



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 05:25 AM UTC

PDB ID : 8AFF / pdb_00008aff
Title : Wild type oxalyl-CoA synthetase Pcs60p
Authors : Burgi, J.; Chojnowski, G.; Giannopoulou, E.A.; Wilmanns, M.
Deposited on : 2022-07-17
Resolution : 2.87 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

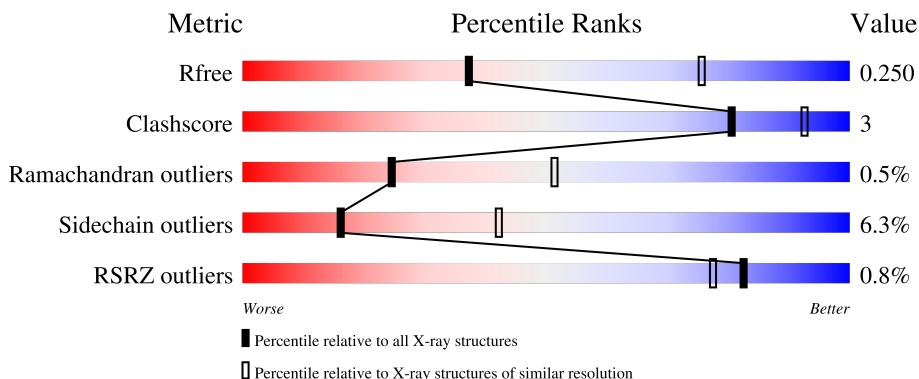
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.87 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	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

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	543	82% 12% . .
1	B	543	68% 9% . 21%
1	C	543	67% 10% . 21%
1	D	543	% 81% 11% . 6%
1	E	543	69% 8% . 22%

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Mol	Chain	Length	Quality of chain
1	F	543	 68% 10% • 21%
1	G	543	 % 67% 9% • 22%
1	H	543	 % 68% 9% • 21%
1	I	543	 % 82% 12% • 5%
1	J	543	 69% 8% • 21%
1	K	543	 % 69% 8% • 22%
1	L	543	 2% 68% 9% • 22%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 42783 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 Oxalate–CoA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	525	Total 4134	C 2660	N 698	O 758	S 18	0	0	0
1	B	428	Total 3370	C 2163	N 571	O 621	S 15	0	0	0
1	C	430	Total 3386	C 2173	N 574	O 624	S 15	0	0	0
1	D	511	Total 4023	C 2590	N 676	O 739	S 18	0	0	0
1	E	426	Total 3353	C 2152	N 569	O 617	S 15	0	0	0
1	F	429	Total 3378	C 2169	N 572	O 622	S 15	0	0	0
1	G	423	Total 3325	C 2134	N 562	O 614	S 15	0	0	0
1	H	427	Total 3362	C 2157	N 570	O 620	S 15	0	0	0
1	I	518	Total 4076	C 2622	N 691	O 746	S 17	0	0	0
1	J	427	Total 3362	C 2157	N 570	O 620	S 15	0	0	0
1	K	425	Total 3344	C 2146	N 567	O 616	S 15	0	0	0
1	L	426	Total 3353	C 2152	N 569	O 617	S 15	0	0	0

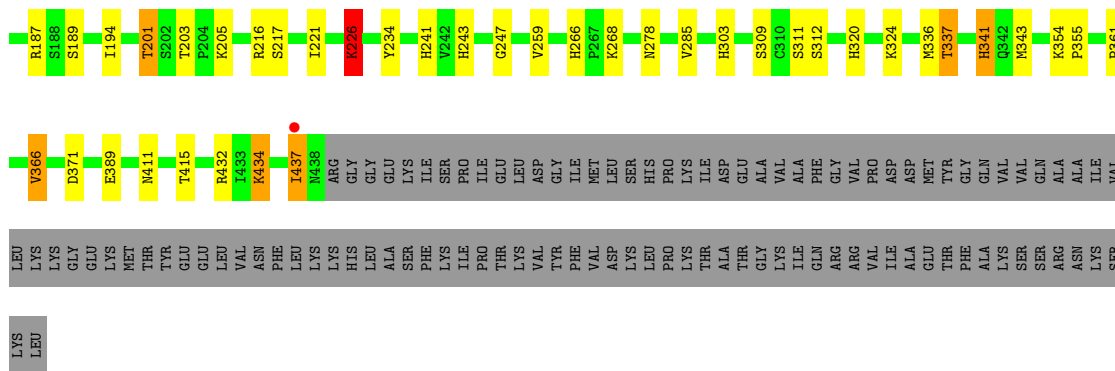
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	31	Total 31	O 31	0	0
2	B	36	Total 36	O 36	0	0

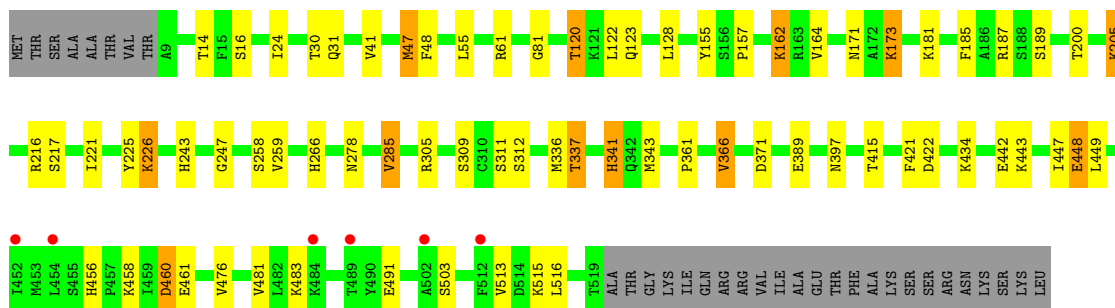
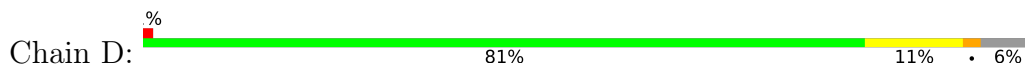
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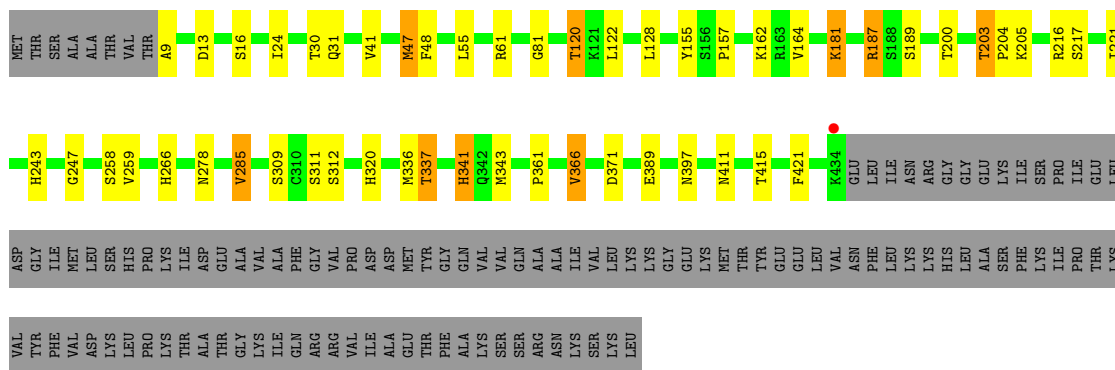
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	58	Total 58	O 58	0	0
2	D	58	Total 58	O 58	0	0
2	E	18	Total 18	O 18	0	0
2	F	33	Total 33	O 33	0	0
2	G	13	Total 13	O 13	0	0
2	H	14	Total 14	O 14	0	0
2	I	25	Total 25	O 25	0	0
2	J	20	Total 20	O 20	0	0
2	K	9	Total 9	O 9	0	0
2	L	2	Total 2	O 2	0	0



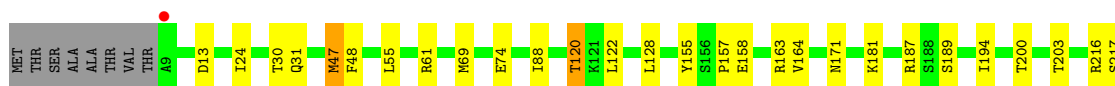
• Molecule 1: Oxalate–CoA ligase

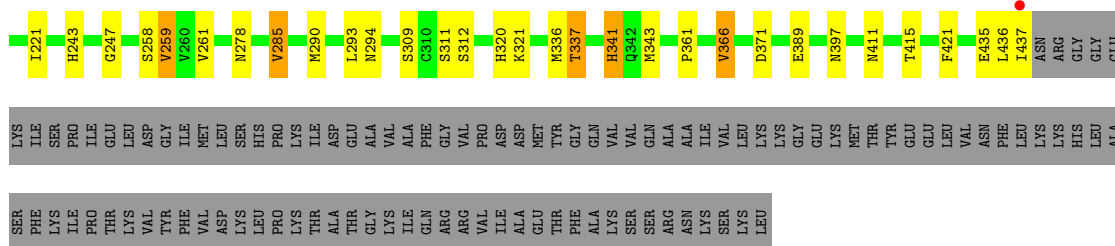


• Molecule 1: Oxalate–CoA ligase

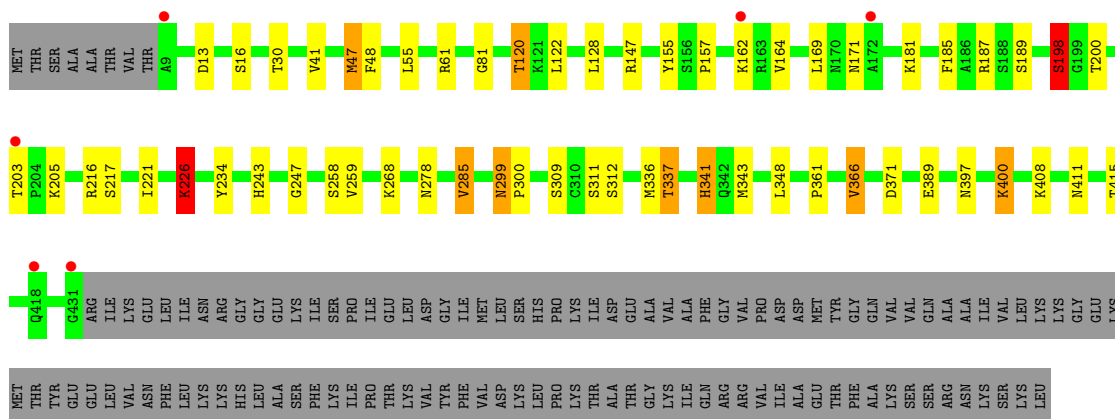


• Molecule 1: Oxalate–CoA ligase

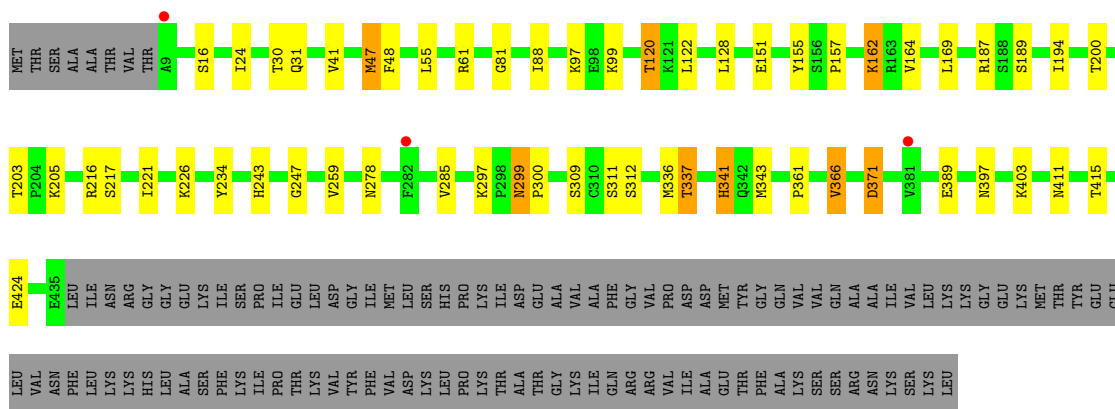




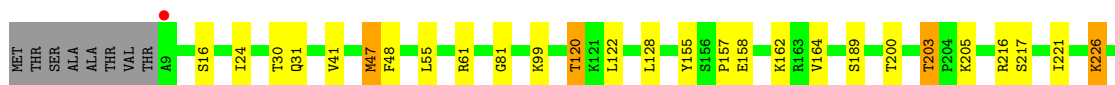
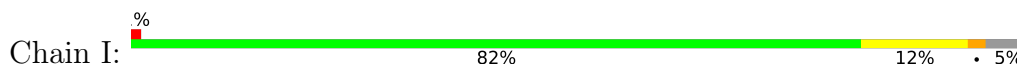
● Molecule 1: Oxalate-CoA ligase

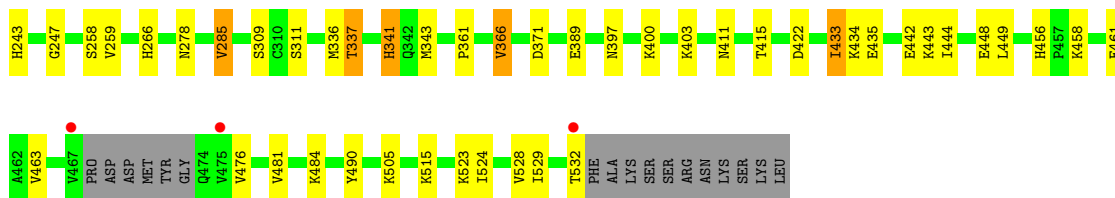


● Molecule 1: Oxalate-CoA ligase



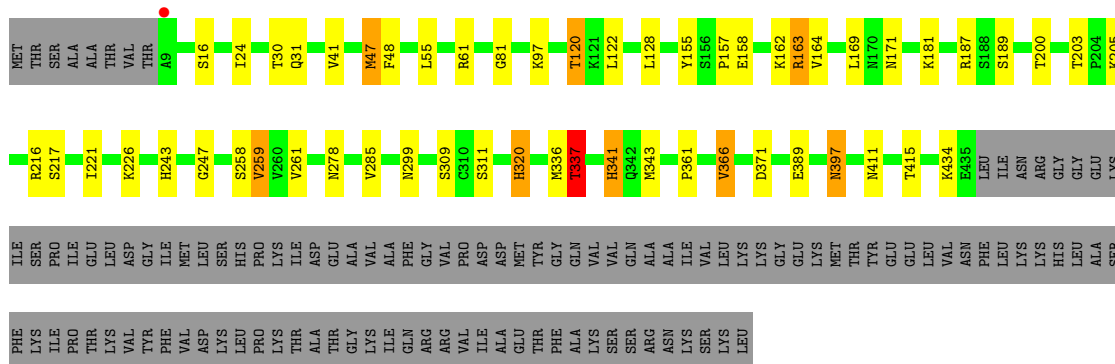
● Molecule 1: Oxalate-CoA ligase





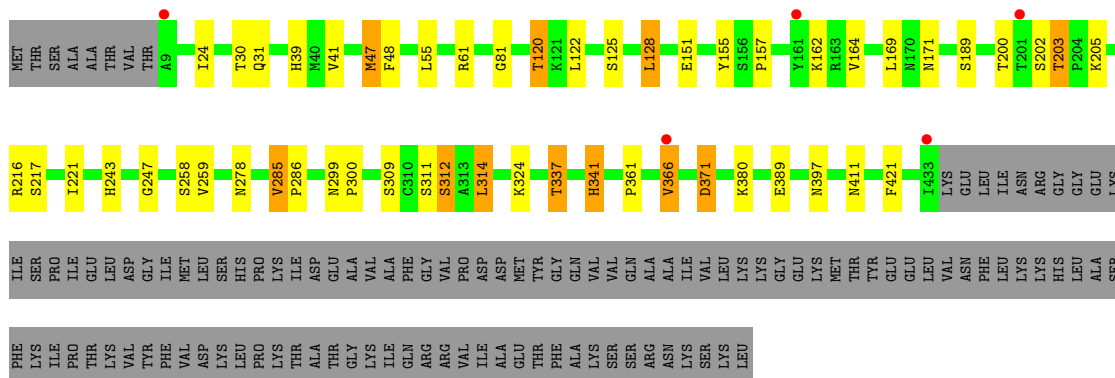
- Molecule 1: Oxalate-CoA ligase

Chain J: 69% 8% 21%



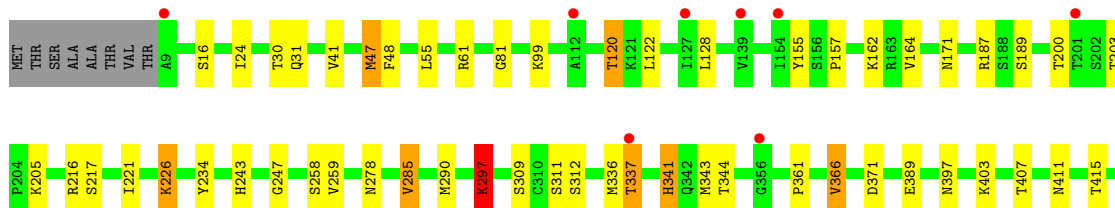
- Molecule 1: Oxalate-CoA ligase

Chain K: 69% 8% 22%



- Molecule 1: Oxalate-CoA ligase

Chain L: 68% 9% 22%



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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	109.03Å 93.72Å 356.49Å 90.00° 93.81° 90.00°	Depositor
Resolution (Å)	29.98 – 2.87 29.98 – 2.87	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.98-2.87) 99.0 (29.98-2.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.85Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.227 , 0.250 0.227 , 0.250	Depositor DCC
R_{free} test set	8269 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	60.1	Xtrriage
Anisotropy	0.531	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	42783	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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	0.70	3/4237 (0.1%)	1.37	20/5753 (0.3%)
1	B	0.71	3/3458 (0.1%)	1.34	16/4704 (0.3%)
1	C	0.72	2/3474 (0.1%)	1.35	20/4726 (0.4%)
1	D	0.71	0/4125	1.37	23/5603 (0.4%)
1	E	0.68	2/3441 (0.1%)	1.31	11/4681 (0.2%)
1	F	0.68	0/3466	1.32	11/4715 (0.2%)
1	G	0.62	0/3413	1.33	17/4645 (0.4%)
1	H	0.60	0/3450	1.30	13/4693 (0.3%)
1	I	0.67	1/4175 (0.0%)	1.36	17/5667 (0.3%)
1	J	0.67	1/3450 (0.0%)	1.30	14/4693 (0.3%)
1	K	0.64	1/3432 (0.0%)	1.31	12/4670 (0.3%)
1	L	0.60	0/3441	1.30	16/4681 (0.3%)
All	All	0.67	13/43562 (0.0%)	1.33	190/59231 (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	H	0	1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	266	HIS	CE1-NE2	7.82	1.40	1.32
1	A	303	HIS	CE1-NE2	7.29	1.39	1.32
1	C	241	HIS	CE1-NE2	6.91	1.39	1.32
1	K	39	HIS	CE1-NE2	6.57	1.39	1.32
1	E	9	ALA	N-CA	6.16	1.57	1.46

The worst 5 of 190 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	167	ARG	CG-CD-NE	9.71	133.37	112.00
1	D	187	ARG	CB-CG-CD	-9.32	89.86	111.30
1	B	187	ARG	CB-CG-CD	-8.75	91.17	111.30
1	E	285	VAL	N-CA-CB	-8.38	106.05	111.83
1	I	285	VAL	N-CA-CB	-8.33	106.08	111.83

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	299	ASN	Peptide

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	4134	0	4152	21	0
1	B	3370	0	3348	20	0
1	C	3386	0	3365	23	0
1	D	4023	0	4032	21	0
1	E	3353	0	3331	18	0
1	F	3378	0	3359	21	0
1	G	3325	0	3294	18	0
1	H	3362	0	3337	17	0
1	I	4076	0	4106	19	0
1	J	3362	0	3337	16	0
1	K	3344	0	3318	17	0
1	L	3353	0	3331	17	0
2	A	31	0	0	0	0
2	B	36	0	0	2	0
2	C	58	0	0	6	0
2	D	58	0	0	3	0
2	E	18	0	0	2	0
2	F	33	0	0	3	0
2	G	13	0	0	2	0
2	H	14	0	0	1	0
2	I	25	0	0	0	0
2	J	20	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	9	0	0	0	0
2	L	2	0	0	1	0
All	All	42783	0	42310	217	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.

The worst 5 of 217 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:L:336:MET:HE1	1:L:415:THR:HB	1.45	0.97
1:H:336:MET:HE1	1:H:415:THR:HB	1.46	0.95
1:K:125:SER:OG	1:K:128:LEU:HB2	1.73	0.89
1:D:205:LYS:HE2	2:D:655:HOH:O	1.77	0.84
1:A:438:ASN:HD21	1:A:443:LYS:HE2	1.45	0.81

There are no symmetry-related clashes.

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	523/543 (96%)	505 (97%)	16 (3%)	2 (0%)	30	56
1	B	426/543 (78%)	414 (97%)	10 (2%)	2 (0%)	24	51
1	C	428/543 (79%)	418 (98%)	8 (2%)	2 (0%)	24	51
1	D	509/543 (94%)	493 (97%)	14 (3%)	2 (0%)	30	56
1	E	424/543 (78%)	412 (97%)	10 (2%)	2 (0%)	24	51
1	F	427/543 (79%)	415 (97%)	10 (2%)	2 (0%)	24	51
1	G	421/543 (78%)	407 (97%)	11 (3%)	3 (1%)	18	44
1	H	425/543 (78%)	412 (97%)	11 (3%)	2 (0%)	24	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	514/543 (95%)	496 (96%)	16 (3%)	2 (0%)	30	56
1	J	425/543 (78%)	413 (97%)	10 (2%)	2 (0%)	24	51
1	K	423/543 (78%)	410 (97%)	11 (3%)	2 (0%)	24	51
1	L	424/543 (78%)	413 (97%)	9 (2%)	2 (0%)	24	51
All	All	5369/6516 (82%)	5208 (97%)	136 (2%)	25 (0%)	24	51

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	312	SER
1	A	341	HIS
1	B	341	HIS
1	C	311	SER
1	C	341	HIS

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	461/476 (97%)	428 (93%)	33 (7%)	13	36
1	B	378/476 (79%)	354 (94%)	24 (6%)	16	42
1	C	380/476 (80%)	353 (93%)	27 (7%)	13	37
1	D	450/476 (94%)	421 (94%)	29 (6%)	16	42
1	E	376/476 (79%)	357 (95%)	19 (5%)	21	50
1	F	379/476 (80%)	359 (95%)	20 (5%)	20	49
1	G	373/476 (78%)	347 (93%)	26 (7%)	14	37
1	H	377/476 (79%)	354 (94%)	23 (6%)	17	43
1	I	455/476 (96%)	423 (93%)	32 (7%)	14	37
1	J	377/476 (79%)	354 (94%)	23 (6%)	17	43
1	K	375/476 (79%)	352 (94%)	23 (6%)	17	43
1	L	376/476 (79%)	354 (94%)	22 (6%)	18	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4757/5712 (83%)	4456 (94%)	301 (6%)	16 42

5 of 301 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	528	VAL
1	L	189	SER
1	J	128	LEU
1	K	164	VAL
1	L	397	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	374	ASN
1	I	171	ASN
1	L	374	ASN
1	H	31	GLN
1	H	266	HIS

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 [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	525/543 (96%)	-0.05	2 (0%) 88 86	52, 63, 114, 174	0
1	B	428/543 (78%)	-0.24	0 100 100	50, 58, 81, 109	0
1	C	430/543 (79%)	-0.22	2 (0%) 87 83	49, 56, 66, 115	0
1	D	511/543 (94%)	-0.04	6 (1%) 76 70	48, 57, 149, 206	0
1	E	426/543 (78%)	-0.13	1 (0%) 91 89	53, 66, 113, 136	0
1	F	429/543 (79%)	-0.04	2 (0%) 87 83	53, 79, 118, 151	0
1	G	423/543 (77%)	0.38	6 (1%) 73 66	66, 105, 143, 174	0
1	H	427/543 (78%)	0.29	3 (0%) 84 80	62, 103, 133, 143	0
1	I	518/543 (95%)	-0.03	4 (0%) 82 77	51, 64, 145, 174	0
1	J	427/543 (78%)	-0.15	1 (0%) 91 89	52, 62, 92, 131	0
1	K	425/543 (78%)	0.28	5 (1%) 76 70	54, 91, 121, 156	0
1	L	426/543 (78%)	0.49	9 (2%) 63 55	65, 106, 151, 188	0
All	All	5395/6516 (82%)	0.04	41 (0%) 82 77	48, 72, 132, 206	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	337	THR	3.9
1	G	9	ALA	3.4
1	L	139	VAL	3.3
1	D	484	LYS	3.2
1	K	9	ALA	3.1

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

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

6.3 Carbohydrates [i](#)

There are no 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.