



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 05:25 AM UTC

PDB ID : 4HT7 / pdb_00004ht7
Title : CO2 concentrating mechanism protein P, CcmP form 2
Authors : Cai, F.; Sutter, M.; Kerfeld, C.A.
Deposited on : 2012-10-31
Resolution : 3.30 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

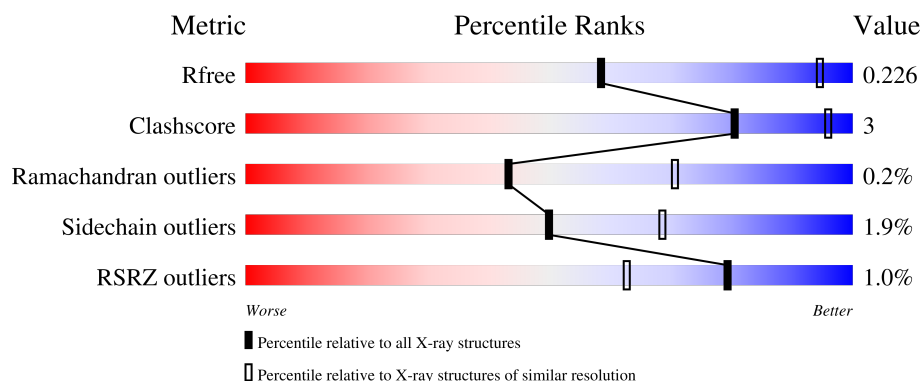
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	227	80% 9% 11%
1	B	227	2% 82% 7% 11%
1	C	227	82% 7% 11%
1	D	227	83% 6% 11%
1	E	227	% 83% 6% 11%

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Mol	Chain	Length	Quality of chain
1	F	227	% 83%6% • 11%
1	G	227	% 82%7% 11%
1	H	227	% 81%8% 11%
1	I	227	81%7% 11%
1	J	227	% 81%7% • 11%
1	K	227	% 83%6% 11%
1	L	227	% 83%5% • 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18655 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 CO2 concentrating mechanism protein P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	203	Total	C	N	O	S	0	0	0
			1553	976	284	289	4			
1	B	203	Total	C	N	O	S	0	0	0
			1553	976	284	289	4			
1	C	203	Total	C	N	O	S	0	0	0
			1553	976	284	289	4			
1	G	203	Total	C	N	O	S	0	0	0
			1553	976	284	289	4			
1	H	203	Total	C	N	O	S	0	0	0
			1553	976	284	289	4			
1	I	203	Total	C	N	O	S	0	0	0
			1553	976	284	289	4			
1	D	203	Total	C	N	O	S	0	0	0
			1553	976	284	289	4			
1	E	203	Total	C	N	O	S	0	0	0
			1553	976	284	289	4			
1	F	203	Total	C	N	O	S	0	0	0
			1553	976	284	289	4			
1	J	203	Total	C	N	O	S	0	0	0
			1553	976	284	289	4			
1	K	203	Total	C	N	O	S	0	0	0
			1553	976	284	289	4			
1	L	203	Total	C	N	O	S	0	0	0
			1553	976	284	289	4			

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q5N3D0
A	2	GLY	-	expression tag	UNP Q5N3D0
A	3	SER	-	expression tag	UNP Q5N3D0
A	4	SER	-	expression tag	UNP Q5N3D0
A	5	HIS	-	expression tag	UNP Q5N3D0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	6	HIS	-	expression tag	UNP Q5N3D0
A	7	HIS	-	expression tag	UNP Q5N3D0
A	8	HIS	-	expression tag	UNP Q5N3D0
A	9	HIS	-	expression tag	UNP Q5N3D0
A	10	HIS	-	expression tag	UNP Q5N3D0
A	11	SER	-	expression tag	UNP Q5N3D0
A	12	GLN	-	expression tag	UNP Q5N3D0
A	13	ASP	-	expression tag	UNP Q5N3D0
A	14	PRO	-	expression tag	UNP Q5N3D0
B	1	MET	-	expression tag	UNP Q5N3D0
B	2	GLY	-	expression tag	UNP Q5N3D0
B	3	SER	-	expression tag	UNP Q5N3D0
B	4	SER	-	expression tag	UNP Q5N3D0
B	5	HIS	-	expression tag	UNP Q5N3D0
B	6	HIS	-	expression tag	UNP Q5N3D0
B	7	HIS	-	expression tag	UNP Q5N3D0
B	8	HIS	-	expression tag	UNP Q5N3D0
B	9	HIS	-	expression tag	UNP Q5N3D0
B	10	HIS	-	expression tag	UNP Q5N3D0
B	11	SER	-	expression tag	UNP Q5N3D0
B	12	GLN	-	expression tag	UNP Q5N3D0
B	13	ASP	-	expression tag	UNP Q5N3D0
B	14	PRO	-	expression tag	UNP Q5N3D0
C	1	MET	-	expression tag	UNP Q5N3D0
C	2	GLY	-	expression tag	UNP Q5N3D0
C	3	SER	-	expression tag	UNP Q5N3D0
C	4	SER	-	expression tag	UNP Q5N3D0
C	5	HIS	-	expression tag	UNP Q5N3D0
C	6	HIS	-	expression tag	UNP Q5N3D0
C	7	HIS	-	expression tag	UNP Q5N3D0
C	8	HIS	-	expression tag	UNP Q5N3D0
C	9	HIS	-	expression tag	UNP Q5N3D0
C	10	HIS	-	expression tag	UNP Q5N3D0
C	11	SER	-	expression tag	UNP Q5N3D0
C	12	GLN	-	expression tag	UNP Q5N3D0
C	13	ASP	-	expression tag	UNP Q5N3D0
C	14	PRO	-	expression tag	UNP Q5N3D0
G	1	MET	-	expression tag	UNP Q5N3D0
G	2	GLY	-	expression tag	UNP Q5N3D0
G	3	SER	-	expression tag	UNP Q5N3D0
G	4	SER	-	expression tag	UNP Q5N3D0
G	5	HIS	-	expression tag	UNP Q5N3D0

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Chain	Residue	Modelled	Actual	Comment	Reference
G	6	HIS	-	expression tag	UNP Q5N3D0
G	7	HIS	-	expression tag	UNP Q5N3D0
G	8	HIS	-	expression tag	UNP Q5N3D0
G	9	HIS	-	expression tag	UNP Q5N3D0
G	10	HIS	-	expression tag	UNP Q5N3D0
G	11	SER	-	expression tag	UNP Q5N3D0
G	12	GLN	-	expression tag	UNP Q5N3D0
G	13	ASP	-	expression tag	UNP Q5N3D0
G	14	PRO	-	expression tag	UNP Q5N3D0
H	1	MET	-	expression tag	UNP Q5N3D0
H	2	GLY	-	expression tag	UNP Q5N3D0
H	3	SER	-	expression tag	UNP Q5N3D0
H	4	SER	-	expression tag	UNP Q5N3D0
H	5	HIS	-	expression tag	UNP Q5N3D0
H	6	HIS	-	expression tag	UNP Q5N3D0
H	7	HIS	-	expression tag	UNP Q5N3D0
H	8	HIS	-	expression tag	UNP Q5N3D0
H	9	HIS	-	expression tag	UNP Q5N3D0
H	10	HIS	-	expression tag	UNP Q5N3D0
H	11	SER	-	expression tag	UNP Q5N3D0
H	12	GLN	-	expression tag	UNP Q5N3D0
H	13	ASP	-	expression tag	UNP Q5N3D0
H	14	PRO	-	expression tag	UNP Q5N3D0
I	1	MET	-	expression tag	UNP Q5N3D0
I	2	GLY	-	expression tag	UNP Q5N3D0
I	3	SER	-	expression tag	UNP Q5N3D0
I	4	SER	-	expression tag	UNP Q5N3D0
I	5	HIS	-	expression tag	UNP Q5N3D0
I	6	HIS	-	expression tag	UNP Q5N3D0
I	7	HIS	-	expression tag	UNP Q5N3D0
I	8	HIS	-	expression tag	UNP Q5N3D0
I	9	HIS	-	expression tag	UNP Q5N3D0
I	10	HIS	-	expression tag	UNP Q5N3D0
I	11	SER	-	expression tag	UNP Q5N3D0
I	12	GLN	-	expression tag	UNP Q5N3D0
I	13	ASP	-	expression tag	UNP Q5N3D0
I	14	PRO	-	expression tag	UNP Q5N3D0
D	1	MET	-	expression tag	UNP Q5N3D0
D	2	GLY	-	expression tag	UNP Q5N3D0
D	3	SER	-	expression tag	UNP Q5N3D0
D	4	SER	-	expression tag	UNP Q5N3D0
D	5	HIS	-	expression tag	UNP Q5N3D0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	6	HIS	-	expression tag	UNP Q5N3D0
D	7	HIS	-	expression tag	UNP Q5N3D0
D	8	HIS	-	expression tag	UNP Q5N3D0
D	9	HIS	-	expression tag	UNP Q5N3D0
D	10	HIS	-	expression tag	UNP Q5N3D0
D	11	SER	-	expression tag	UNP Q5N3D0
D	12	GLN	-	expression tag	UNP Q5N3D0
D	13	ASP	-	expression tag	UNP Q5N3D0
D	14	PRO	-	expression tag	UNP Q5N3D0
E	1	MET	-	expression tag	UNP Q5N3D0
E	2	GLY	-	expression tag	UNP Q5N3D0
E	3	SER	-	expression tag	UNP Q5N3D0
E	4	SER	-	expression tag	UNP Q5N3D0
E	5	HIS	-	expression tag	UNP Q5N3D0
E	6	HIS	-	expression tag	UNP Q5N3D0
E	7	HIS	-	expression tag	UNP Q5N3D0
E	8	HIS	-	expression tag	UNP Q5N3D0
E	9	HIS	-	expression tag	UNP Q5N3D0
E	10	HIS	-	expression tag	UNP Q5N3D0
E	11	SER	-	expression tag	UNP Q5N3D0
E	12	GLN	-	expression tag	UNP Q5N3D0
E	13	ASP	-	expression tag	UNP Q5N3D0
E	14	PRO	-	expression tag	UNP Q5N3D0
F	1	MET	-	expression tag	UNP Q5N3D0
F	2	GLY	-	expression tag	UNP Q5N3D0
F	3	SER	-	expression tag	UNP Q5N3D0
F	4	SER	-	expression tag	UNP Q5N3D0
F	5	HIS	-	expression tag	UNP Q5N3D0
F	6	HIS	-	expression tag	UNP Q5N3D0
F	7	HIS	-	expression tag	UNP Q5N3D0
F	8	HIS	-	expression tag	UNP Q5N3D0
F	9	HIS	-	expression tag	UNP Q5N3D0
F	10	HIS	-	expression tag	UNP Q5N3D0
F	11	SER	-	expression tag	UNP Q5N3D0
F	12	GLN	-	expression tag	UNP Q5N3D0
F	13	ASP	-	expression tag	UNP Q5N3D0
F	14	PRO	-	expression tag	UNP Q5N3D0
J	1	MET	-	expression tag	UNP Q5N3D0
J	2	GLY	-	expression tag	UNP Q5N3D0
J	3	SER	-	expression tag	UNP Q5N3D0
J	4	SER	-	expression tag	UNP Q5N3D0
J	5	HIS	-	expression tag	UNP Q5N3D0

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Chain	Residue	Modelled	Actual	Comment	Reference
J	6	HIS	-	expression tag	UNP Q5N3D0
J	7	HIS	-	expression tag	UNP Q5N3D0
J	8	HIS	-	expression tag	UNP Q5N3D0
J	9	HIS	-	expression tag	UNP Q5N3D0
J	10	HIS	-	expression tag	UNP Q5N3D0
J	11	SER	-	expression tag	UNP Q5N3D0
J	12	GLN	-	expression tag	UNP Q5N3D0
J	13	ASP	-	expression tag	UNP Q5N3D0
J	14	PRO	-	expression tag	UNP Q5N3D0
K	1	MET	-	expression tag	UNP Q5N3D0
K	2	GLY	-	expression tag	UNP Q5N3D0
K	3	SER	-	expression tag	UNP Q5N3D0
K	4	SER	-	expression tag	UNP Q5N3D0
K	5	HIS	-	expression tag	UNP Q5N3D0
K	6	HIS	-	expression tag	UNP Q5N3D0
K	7	HIS	-	expression tag	UNP Q5N3D0
K	8	HIS	-	expression tag	UNP Q5N3D0
K	9	HIS	-	expression tag	UNP Q5N3D0
K	10	HIS	-	expression tag	UNP Q5N3D0
K	11	SER	-	expression tag	UNP Q5N3D0
K	12	GLN	-	expression tag	UNP Q5N3D0
K	13	ASP	-	expression tag	UNP Q5N3D0
K	14	PRO	-	expression tag	UNP Q5N3D0
L	1	MET	-	expression tag	UNP Q5N3D0
L	2	GLY	-	expression tag	UNP Q5N3D0
L	3	SER	-	expression tag	UNP Q5N3D0
L	4	SER	-	expression tag	UNP Q5N3D0
L	5	HIS	-	expression tag	UNP Q5N3D0
L	6	HIS	-	expression tag	UNP Q5N3D0
L	7	HIS	-	expression tag	UNP Q5N3D0
L	8	HIS	-	expression tag	UNP Q5N3D0
L	9	HIS	-	expression tag	UNP Q5N3D0
L	10	HIS	-	expression tag	UNP Q5N3D0
L	11	SER	-	expression tag	UNP Q5N3D0
L	12	GLN	-	expression tag	UNP Q5N3D0
L	13	ASP	-	expression tag	UNP Q5N3D0
L	14	PRO	-	expression tag	UNP Q5N3D0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total O 1 1	0	0

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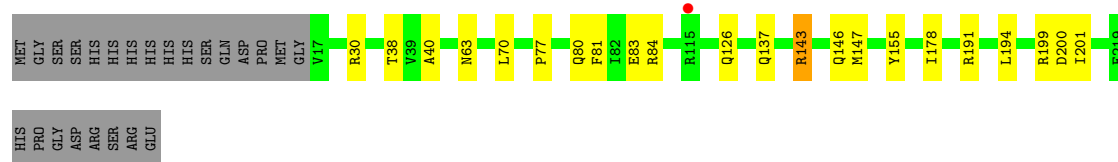
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	2	Total 2	O 2	0	0
2	I	2	Total 2	O 2	0	0
2	D	1	Total 1	O 1	0	0
2	E	2	Total 2	O 2	0	0
2	F	4	Total 4	O 4	0	0
2	J	1	Total 1	O 1	0	0
2	K	4	Total 4	O 4	0	0
2	L	2	Total 2	O 2	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

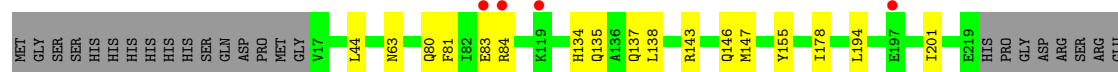
- Molecule 1: CO2 concentrating mechanism protein P

Chain A: 



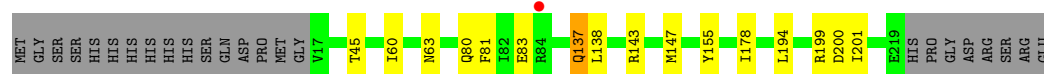
- Molecule 1: CO2 concentrating mechanism protein P

Chain B: 



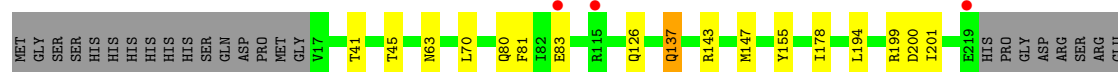
- Molecule 1: CO2 concentrating mechanism protein P

Chain C: 



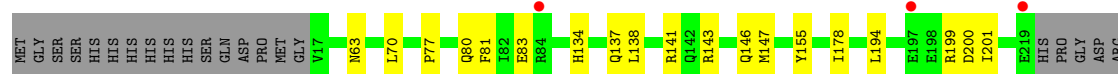
- Molecule 1: CO2 concentrating mechanism protein P

Chain G: 



- Molecule 1: CO2 concentrating mechanism protein P

Chain H: 



SER
ARG
GLU

- Molecule 1: CO2 concentrating mechanism protein P

Chain I:  81% 7% 11%

MET GLY SER SER HIS HIS HIS HIS HIS HIS GLN ASP PRO MET MET GLY V17 T45 I60 N63 Q80 F81 I82 E83 N95 R104 H134 Q137 L138 R143 M147 Y155 I178 L194 R199 D200 I201 E219 HIS PRO GLY ASP ARG SER ARG ARG

GLU

- Molecule 1: CO2 concentrating mechanism protein P

Chain D:  83% 6% 11%

MET GLY SER SER HIS HIS HIS HIS HIS HIS HIS GLN ASP PRO MET MET GLY V17 R30 Y35 Y36 T41 F81 I82 E83 R84 R115 Q137 L138 R141 Q142 R143 Q146 M147 Y155 Q182 L194 E219 HIS PRO GLY ASP ARG SER ARG ARG GLU

- Molecule 1: CO2 concentrating mechanism protein P

Chain E:  83% 6% 11%

MET GLY SER SER HIS HIS HIS HIS HIS HIS HIS GLN ASP PRO MET MET GLY V17 Y35 K71 F81 I82 E83 R84 K119 P120 Q137 L138 R143 Q146 M147 Y155 Q182 L194 R199 E219 HIS PRO GLY ASP ARG SER ARG ARG GLU

- Molecule 1: CO2 concentrating mechanism protein P

Chain F:  83% 6% 11%

MET GLY SER SER HIS HIS HIS HIS HIS HIS HIS GLN ASP PRO MET MET GLY V17 S34 Y35 F43 F81 I82 E83 R84 R100 Q137 L138 R141 Q142 R143 Q146 Y155 Q182 L194 R199 E219 HIS PRO GLY ASP ARG SER ARG ARG GLU

- Molecule 1: CO2 concentrating mechanism protein P

Chain J:  81% 7% 11%

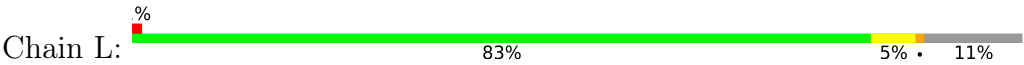
MET GLY SER SER HIS HIS HIS HIS HIS HIS HIS GLN ASP PRO MET MET GLY V17 S34 Y35 L70 K71 P77 F81 I82 E83 R84 N95 E98 Q137 L138 R141 Q142 R143 Q146 Y155 Q182 L194 Y198 R199 E219 HIS PRO GLY ASP ARG SER ARG ARG ARG GLU

- Molecule 1: CO2 concentrating mechanism protein P

Chain K:  83% 6% 11%

MET GLY SER SER HIS HIS HIS HIS HIS HIS HIS GLN ASP PRO MET MET GLY V17 Y35 T41 R64 Q80 F81 I82 E83 R84 Q137 L138 R143 Q146 M147 Y155 Q182 L194 E197 E198 R199 E219 HIS PRO GLY ASP ARG SER ARG ARG ARG GLU

- Molecule 1: CO2 concentrating mechanism protein P



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	175.34Å 176.20Å 200.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.41 – 3.30 39.41 – 3.30	Depositor EDS
% Data completeness (in resolution range)	93.0 (39.41-3.30) 92.1 (39.41-3.30)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	0.21	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 3.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.195 , 0.222 0.201 , 0.226	Depositor DCC
R_{free} test set	2016 reflections (2.15%)	wwPDB-VP
Wilson B-factor (Å ²)	45.2	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.026 for k,h,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	18655	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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](#)

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	0.26	0/1572	0.69	0/2125
1	B	0.26	0/1572	0.69	0/2125
1	C	0.26	0/1572	0.69	0/2125
1	D	0.26	0/1572	0.68	0/2125
1	E	0.26	0/1572	0.68	0/2125
1	F	0.26	0/1572	0.68	0/2125
1	G	0.26	0/1572	0.69	0/2125
1	H	0.26	0/1572	0.68	0/2125
1	I	0.26	0/1572	0.69	0/2125
1	J	0.26	0/1572	0.68	0/2125
1	K	0.26	0/1572	0.68	0/2125
1	L	0.26	0/1572	0.68	0/2125
All	All	0.26	0/18864	0.68	0/25500

There are no bond length outliers.

There are no bond angle outliers.

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	1553	0	1592	20	0
1	B	1553	0	1592	14	0
1	C	1553	0	1592	12	0
1	D	1553	0	1592	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1553	0	1592	7	0
1	F	1553	0	1592	9	0
1	G	1553	0	1592	12	0
1	H	1553	0	1592	13	0
1	I	1553	0	1592	14	0
1	J	1553	0	1592	14	0
1	K	1553	0	1592	8	0
1	L	1553	0	1592	10	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	D	1	0	0	1	0
2	E	2	0	0	0	0
2	F	4	0	0	1	0
2	I	2	0	0	0	0
2	J	1	0	0	0	0
2	K	4	0	0	1	0
2	L	2	0	0	0	0
All	All	18655	0	19104	98	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 (98) 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:126:GLN:NE2	1:C:60:ILE:O	2.16	0.72
1:A:30:ARG:NH1	1:J:95:ASN:OD1	2.28	0.67
1:I:95:ASN:ND2	1:E:71:LYS:HA	2.14	0.61
1:C:45:THR:O	1:F:137:GLN:NE2	2.32	0.61
1:C:63:ASN:ND2	1:C:80:GLN:OE1	2.35	0.60
1:H:63:ASN:ND2	1:H:80:GLN:OE1	2.36	0.58
1:A:63:ASN:ND2	1:A:80:GLN:OE1	2.36	0.58
1:G:63:ASN:ND2	1:G:80:GLN:OE1	2.37	0.58
1:I:63:ASN:ND2	1:I:80:GLN:OE1	2.36	0.58
1:A:146:GLN:HG2	1:D:147:MET:HE2	1.87	0.57
1:B:63:ASN:ND2	1:B:80:GLN:OE1	2.36	0.57
1:H:146:GLN:HG2	1:K:147:MET:HE2	1.88	0.55
1:B:147:MET:HE2	1:E:146:GLN:HG2	1.89	0.54
1:B:146:GLN:HG2	1:E:147:MET:HE2	1.90	0.54
1:G:41:THR:O	1:H:141:ARG:HD3	2.08	0.54
1:A:77:PRO:HB2	1:B:138:LEU:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ARG:NH2	1:C:83:GLU:O	2.42	0.53
1:F:100:ARG:NH1	2:F:303:HOH:O	1.90	0.53
1:H:70:LEU:HD13	1:I:134:HIS:HB2	1.91	0.52
1:A:70:LEU:HD13	1:B:134:HIS:HB2	1.91	0.51
1:J:141:ARG:HD3	1:K:41:THR:O	2.10	0.51
1:H:77:PRO:HB2	1:I:138:LEU:HD11	1.94	0.49
1:H:147:MET:HE2	1:K:146:GLN:HG2	1.94	0.49
1:A:30:ARG:NH1	1:J:98:GLU:HG2	2.28	0.49
1:I:147:MET:HE2	1:L:146:GLN:HG2	1.96	0.48
1:J:70:LEU:HD12	1:L:135:GLN:HB2	1.94	0.48
1:G:155:TYR:HB2	1:G:201:ILE:HG23	1.95	0.48
1:I:45:THR:O	1:L:137:GLN:NE2	2.40	0.48
1:B:155:TYR:HB2	1:B:201:ILE:HG23	1.96	0.48
1:A:155:TYR:HB2	1:A:201:ILE:HG23	1.95	0.48
1:C:155:TYR:HB2	1:C:201:ILE:HG23	1.95	0.48
1:H:155:TYR:HB2	1:H:201:ILE:HG23	1.96	0.47
1:I:137:GLN:OE1	1:L:34:SER:HA	2.15	0.47
1:I:155:TYR:HB2	1:I:201:ILE:HG23	1.95	0.47
1:D:155:TYR:HB3	1:D:194:LEU:HB2	1.97	0.46
1:C:137:GLN:OE1	1:F:34:SER:HA	2.16	0.46
1:G:45:THR:O	1:J:137:GLN:NE2	2.46	0.46
1:H:81:PHE:CD2	1:H:83:GLU:HG2	2.51	0.46
1:E:155:TYR:HB3	1:E:194:LEU:HB2	1.98	0.46
1:G:147:MET:HE2	1:J:146:GLN:HG2	1.97	0.46
1:L:155:TYR:HB3	1:L:194:LEU:HB2	1.98	0.45
1:F:155:TYR:HB3	1:F:194:LEU:HB2	1.98	0.45
1:G:81:PHE:CD2	1:G:83:GLU:HG2	2.52	0.45
1:A:81:PHE:CD2	1:A:83:GLU:HG2	2.52	0.45
1:B:81:PHE:CD2	1:B:83:GLU:HG2	2.51	0.45
1:J:155:TYR:HB3	1:J:194:LEU:HB2	1.98	0.45
1:I:81:PHE:CD2	1:I:83:GLU:HG2	2.52	0.45
1:H:80:GLN:HE21	1:I:138:LEU:HD13	1.82	0.45
1:K:155:TYR:HB3	1:K:194:LEU:HB2	1.98	0.45
1:C:81:PHE:CD2	1:C:83:GLU:HG2	2.52	0.44
1:A:38:THR:HA	1:D:141:ARG:HG2	2.00	0.44
1:J:71:LYS:NZ	1:L:130:ASN:O	2.45	0.44
1:D:35:TYR:OH	1:D:182:GLN:HG2	2.18	0.44
1:J:77:PRO:HB2	1:L:138:LEU:HD11	2.00	0.44
1:G:80:GLN:HB2	1:H:138:LEU:HD13	2.00	0.43
1:J:35:TYR:OH	1:J:182:GLN:HG2	2.18	0.43
1:G:137:GLN:OE1	1:J:34:SER:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:35:TYR:OH	1:E:182:GLN:HG2	2.18	0.43
1:F:35:TYR:OH	1:F:182:GLN:HG2	2.18	0.43
1:L:35:TYR:OH	1:L:182:GLN:HG2	2.18	0.43
1:G:70:LEU:HD13	1:H:134:HIS:HB2	2.00	0.43
1:K:35:TYR:OH	1:K:182:GLN:HG2	2.18	0.43
1:A:178:ILE:HD13	1:A:194:LEU:HD22	2.01	0.42
1:A:80:GLN:HE21	1:B:138:LEU:HD13	1.84	0.42
1:J:81:PHE:CD2	1:J:83:GLU:HG2	2.54	0.42
1:I:178:ILE:H	1:I:178:ILE:HG13	1.75	0.42
1:F:81:PHE:CD2	1:F:83:GLU:HG2	2.55	0.42
1:D:41:THR:O	1:F:141:ARG:HD3	2.20	0.42
1:C:178:ILE:HD13	1:C:194:LEU:HD22	2.01	0.42
1:B:178:ILE:HD13	1:B:194:LEU:HD22	2.01	0.42
1:E:81:PHE:CD2	1:E:83:GLU:HG2	2.55	0.42
1:A:84:ARG:HH12	1:B:84:ARG:HH12	1.66	0.42
1:J:70:LEU:HD13	1:L:134:HIS:HB2	2.02	0.42
1:A:40:ALA:O	1:D:141:ARG:NH2	2.52	0.42
1:G:126:GLN:NE2	1:I:60:ILE:O	2.28	0.42
1:A:199:ARG:HG3	1:A:200:ASP:N	2.35	0.41
1:I:199:ARG:HG3	1:I:200:ASP:N	2.35	0.41
1:B:80:GLN:HE21	1:C:138:LEU:HD13	1.86	0.41
1:C:199:ARG:HG3	1:C:200:ASP:N	2.35	0.41
1:K:64:ARG:NH2	2:K:303:HOH:O	2.52	0.41
1:G:178:ILE:HD13	1:G:194:LEU:HD22	2.02	0.41
1:B:178:ILE:H	1:B:178:ILE:HG13	1.76	0.41
1:I:178:ILE:HD13	1:I:194:LEU:HD22	2.02	0.41
1:H:199:ARG:HG3	1:H:200:ASP:N	2.35	0.41
1:K:81:PHE:CD2	1:K:83:GLU:HG2	2.56	0.41
1:B:44:LEU:HB2	1:F:43:PHE:CE2	2.56	0.41
1:H:178:ILE:HD13	1:H:194:LEU:HD22	2.02	0.41
1:L:81:PHE:CD2	1:L:83:GLU:HG2	2.56	0.41
1:A:126:GLN:NE2	1:C:60:ILE:HG13	2.36	0.41
1:C:147:MET:HE2	1:F:146:GLN:HG2	2.02	0.41
1:G:199:ARG:HG3	1:G:200:ASP:N	2.35	0.41
1:D:81:PHE:CD2	1:D:83:GLU:HG2	2.55	0.41
1:J:138:LEU:HD13	1:K:80:GLN:CB	2.50	0.41
1:A:70:LEU:HD12	1:B:135:GLN:HB2	2.03	0.40
1:E:119:LYS:HA	1:E:120:PRO:HD3	1.98	0.40
1:A:147:MET:HE2	1:D:146:GLN:HG2	2.03	0.40
1:D:30:ARG:NE	2:D:301:HOH:O	2.54	0.40
1:A:143:ARG:CZ	1:A:147:MET:HG2	2.52	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	201/227 (88%)	196 (98%)	5 (2%)	0	100	100
1	B	201/227 (88%)	196 (98%)	5 (2%)	0	100	100
1	C	201/227 (88%)	196 (98%)	5 (2%)	0	100	100
1	D	201/227 (88%)	195 (97%)	5 (2%)	1 (0%)	24	55
1	E	201/227 (88%)	195 (97%)	5 (2%)	1 (0%)	24	55
1	F	201/227 (88%)	195 (97%)	5 (2%)	1 (0%)	24	55
1	G	201/227 (88%)	196 (98%)	5 (2%)	0	100	100
1	H	201/227 (88%)	196 (98%)	5 (2%)	0	100	100
1	I	201/227 (88%)	196 (98%)	5 (2%)	0	100	100
1	J	201/227 (88%)	195 (97%)	5 (2%)	1 (0%)	24	55
1	K	201/227 (88%)	195 (97%)	5 (2%)	1 (0%)	24	55
1	L	201/227 (88%)	195 (97%)	5 (2%)	1 (0%)	24	55
All	All	2412/2724 (88%)	2346 (97%)	60 (2%)	6 (0%)	43	71

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	84	ARG
1	E	84	ARG
1	F	84	ARG
1	J	84	ARG
1	K	84	ARG
1	L	84	ARG

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	158/179 (88%)	156 (99%)	2 (1%)	61	74
1	B	158/179 (88%)	156 (99%)	2 (1%)	61	74
1	C	158/179 (88%)	156 (99%)	2 (1%)	61	74
1	D	158/179 (88%)	154 (98%)	4 (2%)	42	64
1	E	158/179 (88%)	154 (98%)	4 (2%)	42	64
1	F	158/179 (88%)	154 (98%)	4 (2%)	42	64
1	G	158/179 (88%)	156 (99%)	2 (1%)	61	74
1	H	158/179 (88%)	156 (99%)	2 (1%)	61	74
1	I	158/179 (88%)	156 (99%)	2 (1%)	61	74
1	J	158/179 (88%)	154 (98%)	4 (2%)	42	64
1	K	158/179 (88%)	154 (98%)	4 (2%)	42	64
1	L	158/179 (88%)	154 (98%)	4 (2%)	42	64
All	All	1896/2148 (88%)	1860 (98%)	36 (2%)	50	68

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	GLN
1	A	143	ARG
1	B	137	GLN
1	B	143	ARG
1	C	137	GLN
1	C	143	ARG
1	G	137	GLN
1	G	143	ARG
1	H	137	GLN
1	H	143	ARG
1	I	137	GLN
1	I	143	ARG
1	D	83	GLU
1	D	137	GLN

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Mol	Chain	Res	Type
1	D	138	LEU
1	D	143	ARG
1	E	83	GLU
1	E	137	GLN
1	E	138	LEU
1	E	143	ARG
1	F	83	GLU
1	F	137	GLN
1	F	138	LEU
1	F	143	ARG
1	J	83	GLU
1	J	137	GLN
1	J	138	LEU
1	J	143	ARG
1	K	83	GLU
1	K	137	GLN
1	K	138	LEU
1	K	143	ARG
1	L	83	GLU
1	L	137	GLN
1	L	138	LEU
1	L	143	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	80	GLN
1	A	96	GLN
1	B	63	ASN
1	B	80	GLN
1	B	96	GLN
1	B	160	GLN
1	C	96	GLN
1	C	160	GLN
1	G	63	ASN
1	G	80	GLN
1	G	96	GLN
1	H	63	ASN
1	H	80	GLN
1	H	96	GLN
1	H	160	GLN

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Mol	Chain	Res	Type
1	I	63	ASN
1	I	96	GLN
1	I	160	GLN
1	E	32	HIS
1	E	135	GLN
1	L	135	GLN

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 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	203/227 (89%)	-0.09	1 (0%) 87 76	30, 45, 66, 103	0
1	B	203/227 (89%)	-0.08	4 (1%) 65 46	34, 46, 70, 106	0
1	C	203/227 (89%)	-0.16	1 (0%) 87 76	28, 42, 63, 94	0
1	D	203/227 (89%)	-0.09	1 (0%) 87 76	28, 43, 61, 93	0
1	E	203/227 (89%)	-0.14	2 (0%) 79 63	32, 47, 63, 91	0
1	F	203/227 (89%)	-0.05	2 (0%) 79 63	31, 45, 66, 91	0
1	G	203/227 (89%)	-0.14	3 (1%) 72 53	31, 44, 64, 97	0
1	H	203/227 (89%)	-0.07	3 (1%) 72 53	29, 47, 70, 98	0
1	I	203/227 (89%)	-0.12	1 (0%) 87 76	32, 47, 67, 98	0
1	J	203/227 (89%)	-0.02	2 (0%) 79 63	31, 43, 66, 97	0
1	K	203/227 (89%)	-0.12	3 (1%) 72 53	31, 45, 66, 96	0
1	L	203/227 (89%)	-0.08	2 (0%) 79 63	28, 45, 67, 88	0
All	All	2436/2724 (89%)	-0.10	25 (1%) 79 63	28, 45, 67, 106	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	83	GLU	3.8
1	F	83	GLU	3.3
1	B	83	GLU	3.1
1	G	115	ARG	2.9
1	F	199	ARG	2.6
1	C	84	ARG	2.6
1	E	199	ARG	2.6
1	G	219	GLU	2.6
1	K	197	GLU	2.6
1	B	119	LYS	2.5
1	L	199	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	L	219	GLU	2.4
1	D	115	ARG	2.4
1	K	199	ARG	2.4
1	B	84	ARG	2.3
1	B	197	GLU	2.3
1	A	115	ARG	2.3
1	G	83	GLU	2.3
1	H	84	ARG	2.2
1	E	84	ARG	2.1
1	H	197	GLU	2.1
1	I	104	ARG	2.1
1	J	84	ARG	2.0
1	H	219	GLU	2.0
1	K	219	GLU	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 ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.