



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 30, 2023 – 01:01 pm GMT

PDB ID : 8AFF  
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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.31.3  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

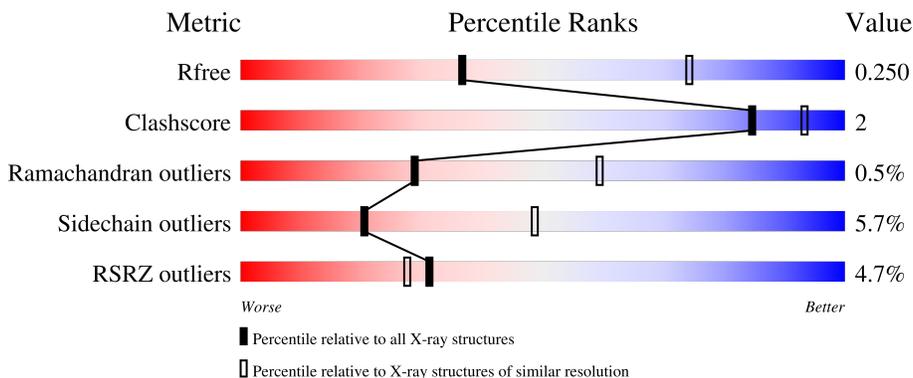
# 1 Overall quality at a glance

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))
$R_{free}$	130704	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (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  $\geq 3$ , 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	
1	B	543	
1	C	543	
1	D	543	
1	E	543	

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Mol	Chain	Length	Quality of chain
1	F	543	<p>2% 70% 8% 21%</p>
1	G	543	<p>7% 70% 7% 22%</p>
1	H	543	<p>5% 71% 7% 21%</p>
1	I	543	<p>5% 84% 10% 5%</p>
1	J	543	<p>% 70% 7% 21%</p>
1	K	543	<p>3% 71% 6% 22%</p>
1	L	543	<p>8% 71% 7% 22%</p>

## 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.

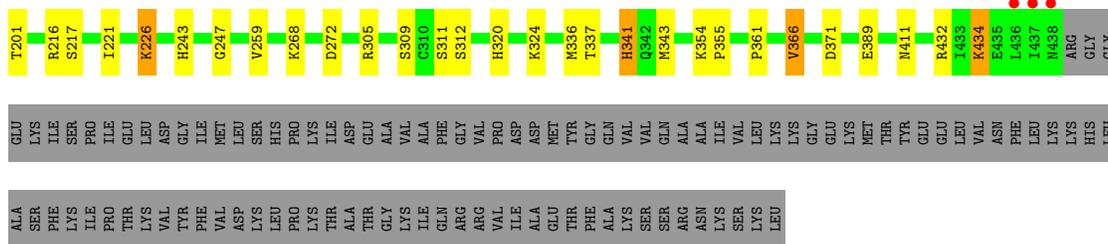
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	31	Total 31	O 31	0	0
2	B	36	Total 36	O 36	0	0

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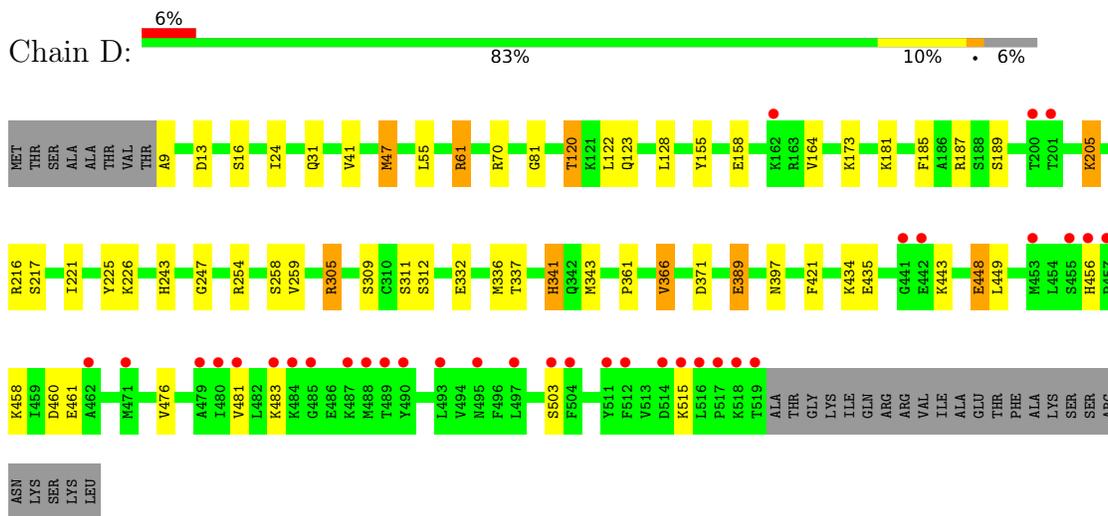
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
2	C	58	Total 58	O 58	0	0
2	D	58	Total 58	O 58	0	0
2	E	18	Total 18	O 18	0	0
2	F	33	Total 33	O 33	0	0
2	G	13	Total 13	O 13	0	0
2	H	14	Total 14	O 14	0	0
2	I	25	Total 25	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

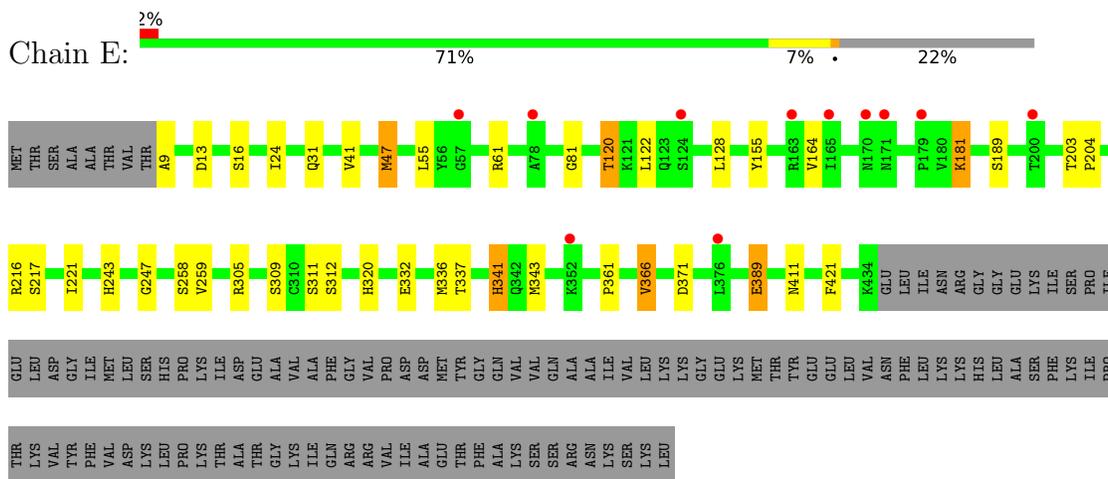




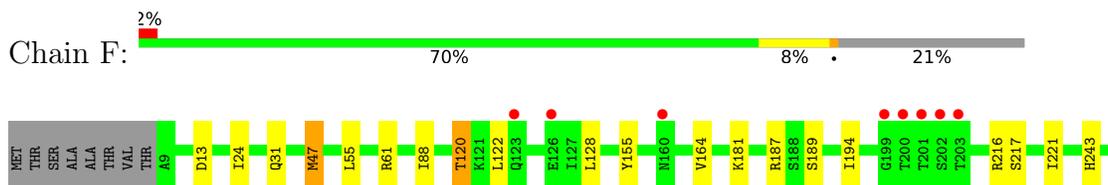
● Molecule 1: Oxalate-CoA ligase



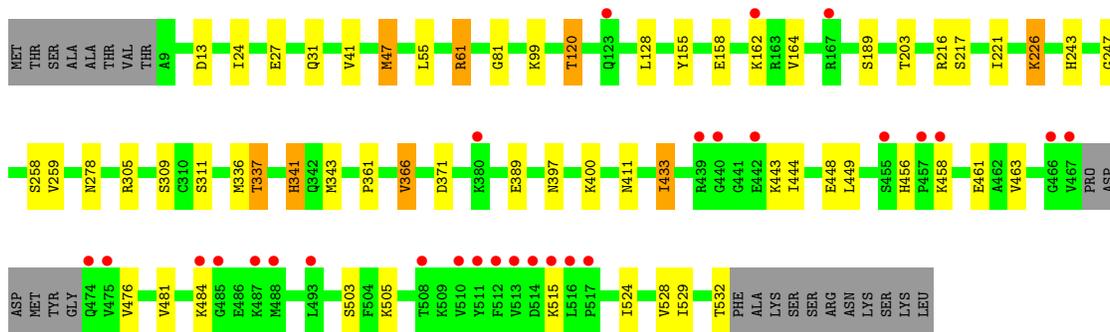
● Molecule 1: Oxalate-CoA ligase



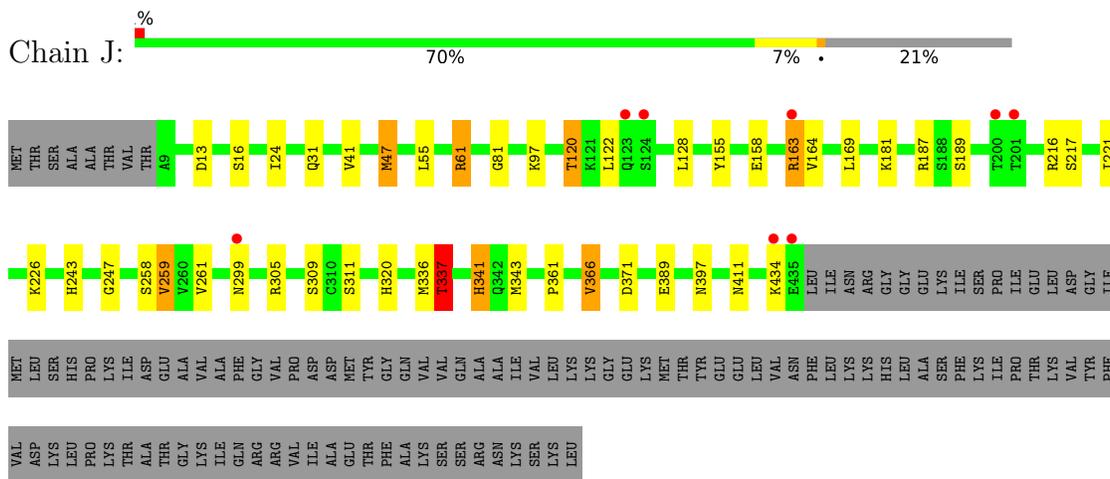
● Molecule 1: Oxalate-CoA ligase



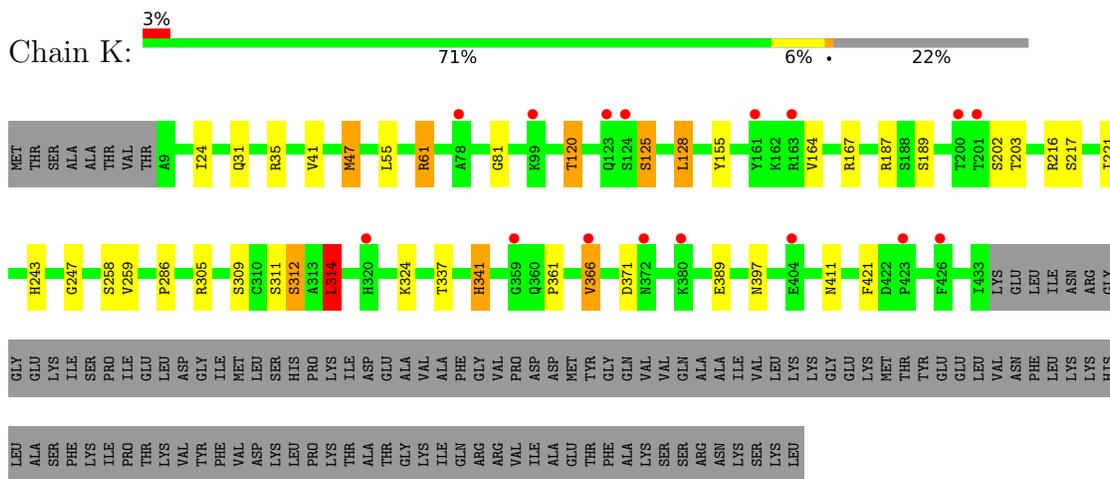




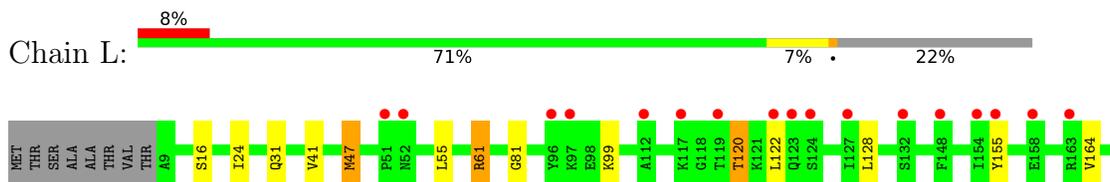
• Molecule 1: Oxalate-CoA ligase

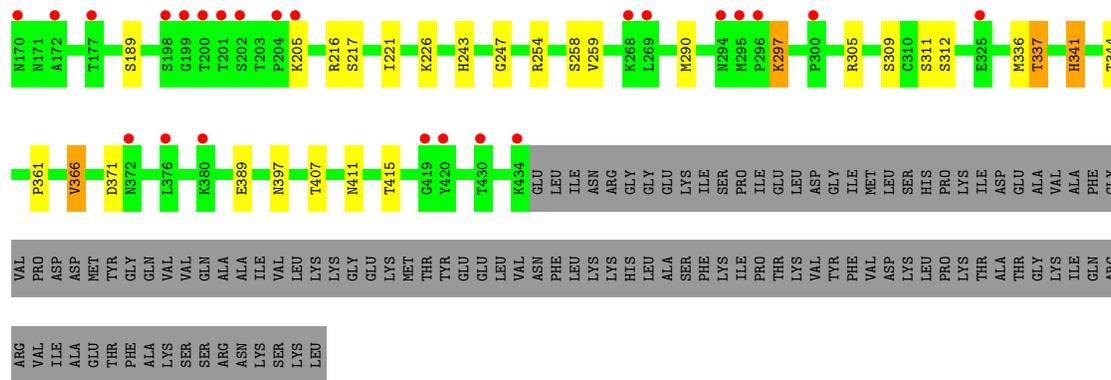


• Molecule 1: Oxalate-CoA ligase



• Molecule 1: Oxalate-CoA ligase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.03Å 93.72Å 356.49Å 90.00° 93.81° 90.00°	Depositor
Resolution (Å)	29.98 – 2.87 29.97 – 2.87	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.98-2.87) 99.1 (29.97-2.87)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 2.85Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.227 , 0.250 0.228 , 0.250	Depositor DCC
$R_{free}$ test set	8186 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.1	Xtrriage
Anisotropy	0.531	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 46.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.53	2/4237 (0.0%)	0.96	6/5753 (0.1%)
1	B	0.56	4/3458 (0.1%)	0.96	6/4704 (0.1%)
1	C	0.54	1/3474 (0.0%)	0.97	9/4726 (0.2%)
1	D	0.57	3/4125 (0.1%)	0.97	7/5603 (0.1%)
1	E	0.51	3/3441 (0.1%)	0.92	3/4681 (0.1%)
1	F	0.50	1/3466 (0.0%)	0.93	4/4715 (0.1%)
1	G	0.43	0/3413	0.93	6/4645 (0.1%)
1	H	0.43	0/3450	0.90	6/4693 (0.1%)
1	I	0.49	1/4175 (0.0%)	0.94	6/5667 (0.1%)
1	J	0.50	0/3450	0.93	7/4693 (0.1%)
1	K	0.46	0/3432	0.92	5/4670 (0.1%)
1	L	0.42	0/3441	0.91	3/4681 (0.1%)
All	All	0.50	15/43562 (0.0%)	0.94	68/59231 (0.1%)

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	H	0	1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	435	GLU	CD-OE1	7.31	1.33	1.25
1	A	442	GLU	CD-OE1	6.47	1.32	1.25
1	F	325	GLU	CD-OE2	6.27	1.32	1.25
1	C	74	GLU	CD-OE2	6.17	1.32	1.25
1	B	158	GLU	CD-OE1	6.14	1.32	1.25

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	167	ARG	CG-CD-NE	10.27	133.37	111.80
1	C	187	ARG	NE-CZ-NH2	-9.40	115.60	120.30
1	D	187	ARG	CB-CG-CD	-8.36	89.86	111.60
1	B	187	ARG	CB-CG-CD	-7.86	91.17	111.60
1	K	314	LEU	CB-CG-CD1	-7.49	98.27	111.00

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	18	0
1	B	3370	0	3348	18	0
1	C	3386	0	3365	21	0
1	D	4023	0	4032	19	0
1	E	3353	0	3331	16	0
1	F	3378	0	3359	18	0
1	G	3325	0	3294	15	0
1	H	3362	0	3337	16	0
1	I	4076	0	4106	17	0
1	J	3362	0	3337	14	0
1	K	3344	0	3318	15	0
1	L	3353	0	3331	16	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	192	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 2.

The worst 5 of 192 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: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
1:G:147:ARG:HB2	2:G:601:HOH:O	1.84	0.77
1:E:13:ASP:OD1	1:E:181:LYS:NZ	2.17	0.74

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%)	34	64
1	B	426/543 (78%)	414 (97%)	10 (2%)	2 (0%)	29	59
1	C	428/543 (79%)	418 (98%)	8 (2%)	2 (0%)	29	59
1	D	509/543 (94%)	493 (97%)	14 (3%)	2 (0%)	34	64
1	E	424/543 (78%)	412 (97%)	10 (2%)	2 (0%)	29	59
1	F	427/543 (79%)	415 (97%)	10 (2%)	2 (0%)	29	59
1	G	421/543 (78%)	407 (97%)	11 (3%)	3 (1%)	22	52
1	H	425/543 (78%)	412 (97%)	11 (3%)	2 (0%)	29	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	514/543 (95%)	496 (96%)	16 (3%)	2 (0%)	34	64
1	J	425/543 (78%)	413 (97%)	10 (2%)	2 (0%)	29	59
1	K	423/543 (78%)	410 (97%)	11 (3%)	2 (0%)	29	59
1	L	424/543 (78%)	413 (97%)	9 (2%)	2 (0%)	29	59
All	All	5369/6516 (82%)	5208 (97%)	136 (2%)	25 (0%)	29	59

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%)	430 (93%)	31 (7%)	16	41
1	B	378/476 (79%)	357 (94%)	21 (6%)	21	49
1	C	380/476 (80%)	358 (94%)	22 (6%)	20	48
1	D	450/476 (94%)	422 (94%)	28 (6%)	18	45
1	E	376/476 (79%)	361 (96%)	15 (4%)	31	63
1	F	379/476 (80%)	363 (96%)	16 (4%)	30	61
1	G	373/476 (78%)	349 (94%)	24 (6%)	17	43
1	H	377/476 (79%)	358 (95%)	19 (5%)	24	54
1	I	455/476 (96%)	426 (94%)	29 (6%)	17	43
1	J	377/476 (79%)	353 (94%)	24 (6%)	17	43
1	K	375/476 (79%)	354 (94%)	21 (6%)	21	49
1	L	376/476 (79%)	354 (94%)	22 (6%)	19	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4757/5712 (83%)	4485 (94%)	272 (6%)	20 49

5 of 272 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	120	THR
1	K	203	THR
1	L	217	SER
1	D	434	LYS
1	D	366	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	171	ASN
1	L	171	ASN
1	G	171	ASN
1	L	299	ASN
1	I	171	ASN

### 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 monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	525/543 (96%)	0.16	25 (4%) 30 26	52, 63, 114, 174	0
1	B	428/543 (78%)	-0.00	4 (0%) 84 84	50, 58, 81, 109	0
1	C	430/543 (79%)	0.03	4 (0%) 84 84	49, 56, 66, 115	0
1	D	511/543 (94%)	0.21	34 (6%) 17 13	48, 57, 149, 206	0
1	E	426/543 (78%)	0.11	11 (2%) 56 53	53, 66, 113, 136	0
1	F	429/543 (79%)	0.06	12 (2%) 53 50	53, 79, 118, 151	0
1	G	423/543 (77%)	0.62	40 (9%) 8 5	66, 105, 143, 174	0
1	H	427/543 (78%)	0.41	28 (6%) 18 14	62, 103, 133, 143	0
1	I	518/543 (95%)	0.22	28 (5%) 25 22	51, 64, 145, 174	0
1	J	427/543 (78%)	-0.00	8 (1%) 66 65	52, 62, 92, 131	0
1	K	425/543 (78%)	0.25	16 (3%) 40 36	54, 91, 121, 156	0
1	L	426/543 (78%)	0.55	41 (9%) 8 5	65, 106, 151, 188	0
All	All	5395/6516 (82%)	0.21	251 (4%) 31 27	48, 72, 132, 206	0

The worst 5 of 251 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	199	GLY	8.2
1	I	475	VAL	7.3
1	I	512	PHE	5.7
1	L	200	THR	5.7
1	I	485	GLY	5.5

### 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 monosaccharides 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.