



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 06:31 PM UTC

PDB ID : 5VRC / pdb_00005vrc
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 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
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

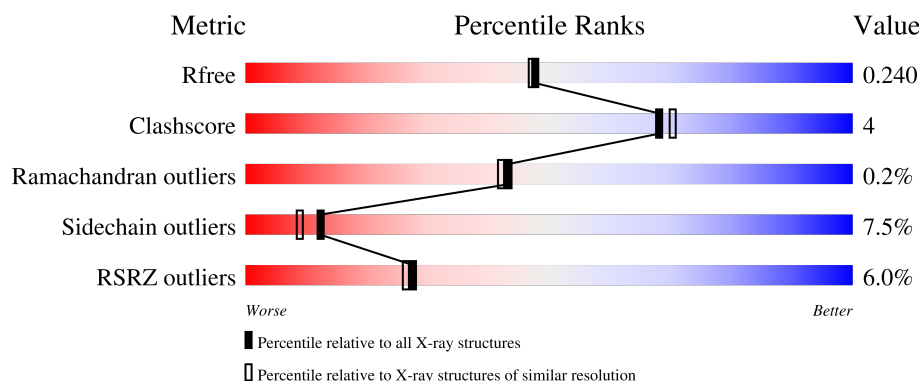
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 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	280	4% 60% 19% .. 19%
1	B	280	2% 60% 18% .. 19%
1	C	280	10% 59% 19% .. 19%
1	D	280	4% 59% 18% .. 20%

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

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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

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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

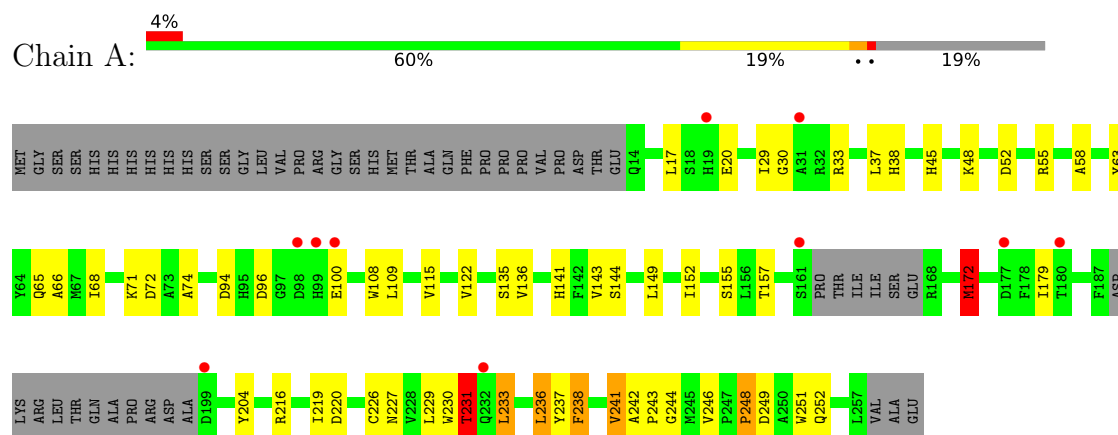
- Molecule 2 is water.

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

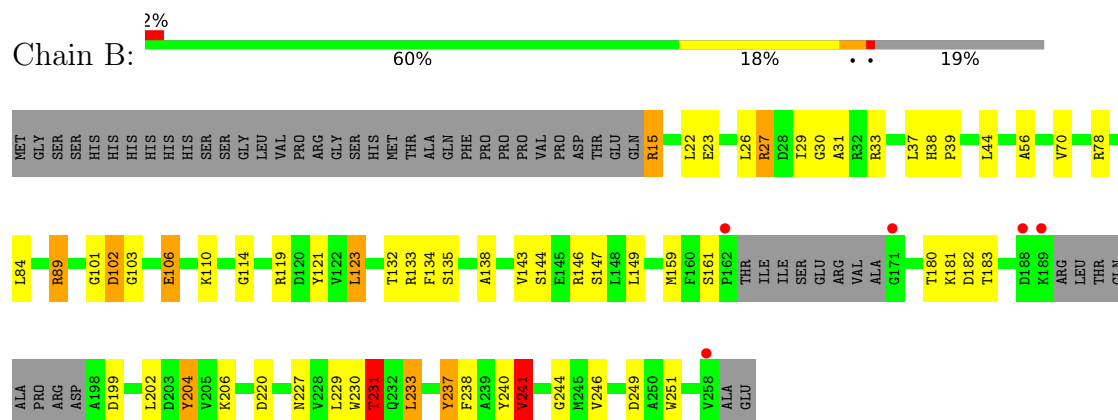
3 Residue-property plots

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.

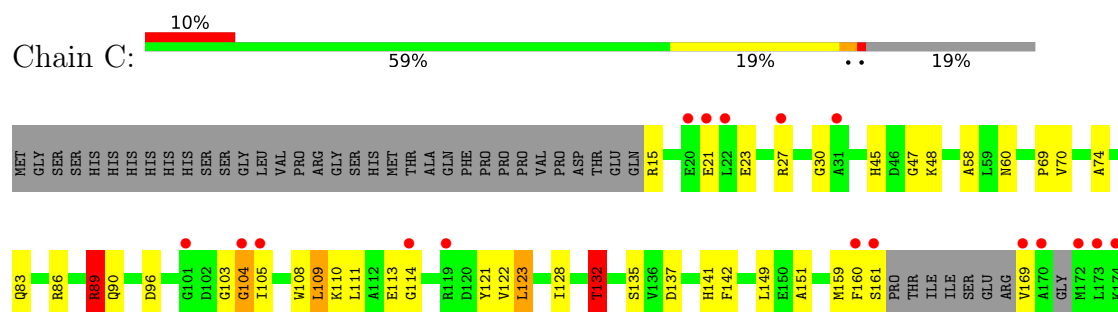
• Molecule 1: Bifunctional coenzyme PQQ synthesis protein C/D

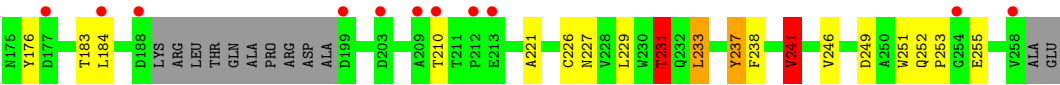


• Molecule 1: Bifunctional coenzyme PQQ synthesis protein C/D

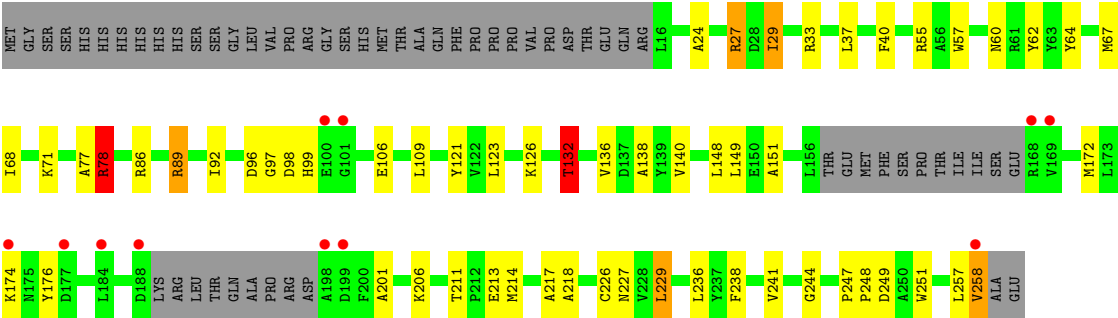


• Molecule 1: Bifunctional coenzyme PQQ synthesis protein C/D





● 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) 97.8 (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 (4.95%)	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 , 60.6	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	1.83	28/1789 (1.6%)	1.52	18/2431 (0.7%)
1	B	1.87	39/1836 (2.1%)	1.50	21/2494 (0.8%)
1	C	1.71	23/1754 (1.3%)	1.53	16/2387 (0.7%)
1	D	1.85	26/1771 (1.5%)	1.62	22/2411 (0.9%)
All	All	1.82	116/7150 (1.6%)	1.54	77/9723 (0.8%)

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 (116) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	249	ASP	N-CA	11.07	1.59	1.46
1	B	144	SER	CA-CB	9.69	1.69	1.53
1	D	126	LYS	C-O	9.24	1.35	1.23
1	C	128	ILE	C-O	-8.95	1.12	1.24
1	D	132	THR	CB-CG2	-8.95	1.23	1.52
1	D	99	HIS	CA-C	8.19	1.62	1.52
1	D	206	LYS	N-CA	8.01	1.55	1.46
1	B	33	ARG	N-CA	7.76	1.56	1.45
1	C	249	ASP	N-CA	7.35	1.55	1.46
1	B	244	GLY	C-O	-7.33	1.13	1.24
1	A	219	ILE	CA-C	7.03	1.61	1.52
1	A	65	GLN	N-CA	7.00	1.54	1.46
1	A	152	ILE	C-O	6.98	1.32	1.24
1	C	221	ALA	C-O	6.96	1.32	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	71	LYS	N-CA	6.95	1.54	1.46
1	A	33	ARG	N-CA	6.91	1.55	1.45
1	B	231	THR	CB-CG2	-6.84	1.29	1.52
1	A	230	TRP	CA-C	6.80	1.61	1.52
1	D	236	LEU	C-O	6.79	1.31	1.24
1	D	151	ALA	N-CA	6.77	1.54	1.46
1	B	31	ALA	CA-CB	6.75	1.63	1.53
1	B	27	ARG	C-O	-6.71	1.16	1.24
1	A	244	GLY	C-O	-6.67	1.15	1.23
1	B	70	VAL	N-CA	-6.53	1.38	1.46
1	B	199	ASP	N-CA	6.49	1.54	1.46
1	A	122	VAL	N-CA	-6.48	1.38	1.46
1	A	246	VAL	C-O	-6.46	1.16	1.24
1	B	240	TYR	C-O	-6.41	1.15	1.24
1	B	30	GLY	N-CA	6.38	1.53	1.45
1	B	44	LEU	CA-C	6.35	1.61	1.52
1	D	217	ALA	CA-C	6.33	1.60	1.52
1	C	226	CYS	N-CA	-6.31	1.38	1.46
1	B	206	LYS	N-CA	6.26	1.53	1.46
1	A	17	LEU	N-CA	6.26	1.53	1.45
1	B	78	ARG	CD-NE	-6.24	1.37	1.46
1	C	21	GLU	C-O	-6.24	1.16	1.24
1	C	255	GLU	C-O	6.23	1.31	1.23
1	A	94	ASP	CA-C	-6.22	1.44	1.52
1	C	132	THR	CB-CG2	-6.22	1.32	1.52
1	A	63	TYR	N-CA	-6.22	1.38	1.46
1	D	251	TRP	C-O	6.17	1.31	1.23
1	A	66	ALA	CA-CB	-6.08	1.42	1.53
1	B	146	ARG	C-O	-6.04	1.16	1.23
1	B	138	ALA	C-O	-6.02	1.17	1.24
1	A	141	HIS	CA-C	5.98	1.60	1.52
1	A	238	PHE	N-CA	5.91	1.53	1.46
1	C	135	SER	N-CA	5.90	1.53	1.46
1	B	180	THR	C-O	5.87	1.31	1.23
1	A	249	ASP	N-CA	5.86	1.53	1.46
1	A	252	GLN	N-CA	5.85	1.52	1.45
1	A	58	ALA	CA-CB	-5.85	1.44	1.53
1	A	38	HIS	C-O	-5.83	1.16	1.24
1	B	133	ARG	CA-CB	5.81	1.62	1.53
1	B	161	SER	CA-C	-5.78	1.46	1.53
1	A	74	ALA	CA-C	5.76	1.60	1.52
1	C	122	VAL	CA-CB	5.76	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	182	ASP	C-O	5.76	1.30	1.24
1	B	135	SER	N-CA	5.69	1.53	1.46
1	B	233	LEU	N-CA	-5.69	1.39	1.46
1	D	78	ARG	CD-NE	-5.67	1.38	1.46
1	D	77	ALA	N-CA	5.67	1.53	1.46
1	C	238	PHE	C-O	-5.64	1.17	1.24
1	C	108	TRP	CA-C	-5.62	1.45	1.52
1	A	251	TRP	C-O	5.61	1.30	1.23
1	D	92	ILE	N-CA	-5.57	1.39	1.46
1	D	227	ASN	CG-ND2	-5.56	1.21	1.33
1	B	22	LEU	N-CA	5.56	1.52	1.46
1	D	226	CYS	CA-C	5.56	1.60	1.52
1	A	216	ARG	C-O	-5.55	1.17	1.24
1	A	72	ASP	CA-C	-5.55	1.45	1.52
1	B	202	LEU	C-O	5.50	1.30	1.24
1	B	121	TYR	C-O	-5.50	1.17	1.24
1	D	148	LEU	C-N	-5.47	1.26	1.33
1	B	246	VAL	CA-C	-5.47	1.47	1.52
1	B	132	THR	N-CA	-5.46	1.39	1.46
1	B	220	ASP	C-O	-5.46	1.17	1.24
1	B	84	LEU	CA-C	-5.45	1.45	1.52
1	C	246	VAL	C-O	-5.45	1.18	1.25
1	B	204	TYR	N-CA	-5.37	1.40	1.46
1	C	74	ALA	C-O	-5.37	1.17	1.24
1	D	218	ALA	C-O	5.36	1.30	1.24
1	D	241	VAL	CA-C	-5.31	1.46	1.52
1	A	220	ASP	CA-C	5.26	1.60	1.52
1	B	38	HIS	CA-C	5.23	1.58	1.53
1	C	237	TYR	CA-C	5.23	1.59	1.52
1	C	121	TYR	CA-C	5.23	1.59	1.52
1	C	210	THR	C-O	-5.21	1.17	1.24
1	C	137	ASP	C-O	5.21	1.30	1.24
1	A	226	CYS	CA-C	5.20	1.59	1.52
1	C	142	PHE	N-CA	5.20	1.52	1.46
1	C	48	LYS	C-O	-5.19	1.17	1.24
1	B	161	SER	N-CA	5.18	1.53	1.46
1	D	213	GLU	C-O	5.18	1.30	1.24
1	D	106	GLU	N-CA	-5.17	1.40	1.46
1	D	244	GLY	C-O	-5.17	1.17	1.24
1	C	58	ALA	CA-C	-5.16	1.46	1.52
1	B	29	ILE	N-CA	5.14	1.52	1.46
1	A	204	TYR	CA-C	5.14	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	15	ARG	N-CA	5.13	1.55	1.46
1	B	251	TRP	CA-C	5.13	1.59	1.52
1	D	229	LEU	C-O	5.12	1.30	1.24
1	A	136	VAL	N-CA	5.11	1.52	1.46
1	A	109	LEU	N-CA	5.09	1.52	1.46
1	D	201	ALA	C-O	-5.09	1.18	1.24
1	D	24	ALA	N-CA	5.08	1.52	1.46
1	D	29	ILE	C-O	-5.08	1.18	1.24
1	B	56	ALA	N-CA	5.08	1.52	1.46
1	B	138	ALA	N-CA	5.06	1.52	1.46
1	B	39	PRO	C-O	5.05	1.30	1.24
1	C	111	LEU	N-CA	5.05	1.52	1.46
1	B	132	THR	CA-CB	5.04	1.61	1.53
1	B	134	PHE	CA-C	5.03	1.59	1.52
1	B	26	LEU	N-CA	5.02	1.52	1.46
1	D	57	TRP	N-CA	5.01	1.52	1.46
1	C	141	HIS	CA-CB	5.01	1.61	1.53
1	D	71	LYS	N-CA	5.01	1.52	1.46

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	103	GLY	CA-C-N	-14.98	99.95	122.28
1	C	103	GLY	C-N-CA	-14.98	99.95	122.28
1	D	78	ARG	NE-CZ-NH2	-13.71	106.86	119.20
1	D	248	PRO	CA-C-N	-13.10	101.68	122.65
1	D	248	PRO	C-N-CA	-13.10	101.68	122.65
1	B	78	ARG	NE-CZ-NH2	-9.95	110.24	119.20
1	A	52	ASP	N-CA-C	9.14	122.39	111.33
1	D	248	PRO	O-C-N	-9.13	111.74	122.24
1	D	138	ALA	N-CA-C	-8.87	101.69	111.36
1	B	233	LEU	N-CA-C	8.51	120.64	111.36
1	A	100	GLU	N-CA-C	8.02	122.49	112.87
1	A	155	SER	N-CA-C	7.81	122.65	113.20
1	D	78	ARG	CD-NE-CZ	7.75	135.26	124.40
1	D	236	LEU	N-CA-C	7.68	120.33	111.11
1	C	103	GLY	O-C-N	-7.65	114.00	122.65
1	B	78	ARG	CD-NE-CZ	6.98	134.17	124.40
1	A	29	ILE	N-CA-C	6.64	117.33	110.36
1	B	78	ARG	NE-CZ-NH1	6.55	128.05	121.50
1	C	89	ARG	NE-CZ-NH2	-6.43	113.42	119.20
1	C	104	GLY	N-CA-C	6.39	123.53	115.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	27	ARG	CG-CD-NE	-6.37	97.99	112.00
1	D	172	MET	CB-CG-SD	-6.31	93.78	112.70
1	D	29	ILE	CB-CA-C	-6.17	104.08	111.97
1	B	102	ASP	N-CA-C	-6.14	101.37	110.46
1	B	230	TRP	N-CA-C	-6.13	104.68	111.36
1	C	74	ALA	N-CA-C	-6.12	104.69	111.36
1	D	78	ARG	CB-CA-C	6.09	121.02	110.72
1	D	40	PHE	N-CA-C	-6.09	104.57	111.14
1	C	83	GLN	N-CA-C	-6.03	104.79	111.36
1	B	78	ARG	CG-CD-NE	-6.03	98.73	112.00
1	A	68	ILE	O-C-N	5.97	124.24	120.42
1	B	29	ILE	CA-C-N	5.93	126.69	119.99
1	B	29	ILE	C-N-CA	5.93	126.69	119.99
1	C	103	GLY	CA-C-O	5.89	125.57	119.27
1	B	31	ALA	N-CA-C	5.88	117.69	111.28
1	B	237	TYR	N-CA-C	-5.83	104.84	111.14
1	B	241	VAL	N-CA-CB	5.79	117.30	111.57
1	A	231	THR	CA-CB-CG2	5.79	120.33	110.50
1	B	147	SER	N-CA-C	-5.79	102.89	110.53
1	D	89	ARG	NE-CZ-NH2	-5.67	114.10	119.20
1	A	231	THR	CA-CB-OG1	5.66	118.09	109.60
1	D	78	ARG	CG-CD-NE	-5.64	99.59	112.00
1	A	108	TRP	N-CA-C	-5.63	105.22	111.36
1	D	98	ASP	N-CA-C	5.57	120.07	113.28
1	C	151	ALA	N-CA-C	-5.56	105.30	111.36
1	C	89	ARG	NE-CZ-NH1	5.50	127.00	121.50
1	D	121	TYR	N-CA-C	-5.49	105.38	111.36
1	B	27	ARG	CG-CD-NE	-5.47	99.97	112.00
1	B	233	LEU	CB-CG-CD1	5.47	127.11	110.70
1	C	70	VAL	N-CA-C	-5.42	105.09	111.00
1	D	248	PRO	N-CA-C	5.41	121.81	113.75
1	A	20	GLU	N-CA-C	5.38	116.82	111.07
1	D	78	ARG	NE-CZ-NH1	5.37	126.87	121.50
1	C	231	THR	CA-CB-CG2	5.37	119.63	110.50
1	B	15	ARG	NE-CZ-NH1	-5.36	116.14	121.50
1	B	144	SER	CA-CB-OG	-5.34	100.41	111.10
1	B	241	VAL	CA-C-O	-5.32	116.18	120.70
1	A	236	LEU	CD1-CG-CD2	5.31	122.48	110.80
1	A	30	GLY	CA-C-O	5.30	126.21	120.75
1	C	122	VAL	N-CA-C	-5.29	105.56	110.53
1	B	15	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	A	248	PRO	N-CA-C	5.24	123.27	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	231	THR	OG1-CB-CG2	5.22	119.73	109.30
1	C	241	VAL	CG1-CB-CG2	5.21	122.26	110.80
1	B	231	THR	CA-CB-OG1	5.16	117.33	109.60
1	D	176	TYR	N-CA-C	-5.13	100.17	108.52
1	C	233	LEU	CB-CG-CD1	5.12	126.07	110.70
1	A	96	ASP	N-CA-C	-5.12	107.20	113.50
1	D	247	PRO	N-CA-C	5.12	116.95	110.70
1	B	89	ARG	NE-CZ-NH2	-5.12	114.59	119.20
1	A	135	SER	CA-CB-OG	-5.12	100.87	111.10
1	D	55	ARG	N-CA-C	5.10	116.53	111.07
1	A	233	LEU	CB-CG-CD1	5.05	125.84	110.70
1	A	172	MET	CB-CG-SD	5.03	127.80	112.70
1	A	109	LEU	N-CA-CB	5.03	117.52	110.12
1	D	140	VAL	N-CA-C	5.01	115.23	110.42
1	A	236	LEU	CA-CB-CG	5.00	133.82	116.30

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 [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	1746	0	1639	6	0
1	B	1790	0	1701	11	0
1	C	1710	0	1567	21	0
1	D	1727	0	1642	15	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	49	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (49) 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: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:78:ARG:HD3	1:D:78:ARG:C	2.31	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:B:227:ASN:O	1:B:231:THR:CG2	2.57	0.51
1:C:27:ARG:NH1	1:C:159:MET:HE3	2.26	0.51
1:B:27:ARG:HG2	1:B:159:MET:HE2	1.93	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:D:211:THR:HG23	1:D:214:MET:HE3	1.96	0.47
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
1:A:242:ALA:HA	1:A:243:PRO:C	2.41	0.45
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:78:ARG:C	1:D:78:ARG:CD	2.91	0.44
1:D:29:ILE:CG2	1:D:33:ARG:HD2	2.48	0.44
1:D:62:TYR:CD2	1:D:62:TYR:C	2.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:86:ARG:HD3	1:D:97:GLY:O	2.20	0.41
1:C:27:ARG:HG2	1:C:159:MET:CE	2.51	0.41
1:C:160:PHE:O	1:C:161:SER:C	2.64	0.41
1:B:204:TYR:CD1	1:B:204:TYR:C	2.99	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
1:C:183:THR:O	1:C:184:LEU:C	2.63	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%)	24	21
1	C	218/280 (78%)	216 (99%)	2 (1%)	0	100	100
1	D	217/280 (78%)	214 (99%)	2 (1%)	1 (0%)	24	21
All	All	879/1120 (78%)	867 (99%)	10 (1%)	2 (0%)	43	42

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%)	148 (91%)	14 (9%)	10	6
1	B	173/234 (74%)	160 (92%)	13 (8%)	12	9
1	C	157/234 (67%)	145 (92%)	12 (8%)	12	9
1	D	163/234 (70%)	153 (94%)	10 (6%)	17	14
All	All	655/936 (70%)	606 (92%)	49 (8%)	12	9

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	48	LYS
1	A	143	VAL
1	A	144	SER
1	A	149	LEU
1	A	157	THR
1	A	172	MET
1	A	179	ILE
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	37	LEU
1	B	89	ARG
1	B	106	GLU
1	B	123	LEU
1	B	143	VAL
1	B	149	LEU
1	B	181	LYS
1	B	183	THR
1	B	229	LEU

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Mol	Chain	Res	Type
1	B	231	THR
1	B	233	LEU
1	B	241	VAL
1	C	45	HIS
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	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
1	D	258	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	208	HIS
1	D	95	HIS
1	D	99	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](#)

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%)	0.17	10 (4%) 39 38	6, 39, 61, 78	1 (0%)
1	B	228/280 (81%)	0.18	5 (2%) 62 61	4, 35, 53, 69	4 (1%)
1	C	226/280 (80%)	1.01	28 (12%) 8 7	11, 40, 60, 67	22 (9%)
1	D	223/280 (79%)	0.20	11 (4%) 35 34	12, 35, 51, 62	8 (3%)
All	All	904/1120 (80%)	0.39	54 (5%) 27 26	4, 37, 58, 78	35 (3%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	189	LYS	33.9
1	D	188	ASP	19.5
1	B	188	ASP	17.7
1	C	199	ASP	17.2
1	C	188	ASP	17.1
1	C	161	SER	17.1
1	C	20	GLU	14.0
1	C	114	GLY	11.6
1	C	177	ASP	8.9
1	C	169	VAL	8.5
1	C	170	ALA	8.2
1	C	212	PRO	8.0
1	C	173	LEU	8.0
1	C	22	LEU	7.0
1	D	198	ALA	6.8
1	B	171	GLY	6.6
1	C	172	MET	6.4
1	C	174	LYS	5.9
1	D	258	VAL	5.9
1	C	210	THR	5.6
1	A	232[A]	GLN	5.2

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Mol	Chain	Res	Type	RSRZ
1	C	21	GLU	5.2
1	C	119	ARG	4.8
1	C	105	ILE	4.8
1	C	27	ARG	4.7
1	D	199	ASP	4.4
1	B	258	VAL	4.0
1	D	174	LYS	3.7
1	C	213	GLU	3.5
1	D	169	VAL	3.0
1	A	31	ALA	3.0
1	C	254	GLY	2.9
1	D	177	ASP	2.9
1	C	184	LEU	2.8
1	A	99	HIS	2.8
1	A	100	GLU	2.8
1	D	168	ARG	2.7
1	B	162	PRO	2.7
1	C	258	VAL	2.7
1	D	184	LEU	2.6
1	A	98	ASP	2.4
1	C	209	ALA	2.3
1	C	203	ASP	2.3
1	A	161	SER	2.3
1	C	31	ALA	2.2
1	C	101	GLY	2.2
1	A	199	ASP	2.1
1	A	19	HIS	2.1
1	D	100	GLU	2.1
1	A	180	THR	2.1
1	A	177	ASP	2.0
1	C	160	PHE	2.0
1	C	104	GLY	2.0
1	D	101	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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.