



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:23 AM UTC

PDB ID : 4FO7 / pdb_00004fo7
Title : Pseudomonas aeruginosa MetAP, in Mn form
Authors : Ye, Q.Z.; Lu, J.P.
Deposited on : 2012-06-20
Resolution : 1.80 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

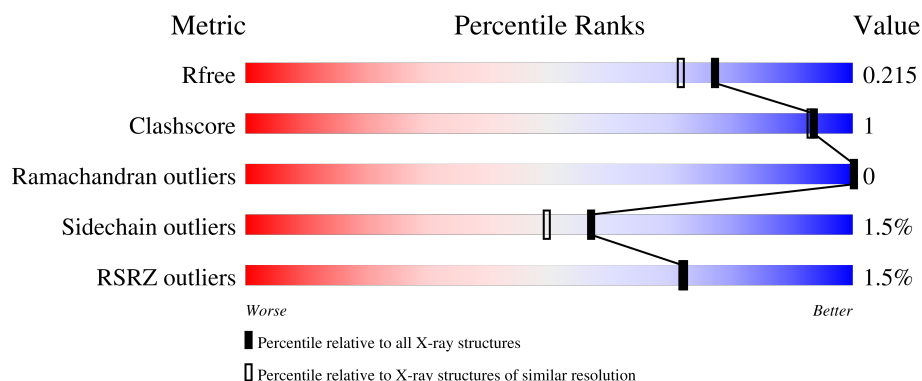
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	0% 72% 19% 8%
1	B	280	0% 70% 21% 7%
1	C	280	2% 75% 16% 8%
1	D	280	0% 74% 18% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8669 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 Methionine aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	1	0
			2036	1288	354	382	12			
1	B	260	Total	C	N	O	S	0	2	0
			2050	1294	357	387	12			
1	C	258	Total	C	N	O	S	0	1	0
			2036	1288	354	382	12			
1	D	258	Total	C	N	O	S	0	2	0
			2037	1285	354	385	13			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	262	GLU	-	expression tag	UNP Q9HXY1
A	263	PHE	-	expression tag	UNP Q9HXY1
A	264	GLU	-	expression tag	UNP Q9HXY1
A	265	LEU	-	expression tag	UNP Q9HXY1
A	266	VAL	-	expression tag	UNP Q9HXY1
A	267	ASP	-	expression tag	UNP Q9HXY1
A	268	LYS	-	expression tag	UNP Q9HXY1
A	269	LEU	-	expression tag	UNP Q9HXY1
A	270	ALA	-	expression tag	UNP Q9HXY1
A	271	ALA	-	expression tag	UNP Q9HXY1
A	272	ALA	-	expression tag	UNP Q9HXY1
A	273	LEU	-	expression tag	UNP Q9HXY1
A	274	GLU	-	expression tag	UNP Q9HXY1
A	275	HIS	-	expression tag	UNP Q9HXY1
A	276	HIS	-	expression tag	UNP Q9HXY1
A	277	HIS	-	expression tag	UNP Q9HXY1
A	278	HIS	-	expression tag	UNP Q9HXY1
A	279	HIS	-	expression tag	UNP Q9HXY1
A	280	HIS	-	expression tag	UNP Q9HXY1
B	262	GLU	-	expression tag	UNP Q9HXY1
B	263	PHE	-	expression tag	UNP Q9HXY1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	264	GLU	-	expression tag	UNP Q9HXY1
B	265	LEU	-	expression tag	UNP Q9HXY1
B	266	VAL	-	expression tag	UNP Q9HXY1
B	267	ASP	-	expression tag	UNP Q9HXY1
B	268	LYS	-	expression tag	UNP Q9HXY1
B	269	LEU	-	expression tag	UNP Q9HXY1
B	270	ALA	-	expression tag	UNP Q9HXY1
B	271	ALA	-	expression tag	UNP Q9HXY1
B	272	ALA	-	expression tag	UNP Q9HXY1
B	273	LEU	-	expression tag	UNP Q9HXY1
B	274	GLU	-	expression tag	UNP Q9HXY1
B	275	HIS	-	expression tag	UNP Q9HXY1
B	276	HIS	-	expression tag	UNP Q9HXY1
B	277	HIS	-	expression tag	UNP Q9HXY1
B	278	HIS	-	expression tag	UNP Q9HXY1
B	279	HIS	-	expression tag	UNP Q9HXY1
B	280	HIS	-	expression tag	UNP Q9HXY1
C	262	GLU	-	expression tag	UNP Q9HXY1
C	263	PHE	-	expression tag	UNP Q9HXY1
C	264	GLU	-	expression tag	UNP Q9HXY1
C	265	LEU	-	expression tag	UNP Q9HXY1
C	266	VAL	-	expression tag	UNP Q9HXY1
C	267	ASP	-	expression tag	UNP Q9HXY1
C	268	LYS	-	expression tag	UNP Q9HXY1
C	269	LEU	-	expression tag	UNP Q9HXY1
C	270	ALA	-	expression tag	UNP Q9HXY1
C	271	ALA	-	expression tag	UNP Q9HXY1
C	272	ALA	-	expression tag	UNP Q9HXY1
C	273	LEU	-	expression tag	UNP Q9HXY1
C	274	GLU	-	expression tag	UNP Q9HXY1
C	275	HIS	-	expression tag	UNP Q9HXY1
C	276	HIS	-	expression tag	UNP Q9HXY1
C	277	HIS	-	expression tag	UNP Q9HXY1
C	278	HIS	-	expression tag	UNP Q9HXY1
C	279	HIS	-	expression tag	UNP Q9HXY1
C	280	HIS	-	expression tag	UNP Q9HXY1
D	262	GLU	-	expression tag	UNP Q9HXY1
D	263	PHE	-	expression tag	UNP Q9HXY1
D	264	GLU	-	expression tag	UNP Q9HXY1
D	265	LEU	-	expression tag	UNP Q9HXY1
D	266	VAL	-	expression tag	UNP Q9HXY1
D	267	ASP	-	expression tag	UNP Q9HXY1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	268	LYS	-	expression tag	UNP Q9HXY1
D	269	LEU	-	expression tag	UNP Q9HXY1
D	270	ALA	-	expression tag	UNP Q9HXY1
D	271	ALA	-	expression tag	UNP Q9HXY1
D	272	ALA	-	expression tag	UNP Q9HXY1
D	273	LEU	-	expression tag	UNP Q9HXY1
D	274	GLU	-	expression tag	UNP Q9HXY1
D	275	HIS	-	expression tag	UNP Q9HXY1
D	276	HIS	-	expression tag	UNP Q9HXY1
D	277	HIS	-	expression tag	UNP Q9HXY1
D	278	HIS	-	expression tag	UNP Q9HXY1
D	279	HIS	-	expression tag	UNP Q9HXY1
D	280	HIS	-	expression tag	UNP Q9HXY1

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total 4	Mn 4	0	0
2	B	3	Total 3	Mn 3	0	0
2	C	3	Total 3	Mn 3	0	0
2	D	4	Total 4	Mn 4	0	0

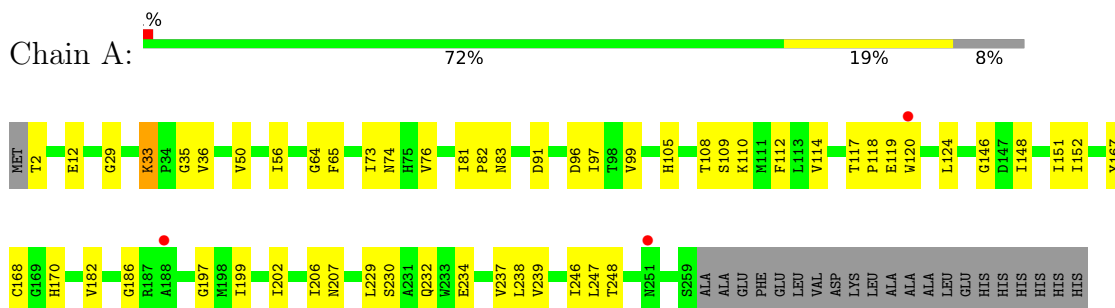
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	130	Total 130	O 130	0	0
3	B	148	Total 148	O 148	0	0
3	C	102	Total 102	O 102	0	0
3	D	116	Total 116	O 116	0	0

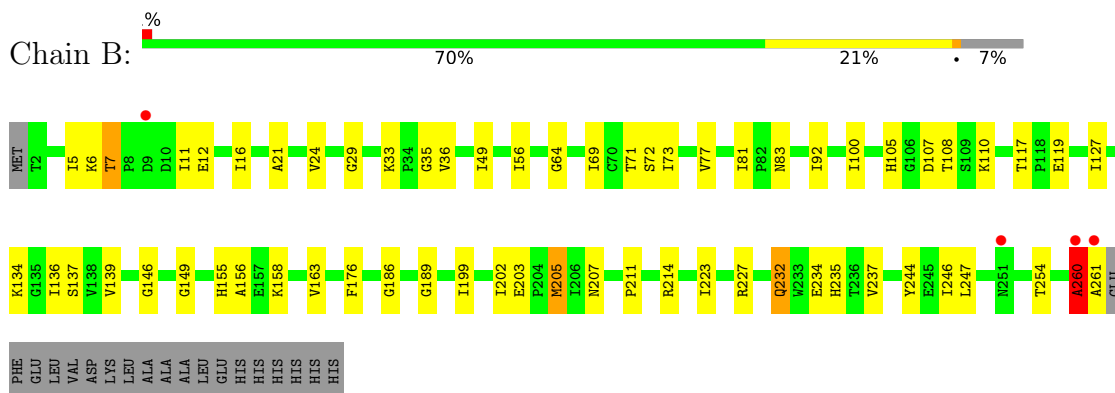
3 Residue-property plots [i](#)

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.

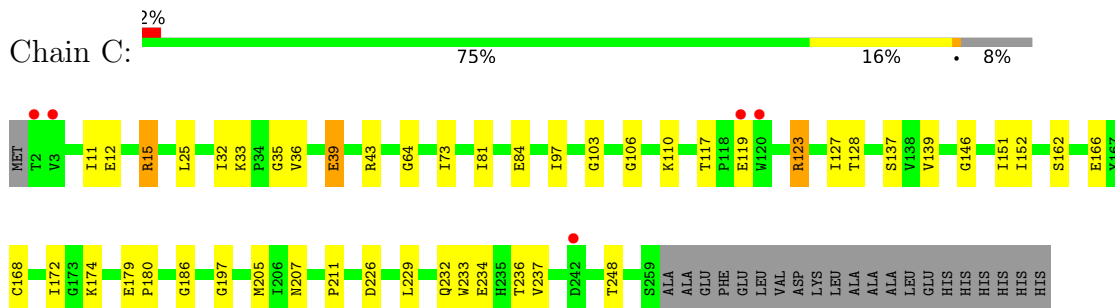
• Molecule 1: Methionine aminopeptidase



• Molecule 1: Methionine aminopeptidase

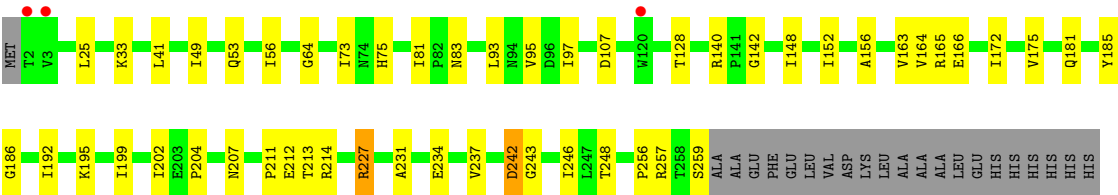


• Molecule 1: Methionine aminopeptidase



• Molecule 1: Methionine aminopeptidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.02Å 111.42Å 140.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.80 – 1.80 35.80 – 1.80	Depositor EDS
% Data completeness (in resolution range)	92.2 (35.80-1.80) 92.1 (35.80-1.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 1.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.192 , 0.230 (Not available) , 0.215	Depositor DCC
R_{free} test set	6200 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	20.3	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 65.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8669	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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

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

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	2.04	36/2080 (1.7%)	1.70	24/2816 (0.9%)
1	B	2.05	31/2092 (1.5%)	1.70	33/2830 (1.2%)
1	C	1.82	19/2080 (0.9%)	1.66	30/2816 (1.1%)
1	D	1.85	16/2079 (0.8%)	1.73	33/2813 (1.2%)
All	All	1.95	102/8331 (1.2%)	1.70	120/11275 (1.1%)

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	B	0	1

All (102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	49	ILE	CA-CB	8.36	1.64	1.54
1	C	81	ILE	CA-CB	7.53	1.61	1.53
1	A	65	PHE	N-CA	7.12	1.54	1.45
1	A	152	ILE	CA-CB	7.08	1.62	1.54
1	B	81	ILE	N-CA	7.02	1.52	1.46
1	A	81	ILE	N-CA	6.97	1.51	1.46
1	B	92	ILE	CA-CB	6.94	1.63	1.54
1	B	246	ILE	CA-CB	6.51	1.60	1.53
1	A	105	HIS	N-CA	6.45	1.53	1.46
1	A	182	VAL	CA-CB	6.43	1.61	1.53
1	A	234	GLU	N-CA	6.39	1.53	1.46
1	B	107	ASP	N-CA	6.38	1.53	1.46
1	A	232	GLN	N-CA	6.38	1.53	1.46
1	A	230	SER	CA-C	6.27	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	128	THR	CA-CB	6.26	1.63	1.53
1	A	33	LYS	N-CA	6.23	1.51	1.46
1	D	97	ILE	CA-CB	6.23	1.62	1.54
1	D	164	VAL	CA-CB	6.18	1.61	1.54
1	C	234	GLU	N-CA	6.06	1.53	1.46
1	D	152	ILE	CA-CB	6.00	1.61	1.54
1	B	235	HIS	N-CA	5.99	1.53	1.45
1	D	107	ASP	CA-C	5.95	1.59	1.52
1	B	108	THR	N-CA	5.92	1.53	1.46
1	D	202	ILE	CA-CB	5.90	1.61	1.53
1	C	36	VAL	CA-CB	5.90	1.60	1.54
1	A	232	GLN	CA-C	5.88	1.59	1.52
1	C	127	ILE	CA-CB	5.86	1.61	1.54
1	A	97	ILE	N-CA	5.86	1.53	1.46
1	D	234	GLU	N-CA	5.82	1.53	1.46
1	B	202	ILE	CA-CB	5.81	1.61	1.53
1	C	81	ILE	N-CA	5.80	1.50	1.46
1	A	170	HIS	N-CA	5.78	1.53	1.46
1	A	148	ILE	CA-CB	5.74	1.60	1.54
1	B	16	ILE	CA-CB	5.73	1.61	1.54
1	A	96	ASP	N-CA	5.73	1.53	1.46
1	B	139	VAL	CA-CB	5.72	1.60	1.53
1	A	81	ILE	CA-CB	5.71	1.59	1.53
1	B	199	ILE	CA-CB	5.69	1.61	1.54
1	A	239	VAL	CA-CB	5.66	1.60	1.53
1	D	95	VAL	CA-CB	5.66	1.60	1.54
1	A	114	VAL	CA-CB	5.63	1.59	1.53
1	A	112	PHE	N-CA	5.63	1.52	1.46
1	B	234	GLU	N-CA	5.62	1.52	1.46
1	A	238	LEU	N-CA	5.61	1.52	1.46
1	D	246	ILE	CA-CB	5.61	1.60	1.53
1	A	56	ILE	CA-C	5.60	1.58	1.52
1	B	71	THR	CA-CB	5.59	1.61	1.53
1	B	232	GLN	N-CA	5.59	1.52	1.46
1	C	205	MET	CA-C	5.59	1.59	1.52
1	C	152	ILE	CA-CB	5.50	1.60	1.54
1	C	81	ILE	CA-C	5.50	1.57	1.53
1	D	199	ILE	CA-CB	5.49	1.61	1.54
1	A	124	LEU	CA-C	5.46	1.60	1.52
1	B	56	ILE	CA-C	5.43	1.58	1.52
1	B	108	THR	CA-CB	5.43	1.62	1.53
1	B	100	ILE	CA-CB	5.42	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	THR	CA-CB	5.39	1.62	1.53
1	A	167	TYR	CA-C	5.37	1.59	1.52
1	A	117	THR	CA-CB	5.36	1.60	1.53
1	A	202	ILE	CA-CB	5.36	1.60	1.54
1	B	21	ALA	CA-CB	5.36	1.61	1.53
1	D	56	ILE	CA-C	5.35	1.58	1.52
1	D	172	ILE	CA-CB	5.32	1.62	1.55
1	B	163	VAL	CA-CB	5.27	1.60	1.54
1	D	185	TYR	N-CA	5.26	1.52	1.45
1	C	232	GLN	N-CA	5.25	1.52	1.46
1	A	246	ILE	CA-CB	5.25	1.59	1.53
1	C	97	ILE	CA-C	5.25	1.58	1.52
1	C	128	THR	CA-CB	5.24	1.61	1.53
1	B	205	MET	N-CA	5.21	1.52	1.46
1	B	36	VAL	CA-CB	5.20	1.60	1.54
1	C	229	LEU	N-CA	5.20	1.52	1.45
1	B	100	ILE	N-CA	5.20	1.52	1.46
1	C	237	VAL	N-CA	5.18	1.52	1.46
1	A	206	ILE	CA-CB	5.17	1.61	1.54
1	A	237	VAL	CA-C	5.17	1.59	1.52
1	B	72	SER	CA-C	5.17	1.58	1.52
1	B	244	TYR	N-CA	5.17	1.52	1.45
1	B	24	VAL	CA-CB	5.16	1.60	1.54
1	A	73	ILE	N-CA	5.16	1.52	1.46
1	D	199	ILE	N-CA	5.14	1.52	1.46
1	A	248	THR	CA-CB	5.11	1.60	1.53
1	C	73	ILE	CA-CB	5.11	1.61	1.54
1	A	91	ASP	N-CA	5.11	1.52	1.45
1	B	136	ILE	CA-CB	5.11	1.60	1.54
1	B	29	GLY	N-CA	5.10	1.52	1.45
1	C	117	THR	CA-CB	5.10	1.61	1.53
1	B	107	ASP	CA-C	5.10	1.58	1.52
1	C	172	ILE	CA-C	5.10	1.58	1.52
1	A	199	ILE	N-CA	5.09	1.52	1.46
1	B	49	ILE	CA-CB	5.09	1.60	1.54
1	B	237	VAL	CA-CB	5.08	1.60	1.54
1	A	82	PRO	CA-C	5.08	1.58	1.52
1	C	233	TRP	CA-C	5.08	1.58	1.52
1	D	148	ILE	CA-CB	5.07	1.60	1.54
1	C	248	THR	CA-CB	5.07	1.60	1.53
1	A	99	VAL	CA-C	5.06	1.58	1.52
1	A	109	SER	N-CA	5.05	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	247	LEU	N-CA	5.05	1.52	1.46
1	A	207	ASN	N-CA	5.04	1.52	1.46
1	C	236	THR	CA-CB	5.02	1.60	1.53
1	B	176	PHE	N-CA	5.01	1.52	1.46

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	260	ALA	N-CA-C	11.46	123.52	111.14
1	A	81	ILE	N-CA-C	10.26	118.12	107.76
1	C	186	GLY	N-CA-C	9.46	123.21	110.43
1	A	186	GLY	N-CA-C	8.40	122.47	110.46
1	A	83	ASN	N-CA-C	8.38	119.01	108.45
1	A	35	GLY	N-CA-C	8.29	124.94	115.08
1	D	83	ASN	N-CA-C	8.27	118.87	108.45
1	B	64	GLY	N-CA-C	8.10	126.13	115.36
1	C	81	ILE	N-CA-C	7.79	115.63	107.76
1	D	186	GLY	N-CA-C	7.75	120.90	110.43
1	B	117	THR	CA-C-N	-7.60	112.86	120.31
1	B	117	THR	C-N-CA	-7.60	112.86	120.31
1	B	77	VAL	N-CA-C	7.38	117.98	110.82
1	C	151	ILE	N-CA-C	7.17	117.94	110.62
1	A	168	CYS	N-CA-C	7.06	119.48	108.96
1	C	168	CYS	N-CA-C	6.99	119.55	109.14
1	D	166	GLU	N-CA-C	6.92	121.43	112.92
1	B	81	ILE	N-CA-C	6.89	115.49	107.77
1	D	81	ILE	N-CA-C	6.80	114.63	107.76
1	C	25	LEU	N-CA-C	6.77	118.66	111.28
1	B	146	GLY	N-CA-C	6.70	122.18	113.27
1	B	119	GLU	N-CA-C	6.70	119.43	111.33
1	C	84	GLU	N-CA-C	6.59	121.17	113.20
1	C	123	ARG	N-CA-C	6.54	118.07	111.07
1	D	156	ALA	N-CA-C	6.50	118.02	111.07
1	C	39	GLU	N-CA-C	6.41	119.08	111.71
1	D	227	ARG	N-CA-C	6.37	120.36	112.47
1	C	137	SER	N-CA-C	6.32	118.97	111.71
1	A	33	LYS	N-CA-C	6.30	115.38	108.14
1	B	33	LYS	N-CA-C	6.30	113.80	108.13
1	B	207	ASN	CA-C-N	6.28	128.60	120.44
1	B	207	ASN	C-N-CA	6.28	128.60	120.44
1	D	248	THR	N-CA-C	6.27	119.87	112.72
1	A	170	HIS	N-CA-C	6.25	118.63	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	254	THR	N-CA-C	6.24	121.04	113.17
1	B	149	GLY	N-CA-C	6.22	120.19	112.73
1	C	32	ILE	N-CA-C	6.18	117.37	107.73
1	C	35	GLY	N-CA-C	6.15	122.40	115.08
1	C	226	ASP	N-CA-C	6.14	120.63	113.20
1	B	186	GLY	N-CA-C	6.13	118.23	110.38
1	B	189	GLY	N-CA-C	6.10	123.47	115.36
1	D	211	PRO	N-CA-C	6.09	122.65	114.18
1	B	69	ILE	CA-C-O	-6.09	115.67	121.64
1	B	110	LYS	N-CA-C	6.05	118.27	109.07
1	C	33	LYS	N-CA-C	6.01	113.63	108.22
1	C	64	GLY	N-CA-C	6.01	123.02	115.21
1	A	247	LEU	N-CA-C	5.99	119.84	112.54
1	A	146	GLY	N-CA-C	5.95	121.61	113.99
1	C	103	GLY	N-CA-C	5.94	123.52	115.32
1	C	211	PRO	N-CA-C	5.91	122.39	114.18
1	A	64	GLY	N-CA-C	5.88	123.18	115.47
1	D	73	ILE	N-CA-C	5.88	117.06	108.53
1	B	176	PHE	CA-CB-CG	5.87	119.67	113.80
1	D	75	HIS	N-CA-C	5.81	119.98	113.01
1	B	203	GLU	N-CA-C	5.80	117.94	109.30
1	A	229	LEU	N-CA-C	5.79	118.67	110.50
1	D	192	ILE	N-CA-C	5.79	116.75	110.21
1	D	237	VAL	N-CA-C	5.78	116.44	108.12
1	C	162	SER	N-CA-C	5.75	118.44	109.52
1	D	93	LEU	N-CA-C	5.75	118.48	108.76
1	C	207	ASN	CA-C-N	5.71	127.87	120.44
1	C	207	ASN	C-N-CA	5.71	127.87	120.44
1	A	197	GLY	N-CA-C	5.71	122.63	115.21
1	D	207	ASN	CA-C-N	5.69	127.91	120.28
1	D	207	ASN	C-N-CA	5.69	127.91	120.28
1	C	152	ILE	N-CA-C	5.66	115.86	110.42
1	B	35	GLY	N-CA-C	5.66	121.81	115.08
1	B	83	ASN	N-CA-C	5.63	115.55	108.45
1	A	105	HIS	N-CA-C	5.62	118.98	109.76
1	C	11	ILE	N-CA-C	5.62	116.26	110.36
1	A	50	VAL	N-CA-C	5.59	116.25	110.82
1	C	197	GLY	N-CA-C	5.59	122.18	114.92
1	B	73	ILE	N-CA-C	5.58	116.63	108.53
1	B	223	ILE	N-CA-C	5.55	117.66	108.99
1	B	108	THR	CA-C-O	-5.55	114.79	120.89
1	C	15	ARG	N-CA-C	5.55	117.33	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	106	GLY	CA-C-O	-5.55	116.61	120.94
1	C	139	VAL	N-CA-C	5.55	116.75	108.54
1	B	7	THR	CA-C-N	5.51	125.46	119.78
1	B	7	THR	C-N-CA	5.51	125.46	119.78
1	A	110	LYS	CA-C-N	5.46	129.22	121.42
1	A	110	LYS	C-N-CA	5.46	129.22	121.42
1	D	256	PRO	N-CA-C	5.43	119.72	111.19
1	D	214	ARG	N-CA-C	5.42	117.31	109.07
1	D	64	GLY	N-CA-C	5.40	122.23	115.21
1	B	127	ILE	N-CA-C	5.39	116.12	110.62
1	D	163	VAL	N-CA-C	5.36	115.57	107.80
1	D	257	ARG	N-CA-C	5.35	117.12	111.28
1	B	137	SER	N-CA-C	5.32	117.83	111.71
1	D	142	GLY	N-CA-C	5.31	122.11	115.21
1	A	118	PRO	N-CA-C	5.31	119.55	111.11
1	B	246	ILE	N-CA-C	5.31	114.91	107.37
1	B	139	VAL	N-CA-C	5.30	115.83	108.84
1	D	242	ASP	N-CA-C	5.28	121.53	113.61
1	D	212	GLU	N-CA-C	5.25	117.84	110.23
1	D	231	ALA	N-CA-C	5.23	117.63	109.52
1	A	74	ASN	N-CA-C	5.22	117.39	108.67
1	A	29	GLY	N-CA-C	5.22	118.95	112.64
1	C	110	LYS	N-CA-C	5.17	116.92	109.07
1	B	156	ALA	N-CA-C	5.15	116.58	111.07
1	C	43	ARG	N-CA-C	5.15	116.89	111.28
1	B	105	HIS	CA-CB-CG	5.14	118.94	113.80
1	D	25	LEU	N-CA-C	5.13	116.87	111.28
1	D	53	GLN	N-CA-C	5.13	117.77	111.82
1	D	41	LEU	N-CA-C	5.12	116.86	111.28
1	D	140	ARG	CA-C-N	-5.11	114.49	119.76
1	D	140	ARG	C-N-CA	-5.11	114.49	119.76
1	A	76	VAL	CA-C-N	5.10	128.03	120.74
1	A	76	VAL	C-N-CA	5.10	128.03	120.74
1	C	146	GLY	N-CA-C	5.08	120.03	113.27
1	A	12	GLU	N-CA-C	5.07	116.81	111.28
1	C	229	LEU	N-CA-C	5.06	117.63	110.50
1	D	140	ARG	N-CA-C	5.05	112.67	108.13
1	C	81	ILE	CA-C-O	-5.04	116.17	119.15
1	D	204	PRO	N-CA-C	5.04	119.11	111.19
1	D	175	VAL	CA-C-N	5.03	127.28	120.44
1	D	175	VAL	C-N-CA	5.03	127.28	120.44
1	A	151	ILE	N-CA-C	5.02	115.74	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	LYS	N-CA-C	5.02	116.70	109.07
1	B	211	PRO	N-CA-C	5.02	121.15	114.18

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	260	ALA	Peptide

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	2036	0	2031	4	0
1	B	2050	0	2049	13	0
1	C	2036	0	2031	3	0
1	D	2037	0	2031	4	0
2	A	4	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	4	0	0	0	0
3	A	130	0	0	0	1
3	B	148	0	0	0	1
3	C	102	0	0	0	0
3	D	116	0	0	1	0
All	All	8669	0	8142	22	1

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 1.

All (22) 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:6:LYS:H	1:D:181:GLN:HE22	1.10	0.98
1:B:214:ARG:HH21	1:B:227:ARG:NH1	1.73	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:LYS:H	1:D:181:GLN:NE2	1.73	0.86
1:C:12:GLU:OE2	1:C:15:ARG:NH1	2.22	0.72
1:B:6:LYS:HD2	1:B:7:THR:H	1.61	0.65
1:B:214:ARG:HH21	1:B:227:ARG:HH12	1.46	0.63
1:D:165:ARG:NH1	3:D:459:HOH:O	2.40	0.54
1:A:120[B]:TRP:CD1	1:A:120[B]:TRP:N	2.77	0.52
1:A:33:LYS:O	1:A:36:VAL:HG12	2.10	0.51
1:B:214:ARG:NH2	1:B:227:ARG:NH1	2.51	0.50
1:C:179:GLU:OE1	1:C:180:PRO:HA	2.13	0.49
1:A:119:GLU:HG3	1:A:120[B]:TRP:CD1	2.48	0.48
1:B:205:MET:HE3	1:B:232:GLN:NE2	2.28	0.48
1:B:205:MET:CE	1:B:232:GLN:NE2	2.78	0.46
1:A:119:GLU:HG3	1:A:120[B]:TRP:HD1	1.80	0.45
1:D:243:GLY:HA3	1:D:259:SER:OG	2.17	0.44
1:B:6:LYS:CD	1:B:7:THR:H	2.29	0.44
1:B:260:ALA:N	1:B:261:ALA:HA	2.33	0.43
1:B:214:ARG:NH2	1:B:227:ARG:HH12	2.14	0.42
1:B:7:THR:HG22	1:B:12[B]:GLU:HG3	2.01	0.41
1:B:134:LYS:HE3	1:B:155:HIS:CD2	2.56	0.41
1:C:123:ARG:HA	1:C:123:ARG:HD3	1.84	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:514:HOH:O	3:B:542:HOH:O[4_545]	1.50	0.70

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	257/280 (92%)	252 (98%)	5 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	260/280 (93%)	256 (98%)	4 (2%)	0	100	100
1	C	257/280 (92%)	253 (98%)	4 (2%)	0	100	100
1	D	258/280 (92%)	252 (98%)	6 (2%)	0	100	100
All	All	1032/1120 (92%)	1013 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	222/238 (93%)	221 (100%)	1 (0%)	81	80
1	B	223/238 (94%)	220 (99%)	3 (1%)	61	54
1	C	222/238 (93%)	218 (98%)	4 (2%)	51	43
1	D	223/238 (94%)	218 (98%)	5 (2%)	45	34
All	All	890/952 (94%)	877 (98%)	13 (2%)	57	49

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	B	5	ILE
1	B	11	ILE
1	B	158	LYS
1	C	39	GLU
1	C	119	GLU
1	C	166	GLU
1	C	174	LYS
1	D	33	LYS
1	D	195	LYS
1	D	213	THR
1	D	227	ARG
1	D	242	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	ASN
1	A	155	HIS
1	A	232	GLN
1	B	46	HIS
1	B	94	ASN
1	B	126	GLN
1	B	129	GLN
1	B	155	HIS
1	B	232	GLN
1	C	46	HIS
1	C	144	HIS
1	C	155	HIS
1	C	232	GLN
1	D	46	HIS
1	D	79	HIS
1	D	181	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](#)

Of 14 ligands modelled in this entry, 14 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	258/280 (92%)	-0.09	3 (1%) 76 77	9, 18, 33, 41	1 (0%)
1	B	260/280 (92%)	-0.18	4 (1%) 72 72	8, 17, 33, 40	2 (0%)
1	C	258/280 (92%)	0.16	5 (1%) 66 66	13, 22, 40, 52	1 (0%)
1	D	258/280 (92%)	-0.04	3 (1%) 76 77	10, 21, 36, 47	2 (0%)
All	All	1034/1120 (92%)	-0.04	15 (1%) 72 72	8, 19, 36, 52	6 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	120[A]	TRP	4.6
1	B	261	ALA	4.0
1	A	120[A]	TRP	4.0
1	D	2	THR	3.8
1	B	251	ASN	2.6
1	B	260	ALA	2.5
1	C	242	ASP	2.5
1	C	3	VAL	2.4
1	D	3	VAL	2.3
1	D	120	TRP	2.3
1	A	188	ALA	2.3
1	B	9	ASP	2.3
1	C	2	THR	2.2
1	C	119	GLU	2.2
1	A	251	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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($\text{\AA}^2$)	Q<0.9
2	MN	D	303	1/1	0.95	0.08	71,71,71,71	0
2	MN	B	303	1/1	0.98	0.03	21,21,21,21	1
2	MN	D	304	1/1	0.98	0.06	24,24,24,24	1
2	MN	C	301	1/1	0.99	0.02	17,17,17,17	0
2	MN	C	303	1/1	0.99	0.07	19,19,19,19	1
2	MN	A	303	1/1	0.99	0.02	19,19,19,19	0
2	MN	A	301	1/1	0.99	0.02	13,13,13,13	0
2	MN	A	304	1/1	1.00	0.03	17,17,17,17	1
2	MN	C	302	1/1	1.00	0.01	14,14,14,14	0
2	MN	B	301	1/1	1.00	0.01	11,11,11,11	0
2	MN	D	301	1/1	1.00	0.01	16,16,16,16	0
2	MN	D	302	1/1	1.00	0.01	14,14,14,14	0
2	MN	B	302	1/1	1.00	0.01	10,10,10,10	0
2	MN	A	302	1/1	1.00	0.01	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.