



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 07:08 PM UTC

PDB ID : 4D80 / pdb_00004d80
Title : Metallosphera sedula Vps4 crystal structure
Authors : Caillat, C.; Macheboeuf, P.; Wu, Y.; McCarthy, A.A.; Boeri-Erba, E.; Effantin, G.; Gottlinger, H.G.; Weissenhorn, W.; Renesto, P.
Deposited on : 2014-12-02
Resolution : 3.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

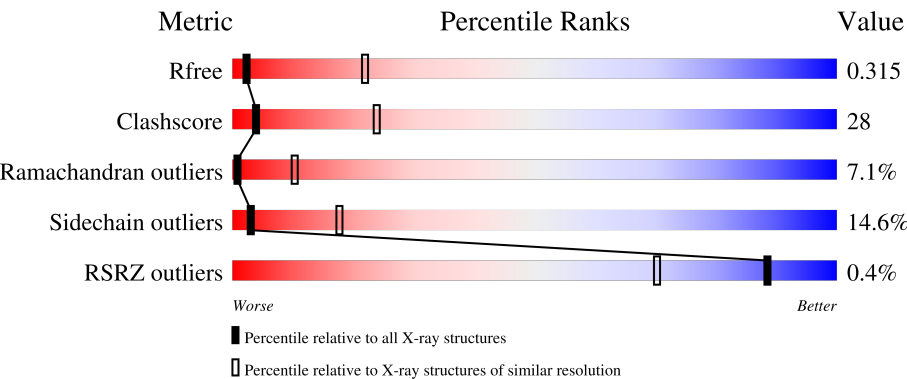
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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	316	% 42%31%9%•15%
1	B	316	% 43%26%10%•19%
1	C	316	44%30%10%•14%
1	D	316	43%31%11%•14%
1	E	316	43%28%10%•17%

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Mol	Chain	Length	Quality of chain
1	F	316	41% 33% 11% • 13%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12875 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 AAA ATPASE, CENTRAL DOMAIN PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			2152	1376	371	397	8			
1	B	257	Total	C	N	O	S	0	0	0
			2060	1319	356	377	8			
1	C	272	Total	C	N	O	S	0	0	0
			2177	1394	373	402	8			
1	D	273	Total	C	N	O	S	0	0	0
			2187	1400	376	403	8			
1	E	262	Total	C	N	O	S	0	0	0
			2106	1347	364	387	8			
1	F	274	Total	C	N	O	S	0	0	0
			2193	1405	378	402	8			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	MET	-	expression tag	UNP A4YHC5
A	55	SER	-	expression tag	UNP A4YHC5
A	56	TYR	-	expression tag	UNP A4YHC5
A	57	TYR	-	expression tag	UNP A4YHC5
A	58	HIS	-	expression tag	UNP A4YHC5
A	59	HIS	-	expression tag	UNP A4YHC5
A	60	HIS	-	expression tag	UNP A4YHC5
A	61	HIS	-	expression tag	UNP A4YHC5
A	62	HIS	-	expression tag	UNP A4YHC5
A	63	HIS	-	expression tag	UNP A4YHC5
A	64	LEU	-	expression tag	UNP A4YHC5
A	65	GLU	-	expression tag	UNP A4YHC5
A	66	SER	-	expression tag	UNP A4YHC5
A	67	THR	-	expression tag	UNP A4YHC5
A	68	SER	-	expression tag	UNP A4YHC5
A	69	LEU	-	expression tag	UNP A4YHC5
A	70	TYR	-	expression tag	UNP A4YHC5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	71	LYS	-	expression tag	UNP A4YHC5
A	72	LYS	-	expression tag	UNP A4YHC5
A	73	ALA	-	expression tag	UNP A4YHC5
A	74	GLY	-	expression tag	UNP A4YHC5
B	54	MET	-	expression tag	UNP A4YHC5
B	55	SER	-	expression tag	UNP A4YHC5
B	56	TYR	-	expression tag	UNP A4YHC5
B	57	TYR	-	expression tag	UNP A4YHC5
B	58	HIS	-	expression tag	UNP A4YHC5
B	59	HIS	-	expression tag	UNP A4YHC5
B	60	HIS	-	expression tag	UNP A4YHC5
B	61	HIS	-	expression tag	UNP A4YHC5
B	62	HIS	-	expression tag	UNP A4YHC5
B	63	HIS	-	expression tag	UNP A4YHC5
B	64	LEU	-	expression tag	UNP A4YHC5
B	65	GLU	-	expression tag	UNP A4YHC5
B	66	SER	-	expression tag	UNP A4YHC5
B	67	THR	-	expression tag	UNP A4YHC5
B	68	SER	-	expression tag	UNP A4YHC5
B	69	LEU	-	expression tag	UNP A4YHC5
B	70	TYR	-	expression tag	UNP A4YHC5
B	71	LYS	-	expression tag	UNP A4YHC5
B	72	LYS	-	expression tag	UNP A4YHC5
B	73	ALA	-	expression tag	UNP A4YHC5
B	74	GLY	-	expression tag	UNP A4YHC5
C	54	MET	-	expression tag	UNP A4YHC5
C	55	SER	-	expression tag	UNP A4YHC5
C	56	TYR	-	expression tag	UNP A4YHC5
C	57	TYR	-	expression tag	UNP A4YHC5
C	58	HIS	-	expression tag	UNP A4YHC5
C	59	HIS	-	expression tag	UNP A4YHC5
C	60	HIS	-	expression tag	UNP A4YHC5
C	61	HIS	-	expression tag	UNP A4YHC5
C	62	HIS	-	expression tag	UNP A4YHC5
C	63	HIS	-	expression tag	UNP A4YHC5
C	64	LEU	-	expression tag	UNP A4YHC5
C	65	GLU	-	expression tag	UNP A4YHC5
C	66	SER	-	expression tag	UNP A4YHC5
C	67	THR	-	expression tag	UNP A4YHC5
C	68	SER	-	expression tag	UNP A4YHC5
C	69	LEU	-	expression tag	UNP A4YHC5
C	70	TYR	-	expression tag	UNP A4YHC5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	71	LYS	-	expression tag	UNP A4YHC5
C	72	LYS	-	expression tag	UNP A4YHC5
C	73	ALA	-	expression tag	UNP A4YHC5
C	74	GLY	-	expression tag	UNP A4YHC5
D	54	MET	-	expression tag	UNP A4YHC5
D	55	SER	-	expression tag	UNP A4YHC5
D	56	TYR	-	expression tag	UNP A4YHC5
D	57	TYR	-	expression tag	UNP A4YHC5
D	58	HIS	-	expression tag	UNP A4YHC5
D	59	HIS	-	expression tag	UNP A4YHC5
D	60	HIS	-	expression tag	UNP A4YHC5
D	61	HIS	-	expression tag	UNP A4YHC5
D	62	HIS	-	expression tag	UNP A4YHC5
D	63	HIS	-	expression tag	UNP A4YHC5
D	64	LEU	-	expression tag	UNP A4YHC5
D	65	GLU	-	expression tag	UNP A4YHC5
D	66	SER	-	expression tag	UNP A4YHC5
D	67	THR	-	expression tag	UNP A4YHC5
D	68	SER	-	expression tag	UNP A4YHC5
D	69	LEU	-	expression tag	UNP A4YHC5
D	70	TYR	-	expression tag	UNP A4YHC5
D	71	LYS	-	expression tag	UNP A4YHC5
D	72	LYS	-	expression tag	UNP A4YHC5
D	73	ALA	-	expression tag	UNP A4YHC5
D	74	GLY	-	expression tag	UNP A4YHC5
E	54	MET	-	expression tag	UNP A4YHC5
E	55	SER	-	expression tag	UNP A4YHC5
E	56	TYR	-	expression tag	UNP A4YHC5
E	57	TYR	-	expression tag	UNP A4YHC5
E	58	HIS	-	expression tag	UNP A4YHC5
E	59	HIS	-	expression tag	UNP A4YHC5
E	60	HIS	-	expression tag	UNP A4YHC5
E	61	HIS	-	expression tag	UNP A4YHC5
E	62	HIS	-	expression tag	UNP A4YHC5
E	63	HIS	-	expression tag	UNP A4YHC5
E	64	LEU	-	expression tag	UNP A4YHC5
E	65	GLU	-	expression tag	UNP A4YHC5
E	66	SER	-	expression tag	UNP A4YHC5
E	67	THR	-	expression tag	UNP A4YHC5
E	68	SER	-	expression tag	UNP A4YHC5
E	69	LEU	-	expression tag	UNP A4YHC5
E	70	TYR	-	expression tag	UNP A4YHC5

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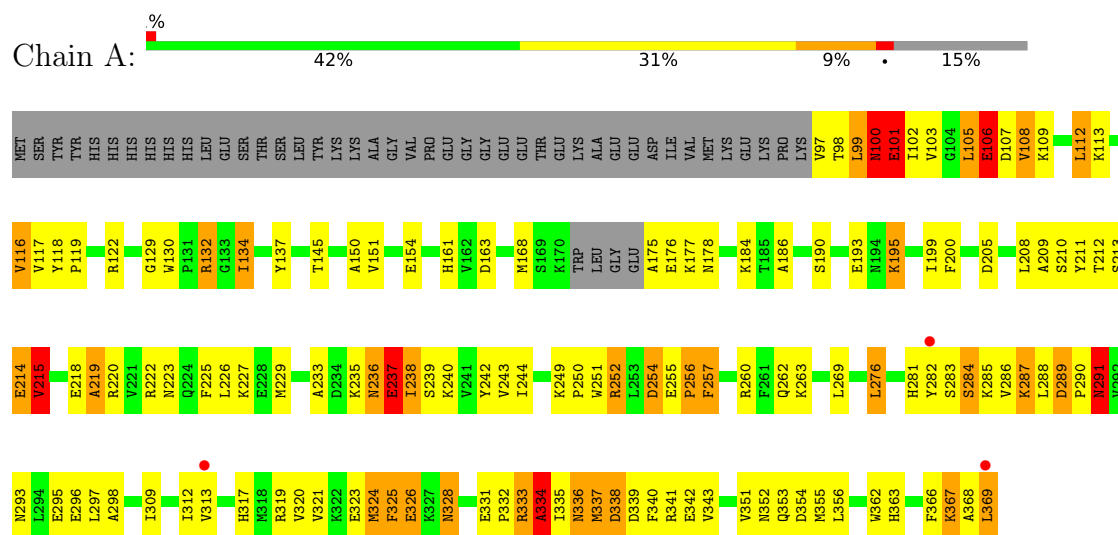
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Chain	Residue	Modelled	Actual	Comment	Reference
E	71	LYS	-	expression tag	UNP A4YHC5
E	72	LYS	-	expression tag	UNP A4YHC5
E	73	ALA	-	expression tag	UNP A4YHC5
E	74	GLY	-	expression tag	UNP A4YHC5
F	54	MET	-	expression tag	UNP A4YHC5
F	55	SER	-	expression tag	UNP A4YHC5
F	56	TYR	-	expression tag	UNP A4YHC5
F	57	TYR	-	expression tag	UNP A4YHC5
F	58	HIS	-	expression tag	UNP A4YHC5
F	59	HIS	-	expression tag	UNP A4YHC5
F	60	HIS	-	expression tag	UNP A4YHC5
F	61	HIS	-	expression tag	UNP A4YHC5
F	62	HIS	-	expression tag	UNP A4YHC5
F	63	HIS	-	expression tag	UNP A4YHC5
F	64	LEU	-	expression tag	UNP A4YHC5
F	65	GLU	-	expression tag	UNP A4YHC5
F	66	SER	-	expression tag	UNP A4YHC5
F	67	THR	-	expression tag	UNP A4YHC5
F	68	SER	-	expression tag	UNP A4YHC5
F	69	LEU	-	expression tag	UNP A4YHC5
F	70	TYR	-	expression tag	UNP A4YHC5
F	71	LYS	-	expression tag	UNP A4YHC5
F	72	LYS	-	expression tag	UNP A4YHC5
F	73	ALA	-	expression tag	UNP A4YHC5
F	74	GLY	-	expression tag	UNP A4YHC5

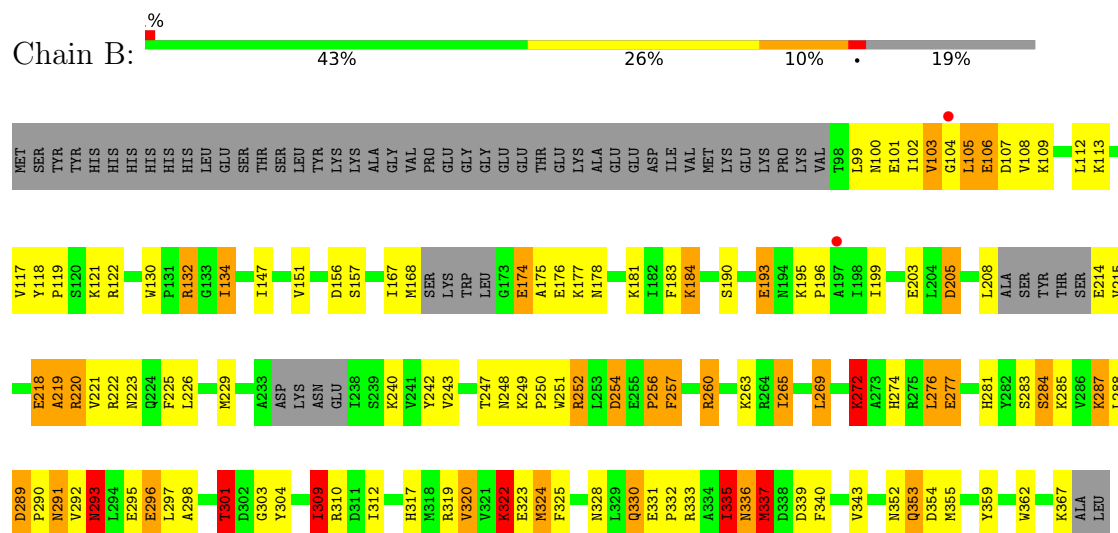
3 Residue-property plots

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: AAA ATPASE, CENTRAL DOMAIN PROTEIN

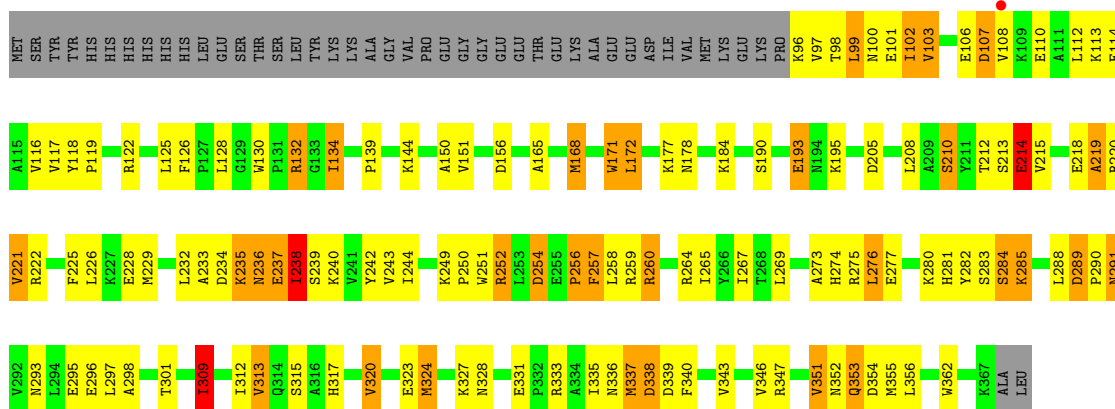


• Molecule 1: AAA ATPASE, CENTRAL DOMAIN PROTEIN

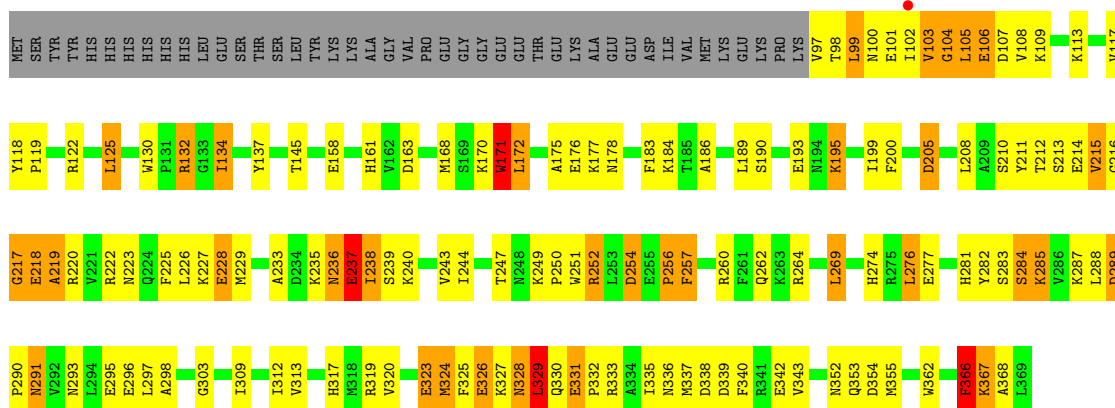


• Molecule 1: AAA ATPASE, CENTRAL DOMAIN PROTEIN

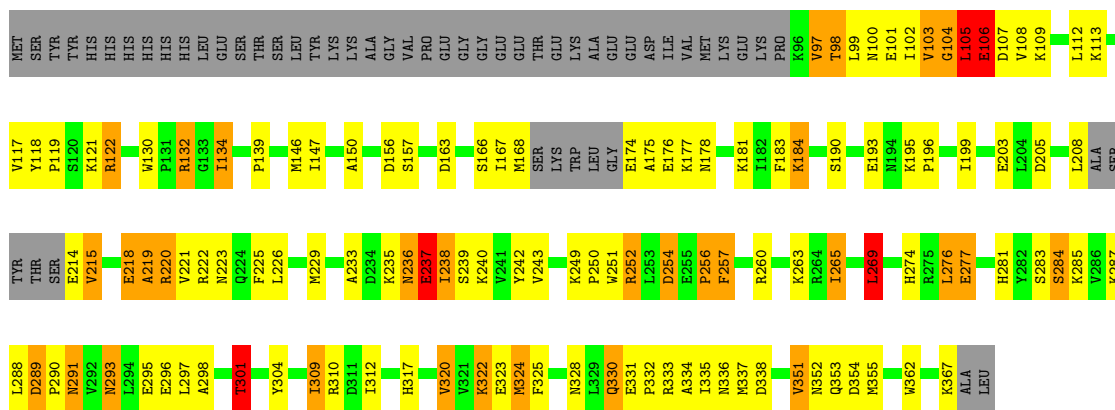




• Molecule 1: AAA ATPASE, CENTRAL DOMAIN PROTEIN



• Molecule 1: AAA ATPASE, CENTRAL DOMAIN PROTEIN



• Molecule 1: AAA ATPASE, CENTRAL DOMAIN PROTEIN



W362	H363	E364	K365	F366	K367	A368	L369	S284	K285	V286	K287	L288	D289	P290	N291	V292	N293	L294	E295	E296	L297	A298	T301	S302	G303	L309	I312	V313	K314	S315	A316	H317	M318	R319	V320	V321	K322	E323	M324	K327	N328	L329	K330	E331	F332	K333	A334	I335	M336	M337	D338	D339	F340	R341	E342	V343	V351	N352	K353	D354	M355	W117	V118	T119	H120	H121	H122	L128	G129	L130	F131	R132	G133	S134	P139	K144	T145	M146	A150	V151	G152	N153	D156	S157	E158	A165	S166	L167	M168	W171	L172	N178	F183	K184	L189	S190	E193	N194	K195	I198	T199	L205	A206	D207	V108	D205	S210	L112	T212	V213	S213	E214	V215	G216	E218	A219	R220	V221	R222	N223	Q224	F225	L226	K227	E228	W229	A233	D234	K235	N236	E237	I238	S239	K240	V243	L244	T247	N248	K249	P250	K251	R252	L253	D254	E255	P256	F257	L258	R259	R260	R264	T267	T268	L269	A273	H274	R275	L276	E277	H281	V282	S283	SER	TRV	HIS	HIS	HIS	HIS	HIS	LEU	GLU	THR	SER	SER	LEU	TRV	LYS	LYS	ALA	GLY	VAL	PRO	GLU	GLU	GLY	GLY	THR	GLU	LYS	ALA	GLU	GLU	ASP	ILE	VAL	MET	LYS	GLU	LYS	PRO	R96	V97	L98	L99	N100	E101	I102	V103	G104	L105	A106	D107	V108	K109	E110	A111	L112	K113
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.70Å 127.39Å 191.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	106.02 – 3.60 106.02 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (106.02-3.60) 99.7 (106.02-3.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.264 , 0.318 0.263 , 0.315	Depositor DCC
R_{free} test set	1464 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	110.9	Xtriage
Anisotropy	0.574	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 89.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12875	wwPDB-VP
Average B, all atoms (Å ²)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.23 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.1588e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.71	0/2191	1.11	10/2952 (0.3%)
1	B	0.70	1/2097 (0.0%)	1.08	10/2823 (0.4%)
1	C	0.75	0/2220	1.08	5/2995 (0.2%)
1	D	0.70	0/2230	1.07	6/3009 (0.2%)
1	E	0.71	0/2144	1.06	8/2887 (0.3%)
1	F	0.71	1/2236 (0.0%)	1.13	10/3016 (0.3%)
All	All	0.71	2/13118 (0.0%)	1.09	49/17682 (0.3%)

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	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	251	TRP	CA-CB	5.58	1.61	1.53
1	B	335	ILE	CA-C	5.23	1.58	1.52

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	104	GLY	N-CA-C	-9.20	97.53	111.42
1	C	108	VAL	N-CA-C	8.80	118.87	110.42
1	F	102	ILE	N-CA-C	8.72	119.56	111.45
1	B	335	ILE	O-C-N	-8.04	114.74	123.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	337	MET	N-CA-C	-7.76	97.98	110.32

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	334	ALA	Peptide
1	B	335	ILE	Peptide
1	C	107	ASP	Peptide
1	D	170	LYS	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	2152	0	2201	153	0
1	B	2060	0	2106	121	0
1	C	2177	0	2219	121	1
1	D	2187	0	2233	130	0
1	E	2106	0	2155	109	0
1	F	2193	0	2244	140	1
All	All	12875	0	13158	737	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 28.

The worst 5 of 737 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:287:LYS:O	1:A:335:ILE:CG2	1.68	1.38
1:A:210:SER:HB3	1:A:211:TYR:N	1.54	1.19
1:B:288:LEU:O	1:B:335:ILE:O	1.66	1.11
1:A:287:LYS:O	1:A:335:ILE:HG21	0.96	1.10
1:A:112:LEU:HD22	1:A:151:VAL:HG11	1.35	1.08

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:PHE:O	1:F:330:GLN:NE2[2_665]	2.19	0.01

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	263/316 (83%)	207 (79%)	34 (13%)	22 (8%)	0	7
1	B	249/316 (79%)	204 (82%)	31 (12%)	14 (6%)	1	14
1	C	270/316 (85%)	218 (81%)	35 (13%)	17 (6%)	1	12
1	D	271/316 (86%)	210 (78%)	38 (14%)	23 (8%)	0	7
1	E	256/316 (81%)	207 (81%)	32 (12%)	17 (7%)	1	12
1	F	272/316 (86%)	214 (79%)	39 (14%)	19 (7%)	1	10
All	All	1581/1896 (83%)	1260 (80%)	209 (13%)	112 (7%)	1	10

5 of 112 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	101	GLU
1	A	106	GLU
1	A	215	VAL
1	A	238	ILE

5.3.2 Protein sidechains [i](#)

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	232/273 (85%)	199 (86%)	33 (14%)	3	19
1	B	221/273 (81%)	185 (84%)	36 (16%)	2	15
1	C	234/273 (86%)	203 (87%)	31 (13%)	4	21
1	D	235/273 (86%)	203 (86%)	32 (14%)	3	20
1	E	227/273 (83%)	193 (85%)	34 (15%)	3	17
1	F	235/273 (86%)	199 (85%)	36 (15%)	3	16
All	All	1384/1638 (84%)	1182 (85%)	202 (15%)	3	18

5 of 202 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	218	GLU
1	E	220	ARG
1	F	351	VAL
1	D	238	ILE
1	D	324	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	100	ASN
1	F	328	ASN
1	C	328	ASN
1	D	161	HIS
1	D	274	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	210:SER	C	211:TYR	N	2.55

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	269/316 (85%)	-0.10	3 (1%)	78 52	84, 149, 228, 279	0
1	B	257/316 (81%)	-0.13	2 (0%)	82 58	71, 135, 218, 262	0
1	C	272/316 (86%)	-0.21	1 (0%)	88 70	86, 134, 200, 216	0
1	D	273/316 (86%)	-0.30	1 (0%)	88 70	81, 135, 208, 251	0
1	E	262/316 (82%)	-0.20	0	100 100	61, 133, 216, 275	0
1	F	274/316 (86%)	-0.30	0	100 100	73, 126, 193, 246	0
All	All	1607/1896 (84%)	-0.21	7 (0%)	88 70	61, 134, 214, 279	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	313	VAL	3.0
1	D	102	ILE	3.0
1	B	197	ALA	2.7
1	B	104	GLY	2.4
1	A	369	LEU	2.3

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.