE2	1:B:251:VAL:HG13	2.29	0.48
1:E:21:GLN:OE1	1:E:81:ARG:HD3	2.13	0.48
1:A:83:ALA:HB1	1:A:88:CYS:O	2.14	0.48
1:B:290:PHE:CG	1:B:291:PRO:HD3	2.48	0.48
1:D:421:MET:HG2	1:D:426:SER:HB2	1.95	0.48
1:A:135:LEU:HD21	1:A:311:MET:HE1	1.95	0.48
1:A:139:THR:HG23	3:A:762:HOH:O	2.14	0.48
1:A:323:PRO:HB2	1:A:327:HIS:HB2	1.95	0.48
1:D:43:GLY:HA2	1:D:53:ARG:O	2.14	0.48
1:F:155:LEU:HD23	1:F:167:VAL:HG22	1.96	0.48
1:D:342:ALA:HB2	1:D:391:THR:HG21	1.96	0.48
1:F:41:HIS:O	1:F:53:ARG:NH1	2.41	0.47
1:E:105:VAL:O	1:E:235:GLY:HA2	2.14	0.47
1:B:139:THR:HG21	3:B:863:HOH:O	2.14	0.47
1:F:12:ILE:O	1:F:16:GLN:HG3	2.15	0.47
1:F:88:CYS:SG	1:F:93:LEU:HD13	2.55	0.47
1:A:158:ASP:HB3	1:A:161:ASP:O	2.15	0.47
1:C:182:MET:HE3	1:C:184:LEU:HD21	1.97	0.47
1:F:121:ILE:HG22	1:F:123:LEU:CD2	2.44	0.47
1:F:417:MET:HE1	1:F:461:PHE:CD1	2.50	0.47
1:C:203:PRO:HB2	1:C:268:GLU:HB3	1.95	0.47
1:A:24:GLU:HG2	1:A:59:MET:HB3	1.97	0.47
1:B:49:LYS:HG2	3:B:796:HOH:O	2.14	0.47
1:C:83:ALA:HB1	1:C:88:CYS:O	2.15	0.47
1:A:442:GLN:CD	1:A:456:SER:HB2	2.39	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:442:GLN:CD	1:C:456:SER:HB2	2.40	0.47
1:F:28:PRO:HG3	1:F:62:ASN:ND2	2.30	0.47
1:F:487:ALA:HB1	1:F:490:TYR:HB3	1.96	0.47
1:B:203:PRO:HB2	1:B:268:GLU:HB3	1.97	0.46
1:F:32:ASN:HA	1:F:139:THR:CG2	2.40	0.46
1:F:35:LEU:HD13	1:F:35:LEU:C	2.39	0.46
1:F:40:ARG:HD2	3:F:732:HOH:O	2.15	0.46
1:A:170:HIS:HB2	1:A:182:MET:HE2	1.98	0.46
1:A:410:SER:HB3	1:B:410:SER:HB3	1.96	0.46
1:C:393:SER:O	1:C:458:LYS:NZ	2.49	0.46
1:F:35:LEU:HD21	1:F:60:PHE:CG	2.49	0.46
1:E:35:LEU:C	1:E:35:LEU:HD23	2.41	0.46
1:B:48:VAL:HG12	1:B:49:LYS:O	2.15	0.46
1:D:374:GLN:NE2	3:D:705:HOH:O	2.48	0.46
1:F:150:CYS:O	1:F:151:LEU:HD23	2.16	0.46
1:D:387:LEU:O	1:D:391:THR:HG23	2.15	0.46
1:D:78:SER:HB3	1:D:81:ARG:HB3	1.97	0.46
1:D:396:LYS:HE2	3:E:792:HOH:O	2.15	0.46
1:B:290:PHE:CZ	1:B:363:LYS:HD3	2.51	0.46
1:E:490:TYR:O	1:E:493:ARG:HG2	2.16	0.46
1:C:320:LEU:HD12	1:C:320:LEU:O	2.16	0.45
1:B:211:GLY:HA2	1:B:318:GLN:OE1	2.16	0.45
1:D:442:GLN:CD	1:D:456:SER:HB2	2.41	0.45
1:A:139:THR:HG22	1:A:147:PRO:HA	1.99	0.45
1:C:41:HIS:CG	1:F:483:PRO:HG3	2.51	0.45
1:A:342:ALA:HB2	1:A:391:THR:HG21	1.98	0.45
1:D:167:VAL:HB	1:D:233:GLU:HB2	1.98	0.45
1:F:137:ALA:O	1:F:147:PRO:HB3	2.17	0.45
1:A:417:MET:O	1:A:421:MET:HE3	2.17	0.45
1:C:53:ARG:NH1	1:F:490:TYR:HH	2.00	0.45
1:C:172:LEU:N	1:C:172:LEU:HD12	2.31	0.45
1:D:83:ALA:HB1	1:D:88:CYS:O	2.17	0.45
1:B:138:PRO:HG2	1:B:319:THR:HG21	1.98	0.45
1:B:275:VAL:CB	1:B:279:GLN:HE22	2.30	0.45
1:B:323:PRO:HB2	1:B:327:HIS:HB2	1.99	0.45
1:F:58:MET:HG2	1:F:60:PHE:CE2	2.52	0.45
1:A:28:PRO:HG3	1:A:62:ASN:ND2	2.32	0.45
1:B:172:LEU:HD12	1:B:172:LEU:N	2.32	0.44
1:A:105:VAL:O	1:A:235:GLY:HA2	2.16	0.44
1:D:483:PRO:HB2	1:D:491:PHE:CZ	2.52	0.44
1:B:287:MET:HB2	1:B:288:PRO:HD2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:410:SER:HB3	1:F:410:SER:HB3	1.99	0.44
1:D:290:PHE:CG	1:D:291:PRO:HD3	2.52	0.44
1:B:154:ALA:HA	1:B:207:THR:O	2.18	0.44
1:C:28:PRO:HB2	1:C:64:LYS:HE2	1.99	0.44
1:F:58:MET:HE3	1:F:58:MET:HB2	1.80	0.44
1:B:158:ASP:HB3	1:B:161:ASP:O	2.17	0.44
1:E:12:ILE:O	1:E:16:GLN:HG3	2.18	0.44
1:B:174:VAL:HG23	1:B:174:VAL:O	2.18	0.44
1:C:188:ARG:HA	1:C:188:ARG:HD2	1.85	0.44
1:E:492:ALA:O	1:E:494:LEU:N	2.50	0.44
1:F:417:MET:HG2	1:F:463:CYS:SG	2.58	0.44
1:B:78:SER:HB3	1:B:81:ARG:HB3	1.98	0.44
1:A:363:LYS:NZ	3:A:708:HOH:O	2.50	0.43
1:C:287:MET:HB2	1:C:288:PRO:CD	2.48	0.43
1:F:194:ARG:CA	1:F:204:LEU:HD12	2.47	0.43
1:B:263:ILE:HD12	1:B:317:LEU:HD12	2.00	0.43
1:B:317:LEU:HA	3:B:718:HOH:O	2.18	0.43
1:F:155:LEU:CD2	1:F:167:VAL:HG22	2.48	0.43
1:F:143:ILE:HD11	1:F:294:CYS:SG	2.59	0.43
1:B:177:ARG:H	1:B:177:ARG:HG2	1.58	0.43
1:D:333:LEU:HB2	1:D:334:PRO:HD3	2.01	0.43
1:F:34:GLU:O	1:F:38:VAL:HG23	2.18	0.43
1:F:138:PRO:HG2	1:F:319:THR:HG21	2.01	0.43
1:C:481:VAL:O	1:C:483:PRO:HD3	2.19	0.43
1:D:276:ARG:HG2	1:D:299:PRO:HA	2.01	0.43
1:F:143:ILE:HD12	1:F:285:HIS:ND1	2.34	0.43
1:C:85:LEU:HA	1:C:85:LEU:HD23	1.83	0.43
1:C:105:VAL:HG22	1:C:238:GLY:C	2.44	0.43
1:E:253:VAL:HG22	1:E:266:GLU:HB3	2.00	0.43
1:B:489:GLU:H	1:B:489:GLU:CD	2.26	0.42
1:F:188:ARG:HG3	1:F:189:HIS:N	2.33	0.42
1:F:347:ILE:HG22	1:F:350:PHE:HB2	2.02	0.42
1:F:487:ALA:O	1:F:491:PHE:HD2	2.02	0.42
1:B:35:LEU:HD23	1:B:35:LEU:C	2.45	0.42
1:B:171:ARG:C	1:B:172:LEU:HD12	2.45	0.42
1:C:138:PRO:HG2	1:C:319:THR:HG21	2.02	0.42
1:F:96:GLU:OE1	1:F:96:GLU:HA	2.19	0.42
1:F:290:PHE:CD1	1:F:291:PRO:HD3	2.54	0.42
1:A:331:ALA:O	1:A:334:PRO:HD2	2.18	0.42
1:B:63:ILE:HG12	1:B:71:ILE:HD12	2.01	0.42
1:B:63:ILE:HD12	1:B:69:SER:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:ARG:HG3	1:D:189:HIS:N	2.35	0.42
1:F:43:GLY:HA2	1:F:53:ARG:O	2.20	0.42
1:F:59:MET:HE3	1:F:71:ILE:C	2.45	0.42
1:D:381:GLN:HG2	1:D:382:GLY:N	2.33	0.42
1:C:35:LEU:C	1:C:35:LEU:HD23	2.45	0.42
1:A:167:VAL:HB	1:A:233:GLU:HB2	2.02	0.42
1:C:484:ARG:HB2	1:C:485:PRO:HD3	2.02	0.42
1:F:131:LEU:HD22	1:F:306:VAL:HG21	2.02	0.42
1:F:153:LEU:HD21	1:F:167:VAL:HG13	2.02	0.42
1:A:124:ALA:HA	1:A:129:PHE:CG	2.55	0.42
1:E:63:ILE:HD12	1:E:63:ILE:N	2.35	0.42
1:E:203:PRO:HB2	1:E:268:GLU:HB3	2.01	0.42
1:E:429:THR:HB	1:E:457:CYS:SG	2.60	0.42
1:A:381:GLN:HG2	1:A:382:GLY:N	2.35	0.41
1:C:59:MET:HE1	1:C:316:ILE:HD13	2.02	0.41
1:D:97:VAL:HG11	1:D:222:PHE:CE1	2.55	0.41
1:F:301:LEU:HD23	1:F:301:LEU:HA	1.95	0.41
1:A:475:ARG:O	1:A:476:ALA:C	2.63	0.41
1:B:466:PRO:O	1:B:467:TRP:C	2.63	0.41
1:F:322:GLY:HA3	1:F:323:PRO:C	2.44	0.41
1:A:331:ALA:C	1:A:334:PRO:HD2	2.45	0.41
1:B:287:MET:HB2	1:B:288:PRO:CD	2.51	0.41
1:E:333:LEU:HB2	1:E:334:PRO:HD3	2.02	0.41
1:F:59:MET:HE2	1:F:70:ARG:HB2	2.01	0.41
1:B:216:ILE:HA	1:B:237:ALA:HB2	2.03	0.41
1:C:86:LEU:HD12	1:C:93:LEU:HD11	2.02	0.41
1:B:105:VAL:O	1:B:235:GLY:HA2	2.21	0.41
1:B:148:PHE:CE1	1:B:173:CYS:HB2	2.56	0.41
1:B:158:ASP:CG	1:B:196:LYS:HZ2	2.25	0.41
1:B:487:ALA:HB1	1:B:490:TYR:HB3	2.02	0.41
1:C:421:MET:HG2	1:C:426:SER:HB2	2.01	0.41
1:E:43:GLY:HA2	1:E:53:ARG:O	2.21	0.41
1:E:120:GLN:O	1:E:310:THR:HA	2.21	0.41
1:E:172:LEU:N	1:E:172:LEU:HD12	2.36	0.41
1:E:426:SER:HB3	1:E:462:ASP:O	2.20	0.41
1:F:298:ASN:HB3	1:F:301:LEU:HG	2.03	0.41
1:F:322:GLY:HA3	1:F:324:GLY:N	2.35	0.41
1:F:331:ALA:O	1:F:334:PRO:HD2	2.21	0.41
1:F:135:LEU:HD22	1:F:263:ILE:HD13	2.03	0.41
1:B:161:ASP:OD1	1:B:161:ASP:C	2.64	0.40
1:B:290:PHE:CE1	1:B:363:LYS:HD3	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:LEU:CD2	1:C:263:ILE:HG21	2.51	0.40
1:E:161:ASP:OD2	1:E:164:LEU:HD23	2.21	0.40
1:A:270:LEU:HD11	1:A:305:LYS:HB2	2.03	0.40
1:D:230:GLY:O	1:D:231:TYR:C	2.65	0.40
1:B:63:ILE:CD1	1:B:70:ARG:HA	2.51	0.40
1:D:216:ILE:HA	1:D:237:ALA:HB2	2.02	0.40
1:C:24:GLU:HG2	1:C:59:MET:HB3	2.02	0.40
1:E:145:ALA:HB2	1:E:285:HIS:O	2.21	0.40
1:E:465:VAL:HG11	1:E:470:LYS:HA	2.03	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	491/522 (94%)	473 (96%)	18 (4%)	0	100	100
1	B	488/522 (94%)	472 (97%)	15 (3%)	1 (0%)	43	48
1	C	487/522 (93%)	469 (96%)	17 (4%)	1 (0%)	43	48
1	D	489/522 (94%)	469 (96%)	19 (4%)	1 (0%)	43	48
1	E	489/522 (94%)	471 (96%)	17 (4%)	1 (0%)	43	48
1	F	486/522 (93%)	466 (96%)	20 (4%)	0	100	100
All	All	2930/3132 (94%)	2820 (96%)	106 (4%)	4 (0%)	48	54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	493	ARG
1	C	491	PHE
1	B	43	GLY
1	D	43	GLY

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	395/419 (94%)	394 (100%)	1 (0%)	86	90
1	B	392/419 (94%)	387 (99%)	5 (1%)	61	71
1	C	392/419 (94%)	388 (99%)	4 (1%)	68	76
1	D	392/419 (94%)	389 (99%)	3 (1%)	73	80
1	E	394/419 (94%)	389 (99%)	5 (1%)	61	71
1	F	390/419 (93%)	385 (99%)	5 (1%)	61	71
All	All	2355/2514 (94%)	2332 (99%)	23 (1%)	68	76

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	LYS
1	B	105	VAL
1	B	140	ASN
1	B	180	LEU
1	B	234	LEU
1	B	484	ARG
1	C	105	VAL
1	C	310	THR
1	C	354	VAL
1	C	374	GLN
1	D	93	LEU
1	D	294	CYS
1	D	354	VAL
1	E	14	LEU
1	E	180	LEU
1	E	226	THR
1	E	426	SER
1	E	493	ARG
1	F	93	LEU
1	F	157	SER
1	F	192	VAL
1	F	204	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	326	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	313	ASN
1	A	472	HIS
1	B	118	GLN
1	B	279	GLN
1	B	352	GLN
1	B	453	ASN
1	B	472	HIS
1	C	6	GLN
1	C	18	HIS
1	C	27	HIS
1	C	68	HIS
1	C	120	GLN
1	C	352	GLN
1	C	453	ASN
1	C	472	HIS
1	D	6	GLN
1	D	18	HIS
1	D	120	GLN
1	D	352	GLN
1	D	453	ASN
1	E	18	HIS
1	F	18	HIS
1	F	92	GLN
1	F	209	ASN
1	F	232	ASN
1	F	352	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	9JE	A	602	-	6,6,6	0.41	0	5,5,5	1.12	0
2	9JE	A	601	-	6,6,6	0.33	0	5,5,5	0.24	0
2	9JE	F	601	-	6,6,6	0.38	0	5,5,5	0.17	0
2	9JE	C	602	-	6,6,6	0.69	0	5,5,5	0.69	0
2	9JE	D	601	-	6,6,6	0.34	0	5,5,5	0.23	0
2	9JE	B	601	-	6,6,6	0.44	0	5,5,5	0.22	0
2	9JE	D	602	-	6,6,6	0.98	0	5,5,5	0.51	0
2	9JE	C	601	-	6,6,6	0.30	0	5,5,5	0.55	0
2	9JE	E	601	-	6,6,6	0.45	0	5,5,5	0.38	0
2	9JE	C	603	-	6,6,6	0.43	0	5,5,5	1.23	1 (20%)

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	9JE	A	602	-	-	1/4/4/4	-
2	9JE	A	601	-	-	2/4/4/4	-
2	9JE	F	601	-	-	1/4/4/4	-
2	9JE	C	602	-	-	2/4/4/4	-
2	9JE	D	601	-	-	0/4/4/4	-
2	9JE	B	601	-	-	1/4/4/4	-
2	9JE	D	602	-	-	3/4/4/4	-
2	9JE	C	601	-	-	3/4/4/4	-
2	9JE	E	601	-	-	1/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	9JE	C	603	-	-	3/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	603	9JE	O01-C02-C03	-2.24	97.22	111.44

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	601	9JE	C02-C03-C04-C05
2	F	601	9JE	O01-C02-C03-C04
2	A	601	9JE	C02-C03-C04-C05
2	D	602	9JE	C02-C03-C04-C05
2	C	603	9JE	C03-C04-C05-C06
2	C	603	9JE	C04-C05-C06-O07
2	C	602	9JE	C02-C03-C04-C05
2	A	602	9JE	C04-C05-C06-O07
2	B	601	9JE	C04-C05-C06-O07
2	A	601	9JE	O01-C02-C03-C04
2	C	601	9JE	C04-C05-C06-O07
2	C	601	9JE	C03-C04-C05-C06
2	D	602	9JE	C04-C05-C06-O07
2	C	602	9JE	C03-C04-C05-C06
2	D	602	9JE	C03-C04-C05-C06
2	E	601	9JE	C02-C03-C04-C05
2	C	603	9JE	C02-C03-C04-C05

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	493/522 (94%)	-0.49	4 (0%) 82 84	25, 44, 68, 85	0
1	B	490/522 (93%)	-0.12	14 (2%) 53 54	24, 55, 100, 116	0
1	C	489/522 (93%)	-0.36	3 (0%) 85 87	25, 50, 72, 103	0
1	D	491/522 (94%)	-0.67	2 (0%) 88 90	23, 36, 58, 83	0
1	E	491/522 (94%)	-0.51	1 (0%) 91 92	24, 44, 62, 76	0
1	F	488/522 (93%)	0.07	9 (1%) 67 69	25, 70, 102, 125	0
All	All	2942/3132 (93%)	-0.35	33 (1%) 78 79	23, 46, 91, 125	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	492	ALA	6.0
1	F	492	ALA	5.6
1	D	494	LEU	4.6
1	B	192	VAL	3.4
1	C	4	PRO	3.3
1	F	490	TYR	3.3
1	B	4	PRO	3.2
1	A	492	ALA	3.2
1	F	160	VAL	3.1
1	F	303	VAL	3.0
1	B	247	LEU	2.8
1	F	159	PRO	2.8
1	E	494	LEU	2.8
1	B	160	VAL	2.7
1	B	248	VAL	2.6
1	B	199	ALA	2.6
1	B	493	ARG	2.5
1	F	162	ALA	2.5
1	B	492	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	243	ARG	2.5
1	D	490	TYR	2.5
1	A	496	LYS	2.3
1	B	490	TYR	2.3
1	B	108	VAL	2.2
1	B	146	GLY	2.2
1	F	302	PRO	2.2
1	A	4	PRO	2.1
1	B	6	GLN	2.1
1	F	68	HIS	2.1
1	A	108	VAL	2.1
1	F	253	VAL	2.1
1	B	273	VAL	2.1
1	C	272	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
2	9JE	D	602	7/7	0.82	0.19	42,52,57,59	0
2	9JE	C	601	7/7	0.90	0.13	41,46,50,60	0
2	9JE	C	602	7/7	0.91	0.12	45,48,59,62	0
2	9JE	F	601	7/7	0.91	0.11	36,43,46,59	0
2	9JE	A	601	7/7	0.93	0.14	41,51,59,62	0
2	9JE	E	601	7/7	0.93	0.11	37,37,39,47	0
2	9JE	C	603	7/7	0.93	0.13	39,47,56,60	0
2	9JE	B	601	7/7	0.95	0.08	33,36,41,52	0
2	9JE	A	602	7/7	0.96	0.07	33,38,47,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	9JE	D	601	7/7	0.97	0.06	29,32,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.