



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 03:31 am BST

PDB ID : 5VRC
Title : Crystal structure for Methylobacterium extorquens PqqC (truncation of natural CD fusion)
Authors : Evans III, R.L.; Wilmot, C.M.; Esler, M.A.
Deposited on : 2017-05-10
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
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

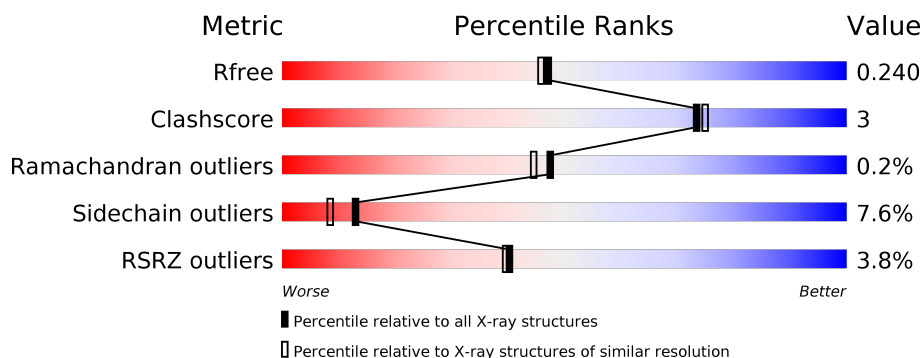
1 Overall quality at a glance

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	280	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>9%</div> <div>••</div> <div>19%</div> </div> </div>
1	B	280	<div> <div>2%</div> <div> <div></div> <div>64%</div> <div>15%</div> <div>••</div> <div>19%</div> </div> </div>
1	C	280	<div> <div>5%</div> <div> <div></div> <div>65%</div> <div>13%</div> <div>••</div> <div>19%</div> </div> </div>
1	D	280	<div> <div>2%</div> <div> <div></div> <div>66%</div> <div>11%</div> <div>••</div> <div>20%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7057 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 Bifunctional coenzyme PQQ synthesis protein C/D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	1	0
			1746	1125	309	306	6			
1	B	228	Total	C	N	O	S	0	0	0
			1790	1151	314	319	6			
1	C	226	Total	C	N	O	S	0	0	0
			1710	1104	294	306	6			
1	D	223	Total	C	N	O	S	0	0	0
			1727	1116	302	304	5			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q49150
A	-18	GLY	-	expression tag	UNP Q49150
A	-17	SER	-	expression tag	UNP Q49150
A	-16	SER	-	expression tag	UNP Q49150
A	-15	HIS	-	expression tag	UNP Q49150
A	-14	HIS	-	expression tag	UNP Q49150
A	-13	HIS	-	expression tag	UNP Q49150
A	-12	HIS	-	expression tag	UNP Q49150
A	-11	HIS	-	expression tag	UNP Q49150
A	-10	HIS	-	expression tag	UNP Q49150
A	-9	SER	-	expression tag	UNP Q49150
A	-8	SER	-	expression tag	UNP Q49150
A	-7	GLY	-	expression tag	UNP Q49150
A	-6	LEU	-	expression tag	UNP Q49150
A	-5	VAL	-	expression tag	UNP Q49150
A	-4	PRO	-	expression tag	UNP Q49150
A	-3	ARG	-	expression tag	UNP Q49150
A	-2	GLY	-	expression tag	UNP Q49150
A	-1	SER	-	expression tag	UNP Q49150
A	0	HIS	-	expression tag	UNP Q49150
B	-19	MET	-	initiating methionine	UNP Q49150

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP Q49150
B	-17	SER	-	expression tag	UNP Q49150
B	-16	SER	-	expression tag	UNP Q49150
B	-15	HIS	-	expression tag	UNP Q49150
B	-14	HIS	-	expression tag	UNP Q49150
B	-13	HIS	-	expression tag	UNP Q49150
B	-12	HIS	-	expression tag	UNP Q49150
B	-11	HIS	-	expression tag	UNP Q49150
B	-10	HIS	-	expression tag	UNP Q49150
B	-9	SER	-	expression tag	UNP Q49150
B	-8	SER	-	expression tag	UNP Q49150
B	-7	GLY	-	expression tag	UNP Q49150
B	-6	LEU	-	expression tag	UNP Q49150
B	-5	VAL	-	expression tag	UNP Q49150
B	-4	PRO	-	expression tag	UNP Q49150
B	-3	ARG	-	expression tag	UNP Q49150
B	-2	GLY	-	expression tag	UNP Q49150
B	-1	SER	-	expression tag	UNP Q49150
B	0	HIS	-	expression tag	UNP Q49150
C	-19	MET	-	initiating methionine	UNP Q49150
C	-18	GLY	-	expression tag	UNP Q49150
C	-17	SER	-	expression tag	UNP Q49150
C	-16	SER	-	expression tag	UNP Q49150
C	-15	HIS	-	expression tag	UNP Q49150
C	-14	HIS	-	expression tag	UNP Q49150
C	-13	HIS	-	expression tag	UNP Q49150
C	-12	HIS	-	expression tag	UNP Q49150
C	-11	HIS	-	expression tag	UNP Q49150
C	-10	HIS	-	expression tag	UNP Q49150
C	-9	SER	-	expression tag	UNP Q49150
C	-8	SER	-	expression tag	UNP Q49150
C	-7	GLY	-	expression tag	UNP Q49150
C	-6	LEU	-	expression tag	UNP Q49150
C	-5	VAL	-	expression tag	UNP Q49150
C	-4	PRO	-	expression tag	UNP Q49150
C	-3	ARG	-	expression tag	UNP Q49150
C	-2	GLY	-	expression tag	UNP Q49150
C	-1	SER	-	expression tag	UNP Q49150
C	0	HIS	-	expression tag	UNP Q49150
D	-19	MET	-	initiating methionine	UNP Q49150
D	-18	GLY	-	expression tag	UNP Q49150
D	-17	SER	-	expression tag	UNP Q49150

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP Q49150
D	-15	HIS	-	expression tag	UNP Q49150
D	-14	HIS	-	expression tag	UNP Q49150
D	-13	HIS	-	expression tag	UNP Q49150
D	-12	HIS	-	expression tag	UNP Q49150
D	-11	HIS	-	expression tag	UNP Q49150
D	-10	HIS	-	expression tag	UNP Q49150
D	-9	SER	-	expression tag	UNP Q49150
D	-8	SER	-	expression tag	UNP Q49150
D	-7	GLY	-	expression tag	UNP Q49150
D	-6	LEU	-	expression tag	UNP Q49150
D	-5	VAL	-	expression tag	UNP Q49150
D	-4	PRO	-	expression tag	UNP Q49150
D	-3	ARG	-	expression tag	UNP Q49150
D	-2	GLY	-	expression tag	UNP Q49150
D	-1	SER	-	expression tag	UNP Q49150
D	0	HIS	-	expression tag	UNP Q49150

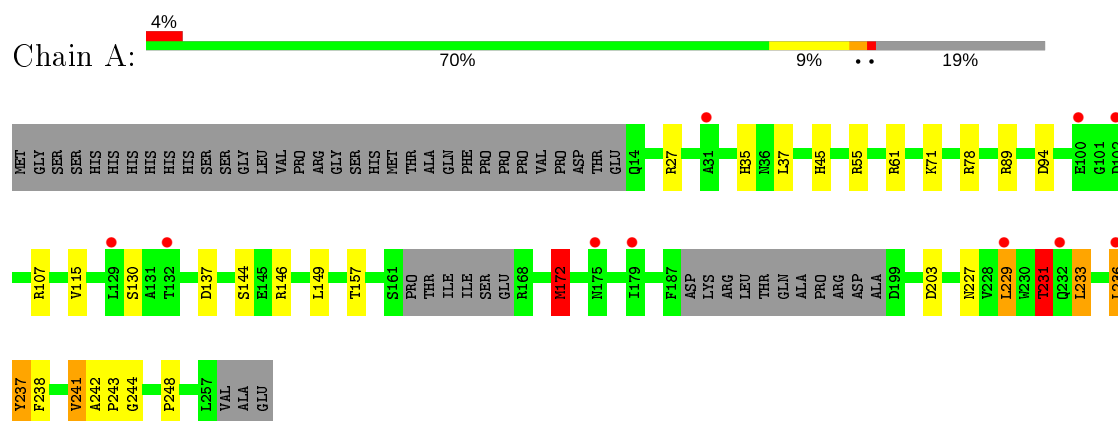
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	16	Total O 16 16	0	0
2	B	26	Total O 26 26	0	0
2	C	17	Total O 17 17	0	0
2	D	25	Total O 25 25	0	0

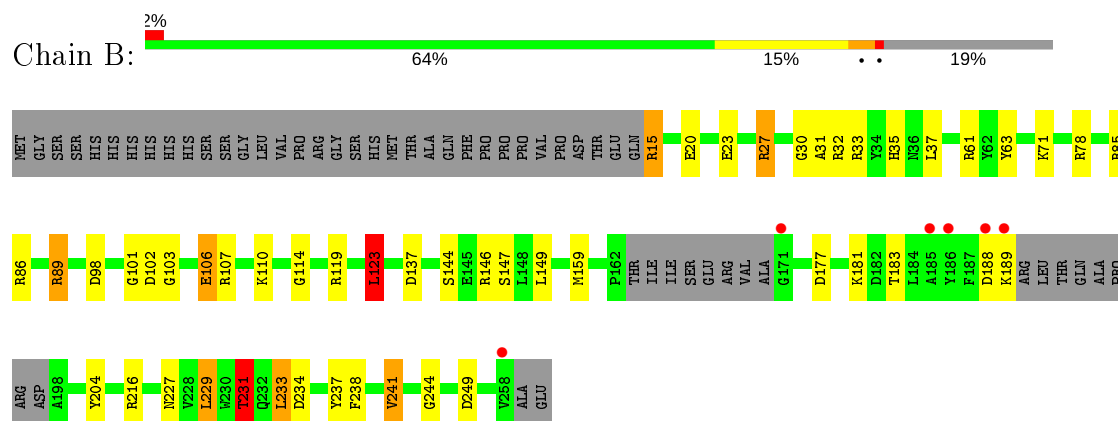
3 Residue-property plots [i](#)

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.

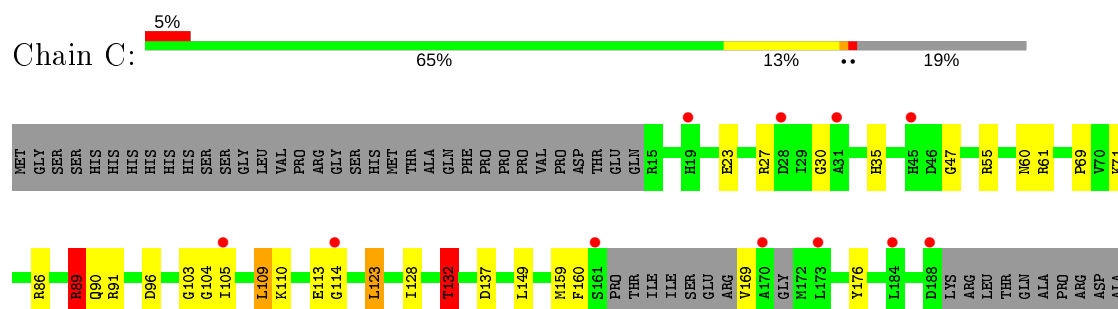
- Molecule 1: Bifunctional coenzyme PQQ synthesis protein C/D

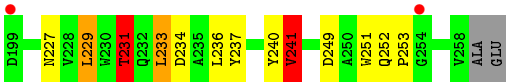


- Molecule 1: Bifunctional coenzyme PQQ synthesis protein C/D

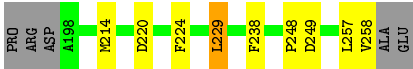
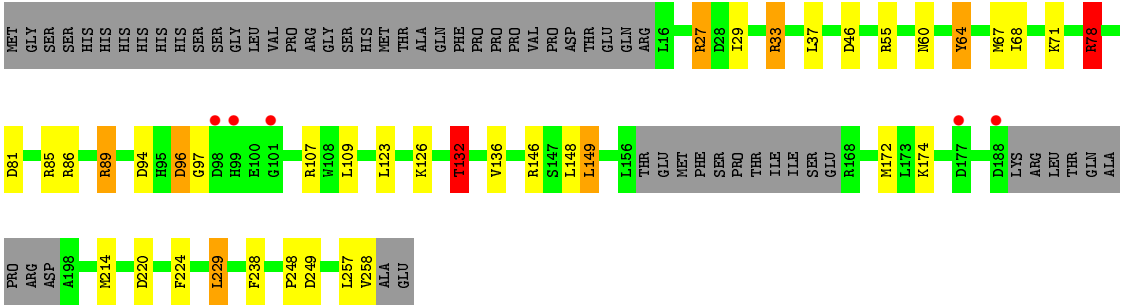


- Molecule 1: Bifunctional coenzyme PQQ synthesis protein C/D





● Molecule 1: Bifunctional coenzyme PQQ synthesis protein C/D



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.50Å 114.19Å 145.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.51 – 2.00 29.51 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.8 (29.51-2.00) 97.9 (29.51-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.197 , 0.236 0.204 , 0.240	Depositor DCC
R_{free} test set	3495 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 69.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7057	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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

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	1.35	3/1789 (0.2%)	1.36	20/2431 (0.8%)
1	B	1.42	12/1836 (0.7%)	1.46	27/2494 (1.1%)
1	C	1.27	3/1754 (0.2%)	1.31	17/2387 (0.7%)
1	D	1.41	5/1771 (0.3%)	1.52	30/2411 (1.2%)
All	All	1.36	23/7150 (0.3%)	1.42	94/9723 (1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	1
All	All	0	2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	144	SER	CA-CB	10.81	1.69	1.52
1	D	132	THR	CB-CG2	-8.89	1.23	1.52
1	D	249	ASP	N-CA	6.80	1.59	1.46
1	B	231	THR	CB-CG2	-6.78	1.29	1.52
1	B	244	GLY	C-O	-6.34	1.13	1.23
1	A	130	SER	CB-OG	-6.31	1.34	1.42
1	D	126	LYS	C-O	6.29	1.35	1.23
1	C	132	THR	CB-CG2	-6.16	1.32	1.52
1	C	128	ILE	C-O	-5.80	1.12	1.23
1	A	237	TYR	CZ-OH	-5.72	1.28	1.37
1	D	224	PHE	CG-CD2	-5.70	1.30	1.38
1	B	63	TYR	CE2-CZ	5.63	1.45	1.38
1	B	147	SER	CA-CB	5.57	1.61	1.52
1	D	64	TYR	CG-CD1	-5.55	1.31	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	244	GLY	C-O	-5.46	1.15	1.23
1	B	31	ALA	CA-CB	5.42	1.63	1.52
1	C	240	TYR	CE1-CZ	-5.36	1.31	1.38
1	B	78	ARG	CD-NE	-5.26	1.37	1.46
1	B	33	ARG	N-CA	5.25	1.56	1.46
1	B	33	ARG	CZ-NH1	-5.23	1.26	1.33
1	B	30	GLY	N-CA	5.08	1.53	1.46
1	B	20	GLU	CD-OE1	5.03	1.31	1.25
1	B	204	TYR	CB-CG	-5.02	1.44	1.51

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	78	ARG	NE-CZ-NH2	-26.88	106.86	120.30
1	B	78	ARG	NE-CZ-NH2	-20.12	110.24	120.30
1	B	78	ARG	NE-CZ-NH1	15.51	128.05	120.30
1	C	89	ARG	NE-CZ-NH2	-13.77	113.42	120.30
1	C	89	ARG	NE-CZ-NH1	13.39	127.00	120.30
1	D	78	ARG	NE-CZ-NH1	13.15	126.87	120.30
1	D	89	ARG	NE-CZ-NH2	-12.40	114.10	120.30
1	D	89	ARG	NE-CZ-NH1	12.21	126.41	120.30
1	B	89	ARG	NE-CZ-NH2	-11.41	114.59	120.30
1	B	89	ARG	NE-CZ-NH1	11.15	125.87	120.30
1	B	27	ARG	NE-CZ-NH2	-10.72	114.94	120.30
1	C	103	GLY	C-N-CA	-10.64	99.95	122.30
1	B	27	ARG	NE-CZ-NH1	10.02	125.31	120.30
1	B	233	LEU	CB-CG-CD1	9.47	127.11	111.00
1	B	86	ARG	NE-CZ-NH1	9.29	124.95	120.30
1	A	27	ARG	NE-CZ-NH1	9.27	124.93	120.30
1	A	78	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	C	233	LEU	CB-CG-CD1	8.87	126.07	111.00
1	A	233	LEU	CB-CG-CD1	8.73	125.84	111.00
1	C	55	ARG	NE-CZ-NH2	-8.61	115.99	120.30
1	D	27	ARG	NE-CZ-NH2	-8.51	116.04	120.30
1	D	78	ARG	CD-NE-CZ	8.33	135.26	123.60
1	B	15	ARG	NE-CZ-NH1	-8.31	116.14	120.30
1	A	78	ARG	NE-CZ-NH1	8.23	124.42	120.30
1	D	33	ARG	NE-CZ-NH2	-8.14	116.23	120.30
1	A	236	LEU	CA-CB-CG	8.05	133.82	115.30
1	A	89	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	D	248	PRO	C-N-CA	-8.01	101.68	121.70
1	D	81	ASP	CB-CG-OD1	7.79	125.31	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	229	LEU	CB-CG-CD1	7.74	124.16	111.00
1	A	203	ASP	CB-CG-OD1	7.73	125.26	118.30
1	B	78	ARG	CD-NE-CZ	7.55	134.17	123.60
1	B	85	ARG	NE-CZ-NH2	-7.45	116.58	120.30
1	B	137	ASP	CB-CG-OD1	7.44	124.99	118.30
1	A	61	ARG	NE-CZ-NH2	-7.39	116.61	120.30
1	A	27	ARG	NE-CZ-NH2	-7.35	116.62	120.30
1	B	15	ARG	NE-CZ-NH2	7.31	123.95	120.30
1	D	146	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	C	241	VAL	CG1-CB-CG2	7.10	122.26	110.90
1	D	55	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	A	146	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	A	107	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	D	248	PRO	O-C-N	-6.85	111.74	122.70
1	D	55	ARG	NE-CZ-NH1	6.81	123.70	120.30
1	A	89	ARG	NE-CZ-NH1	6.77	123.68	120.30
1	B	86	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	C	137	ASP	CB-CG-OD2	-6.59	112.37	118.30
1	D	27	ARG	CG-CD-NE	-6.58	97.99	111.80
1	B	177	ASP	CB-CG-OD1	6.46	124.11	118.30
1	D	85	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	A	61	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	A	137	ASP	CB-CG-OD1	6.35	124.01	118.30
1	A	146	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	D	46	ASP	CB-CG-OD1	6.28	123.95	118.30
1	D	148	LEU	CB-CG-CD2	-6.26	100.36	111.00
1	C	249	ASP	CB-CG-OD1	6.24	123.91	118.30
1	B	78	ARG	CG-CD-NE	-6.22	98.73	111.80
1	D	172	MET	CB-CG-SD	-6.21	93.78	112.40
1	A	172	MET	CG-SD-CE	6.15	110.04	100.20
1	C	61	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	D	94	ASP	CB-CG-OD1	6.11	123.80	118.30
1	B	216	ARG	NE-CZ-NH2	6.00	123.30	120.30
1	C	91	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	C	234	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	D	248	PRO	CA-C-N	5.96	130.30	117.20
1	D	46	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	B	61	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	C	229	LEU	CA-CB-CG	5.86	128.78	115.30
1	B	229	LEU	CB-CG-CD1	5.82	120.90	111.00
1	D	78	ARG	CG-CD-NE	-5.81	99.59	111.80
1	B	123	LEU	CA-CB-CG	5.78	128.60	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	THR	CA-CB-CG2	5.67	120.33	112.40
1	D	214	MET	CG-SD-CE	5.65	109.24	100.20
1	C	61	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	B	241	VAL	CG1-CB-CG2	5.64	119.93	110.90
1	B	27	ARG	CG-CD-NE	-5.64	99.97	111.80
1	A	229	LEU	CB-CG-CD1	5.59	120.51	111.00
1	D	96	ASP	CB-CG-OD1	-5.55	113.30	118.30
1	B	98	ASP	CB-CG-OD1	5.46	123.21	118.30
1	A	94	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	C	103	GLY	O-C-N	-5.41	114.00	123.20
1	D	220	ASP	CB-CG-OD1	5.37	123.13	118.30
1	D	33	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	D	229	LEU	CB-CG-CD1	5.32	120.05	111.00
1	D	78	ARG	CB-CA-C	5.31	121.02	110.40
1	B	234	ASP	CB-CG-OD1	-5.18	113.64	118.30
1	D	149	LEU	CB-CG-CD2	5.18	119.80	111.00
1	B	107	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	B	32	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	C	231	THR	CA-CB-CG2	5.17	119.63	112.40
1	A	172	MET	CB-CG-SD	5.13	127.80	112.40
1	B	241	VAL	CA-CB-CG1	5.10	118.56	110.90
1	C	236	LEU	CB-CG-CD2	-5.06	102.39	111.00
1	D	107	ARG	NE-CZ-NH2	5.05	122.83	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	104	GLY	Peptide
1	D	78	ARG	Sidechain

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	1746	0	1639	6	0
1	B	1790	0	1701	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1710	0	1567	19	0
1	D	1727	0	1642	12	0
2	A	16	0	0	0	0
2	B	26	0	0	0	0
2	C	17	0	0	0	0
2	D	25	0	0	0	0
All	All	7057	0	6549	44	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 (44) 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:188:ASP:O	1:B:189:LYS:O	1.93	0.85
1:A:227:ASN:O	1:A:231:THR:HG23	1.80	0.80
1:A:45:HIS:HA	1:A:172:MET:HG2	1.65	0.78
1:C:227:ASN:O	1:C:231:THR:HG23	1.83	0.76
1:B:227:ASN:O	1:B:231:THR:HG23	1.88	0.73
1:C:237:TYR:HA	1:C:241:VAL:HG13	1.72	0.70
1:D:257:LEU:O	1:D:258:VAL:HB	1.91	0.70
1:C:60:ASN:OD1	1:C:132:THR:HG21	1.92	0.69
1:C:69:PRO:HG3	1:C:105:ILE:HD11	1.77	0.65
1:C:60:ASN:OD1	1:C:132:THR:CG2	2.53	0.57
1:D:78:ARG:O	1:D:78:ARG:HD3	2.04	0.57
1:B:237:TYR:HA	1:B:241:VAL:HG13	1.86	0.56
1:B:119:ARG:HG2	1:B:123:LEU:HD22	1.88	0.55
1:D:60:ASN:OD1	1:D:132:THR:HG21	2.07	0.54
1:C:89:ARG:HG3	1:C:90:GLN:N	2.23	0.53
1:C:86:ARG:NH1	1:D:96:ASP:O	2.42	0.52
1:C:27:ARG:NH1	1:C:159:MET:HE3	2.25	0.51
1:B:227:ASN:O	1:B:231:THR:CG2	2.57	0.51
1:D:78:ARG:C	1:D:78:ARG:HD3	2.31	0.50
1:B:23:GLU:O	1:B:27:ARG:HG3	2.12	0.49
1:B:102:ASP:OD1	1:B:103:GLY:N	2.46	0.49
1:D:67:MET:HG3	1:D:136:VAL:HG11	1.95	0.49
1:A:238:PHE:CD1	1:A:243:PRO:HD2	2.48	0.49
1:C:109:LEU:O	1:C:113:GLU:HG3	2.13	0.48
1:C:23:GLU:O	1:C:27:ARG:HG3	2.14	0.47
1:C:47:GLY:HA2	1:C:176:TYR:CZ	2.50	0.47
1:B:110:LYS:O	1:B:114:GLY:N	2.43	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:TRP:CZ2	1:C:253:PRO:HA	2.52	0.45
1:A:237:TYR:HA	1:A:241:VAL:HG13	1.98	0.44
1:D:29:ILE:CG2	1:D:33:ARG:HD2	2.48	0.44
1:C:110:LYS:O	1:C:114:GLY:N	2.45	0.43
1:C:96:ASP:O	1:D:86:ARG:NH1	2.49	0.42
1:B:101:GLY:HA2	1:B:106:GLU:CG	2.49	0.42
1:B:238:PHE:CD1	1:D:238:PHE:HB2	2.54	0.42
1:C:227:ASN:O	1:C:231:THR:CG2	2.62	0.42
1:D:64:TYR:CZ	1:D:68:ILE:HD11	2.56	0.41
1:A:55:ARG:HG2	1:A:115:VAL:HG23	2.01	0.41
1:A:242:ALA:HA	1:A:243:PRO:C	2.41	0.41
1:C:86:ARG:HD3	1:D:97:GLY:O	2.20	0.41
1:B:27:ARG:HG2	1:B:159:MET:HE2	2.02	0.41
1:C:27:ARG:HG2	1:C:159:MET:CE	2.51	0.41
1:C:109:LEU:HD11	1:C:123:LEU:HD11	2.03	0.41
1:C:30:GLY:HA3	1:C:160:PHE:CZ	2.56	0.40
1:D:60:ASN:OD1	1:D:132:THR:CG2	2.68	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	222/280 (79%)	218 (98%)	4 (2%)	0	100	100
1	B	222/280 (79%)	219 (99%)	2 (1%)	1 (0%)	29	23
1	C	218/280 (78%)	216 (99%)	2 (1%)	0	100	100
1	D	217/280 (78%)	214 (99%)	2 (1%)	1 (0%)	29	23
All	All	879/1120 (78%)	867 (99%)	10 (1%)	2 (0%)	47	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	174	LYS
1	B	249	ASP

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	162/234 (69%)	149 (92%)	13 (8%)	12	7
1	B	173/234 (74%)	159 (92%)	14 (8%)	11	7
1	C	157/234 (67%)	144 (92%)	13 (8%)	11	7
1	D	163/234 (70%)	153 (94%)	10 (6%)	18	14
All	All	655/936 (70%)	605 (92%)	50 (8%)	13	8

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	37	LEU
1	A	71	LYS
1	A	144	SER
1	A	149	LEU
1	A	157	THR
1	A	172	MET
1	A	229	LEU
1	A	231	THR
1	A	233	LEU
1	A	236	LEU
1	A	241	VAL
1	A	248	PRO
1	B	15	ARG
1	B	35	HIS
1	B	37	LEU
1	B	71	LYS
1	B	89	ARG
1	B	106	GLU
1	B	123	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	146	ARG
1	B	149	LEU
1	B	181	LYS
1	B	183	THR
1	B	229	LEU
1	B	231	THR
1	B	233	LEU
1	C	35	HIS
1	C	71	LYS
1	C	89	ARG
1	C	109	LEU
1	C	123	LEU
1	C	132	THR
1	C	149	LEU
1	C	169	VAL
1	C	229	LEU
1	C	231	THR
1	C	233	LEU
1	C	241	VAL
1	C	252	GLN
1	D	27	ARG
1	D	37	LEU
1	D	71	LYS
1	D	78	ARG
1	D	89	ARG
1	D	109	LEU
1	D	123	LEU
1	D	132	THR
1	D	149	LEU
1	D	229	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	95	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	227/280 (81%)	0.27	10 (4%) 34 33	18, 39, 61, 78	1 (0%)
1	B	228/280 (81%)	0.08	6 (2%) 56 54	23, 36, 53, 69	4 (1%)
1	C	226/280 (80%)	0.36	13 (5%) 23 22	24, 43, 60, 67	22 (9%)
1	D	223/280 (79%)	-0.06	5 (2%) 62 60	22, 36, 51, 62	8 (3%)
All	All	904/1120 (80%)	0.16	34 (3%) 40 39	18, 38, 58, 78	35 (3%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	161	SER	8.2
1	A	232[A]	GLN	7.6
1	B	189	LYS	7.0
1	C	188	ASP	6.5
1	C	199	ASP	6.4
1	C	254	GLY	5.1
1	B	188	ASP	4.7
1	A	179	ILE	4.2
1	D	188	ASP	4.1
1	A	31	ALA	4.1
1	C	31	ALA	4.0
1	B	258	VAL	3.8
1	D	98	ASP	3.8
1	D	99	HIS	3.5
1	C	114	GLY	3.4
1	C	105	ILE	3.3
1	A	100	GLU	3.2
1	B	171	GLY	3.0
1	C	28	ASP	2.9
1	B	185	ALA	2.9
1	C	170	ALA	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	45	HIS	2.8
1	D	101	GLY	2.5
1	A	129	LEU	2.5
1	C	184	LEU	2.5
1	B	186	TYR	2.4
1	A	229	LEU	2.3
1	A	102	ASP	2.3
1	D	177	ASP	2.3
1	A	175	ASN	2.2
1	C	19	HIS	2.2
1	A	236	LEU	2.1
1	C	173	LEU	2.1
1	A	132	THR	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.