



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 03:58 PM UTC

PDB ID : 2A1B / pdb_00002a1b
Title : Carboxysome shell protein ccmK2
Authors : Kerfeld, C.A.; Sawaya, M.R.; Tanaka, S.; Nguyen, C.V.; Phillips, M.; Beeby, M.; Yeates, T.O.
Deposited on : 2005-06-20
Resolution : 2.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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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

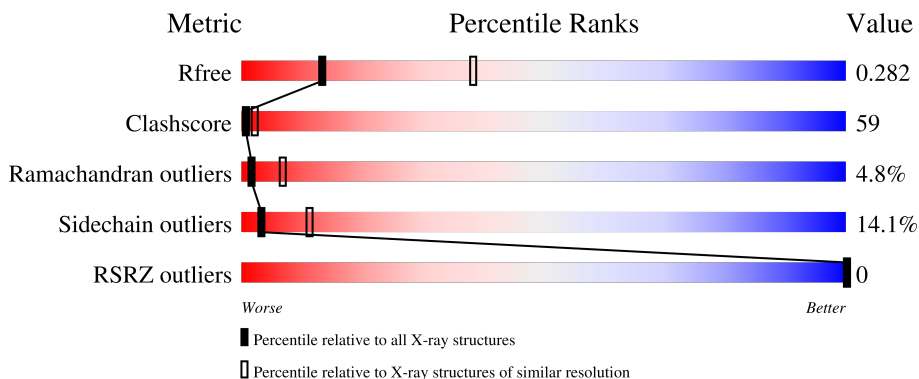
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	116	
1	B	116	
1	C	116	
1	D	116	
1	E	116	

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Mol	Chain	Length	Quality of chain			
1	F	116	24%	51%	12%	13%
1	G	116	26%	48%	12%	13%
1	H	116	25%	50%	11%	13%
1	I	116	20%	55%	12%	13%
1	J	116	25%	49%	13%	13%
1	K	116	22%	51%	14%	13%
1	L	116	28%	47%	12%	13%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 9072 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 Carbon dioxide concentrating mechanism protein ccmK homolog 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	101	756	472	136	146	2	0	0	0
1	B	101	756	472	136	146	2	0	0	0
1	C	101	756	472	136	146	2	0	0	0
1	D	101	756	472	136	146	2	0	0	0
1	E	101	756	472	136	146	2	0	0	0
1	F	101	756	472	136	146	2	0	0	0
1	G	101	756	472	136	146	2	0	0	0
1	H	101	756	472	136	146	2	0	0	0
1	I	101	756	472	136	146	2	0	0	0
1	J	101	756	472	136	146	2	0	0	0
1	K	101	756	472	136	146	2	0	0	0
1	L	101	756	472	136	146	2	0	0	0

There are 180 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P72761
A	52	GLY	GLU	engineered mutation	UNP P72761
A	104	GLY	-	expression tag	UNP P72761
A	105	VAL	-	expression tag	UNP P72761

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Chain	Residue	Modelled	Actual	Comment	Reference
A	106	PRO	-	expression tag	UNP P72761
A	107	ARG	-	expression tag	UNP P72761
A	108	GLY	-	expression tag	UNP P72761
A	109	LEU	-	expression tag	UNP P72761
A	110	GLU	-	expression tag	UNP P72761
A	111	HIS	-	expression tag	UNP P72761
A	112	HIS	-	expression tag	UNP P72761
A	113	HIS	-	expression tag	UNP P72761
A	114	HIS	-	expression tag	UNP P72761
A	115	HIS	-	expression tag	UNP P72761
A	116	HIS	-	expression tag	UNP P72761
B	1	MET	-	initiating methionine	UNP P72761
B	52	GLY	GLU	engineered mutation	UNP P72761
B	104	GLY	-	expression tag	UNP P72761
B	105	VAL	-	expression tag	UNP P72761
B	106	PRO	-	expression tag	UNP P72761
B	107	ARG	-	expression tag	UNP P72761
B	108	GLY	-	expression tag	UNP P72761
B	109	LEU	-	expression tag	UNP P72761
B	110	GLU	-	expression tag	UNP P72761
B	111	HIS	-	expression tag	UNP P72761
B	112	HIS	-	expression tag	UNP P72761
B	113	HIS	-	expression tag	UNP P72761
B	114	HIS	-	expression tag	UNP P72761
B	115	HIS	-	expression tag	UNP P72761
B	116	HIS	-	expression tag	UNP P72761
C	1	MET	-	initiating methionine	UNP P72761
C	52	GLY	GLU	engineered mutation	UNP P72761
C	104	GLY	-	expression tag	UNP P72761
C	105	VAL	-	expression tag	UNP P72761
C	106	PRO	-	expression tag	UNP P72761
C	107	ARG	-	expression tag	UNP P72761
C	108	GLY	-	expression tag	UNP P72761
C	109	LEU	-	expression tag	UNP P72761
C	110	GLU	-	expression tag	UNP P72761
C	111	HIS	-	expression tag	UNP P72761
C	112	HIS	-	expression tag	UNP P72761
C	113	HIS	-	expression tag	UNP P72761
C	114	HIS	-	expression tag	UNP P72761
C	115	HIS	-	expression tag	UNP P72761
C	116	HIS	-	expression tag	UNP P72761
D	1	MET	-	initiating methionine	UNP P72761

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Chain	Residue	Modelled	Actual	Comment	Reference
D	52	GLY	GLU	engineered mutation	UNP P72761
D	104	GLY	-	expression tag	UNP P72761
D	105	VAL	-	expression tag	UNP P72761
D	106	PRO	-	expression tag	UNP P72761
D	107	ARG	-	expression tag	UNP P72761
D	108	GLY	-	expression tag	UNP P72761
D	109	LEU	-	expression tag	UNP P72761
D	110	GLU	-	expression tag	UNP P72761
D	111	HIS	-	expression tag	UNP P72761
D	112	HIS	-	expression tag	UNP P72761
D	113	HIS	-	expression tag	UNP P72761
D	114	HIS	-	expression tag	UNP P72761
D	115	HIS	-	expression tag	UNP P72761
D	116	HIS	-	expression tag	UNP P72761
E	1	MET	-	initiating methionine	UNP P72761
E	52	GLY	GLU	engineered mutation	UNP P72761
E	104	GLY	-	expression tag	UNP P72761
E	105	VAL	-	expression tag	UNP P72761
E	106	PRO	-	expression tag	UNP P72761
E	107	ARG	-	expression tag	UNP P72761
E	108	GLY	-	expression tag	UNP P72761
E	109	LEU	-	expression tag	UNP P72761
E	110	GLU	-	expression tag	UNP P72761
E	111	HIS	-	expression tag	UNP P72761
E	112	HIS	-	expression tag	UNP P72761
E	113	HIS	-	expression tag	UNP P72761
E	114	HIS	-	expression tag	UNP P72761
E	115	HIS	-	expression tag	UNP P72761
E	116	HIS	-	expression tag	UNP P72761
F	1	MET	-	initiating methionine	UNP P72761
F	52	GLY	GLU	engineered mutation	UNP P72761
F	104	GLY	-	expression tag	UNP P72761
F	105	VAL	-	expression tag	UNP P72761
F	106	PRO	-	expression tag	UNP P72761
F	107	ARG	-	expression tag	UNP P72761
F	108	GLY	-	expression tag	UNP P72761
F	109	LEU	-	expression tag	UNP P72761
F	110	GLU	-	expression tag	UNP P72761
F	111	HIS	-	expression tag	UNP P72761
F	112	HIS	-	expression tag	UNP P72761
F	113	HIS	-	expression tag	UNP P72761
F	114	HIS	-	expression tag	UNP P72761

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Chain	Residue	Modelled	Actual	Comment	Reference
F	115	HIS	-	expression tag	UNP P72761
F	116	HIS	-	expression tag	UNP P72761
G	1	MET	-	initiating methionine	UNP P72761
G	52	GLY	GLU	engineered mutation	UNP P72761
G	104	GLY	-	expression tag	UNP P72761
G	105	VAL	-	expression tag	UNP P72761
G	106	PRO	-	expression tag	UNP P72761
G	107	ARG	-	expression tag	UNP P72761
G	108	GLY	-	expression tag	UNP P72761
G	109	LEU	-	expression tag	UNP P72761
G	110	GLU	-	expression tag	UNP P72761
G	111	HIS	-	expression tag	UNP P72761
G	112	HIS	-	expression tag	UNP P72761
G	113	HIS	-	expression tag	UNP P72761
G	114	HIS	-	expression tag	UNP P72761
G	115	HIS	-	expression tag	UNP P72761
G	116	HIS	-	expression tag	UNP P72761
H	1	MET	-	initiating methionine	UNP P72761
H	52	GLY	GLU	engineered mutation	UNP P72761
H	104	GLY	-	expression tag	UNP P72761
H	105	VAL	-	expression tag	UNP P72761
H	106	PRO	-	expression tag	UNP P72761
H	107	ARG	-	expression tag	UNP P72761
H	108	GLY	-	expression tag	UNP P72761
H	109	LEU	-	expression tag	UNP P72761
H	110	GLU	-	expression tag	UNP P72761
H	111	HIS	-	expression tag	UNP P72761
H	112	HIS	-	expression tag	UNP P72761
H	113	HIS	-	expression tag	UNP P72761
H	114	HIS	-	expression tag	UNP P72761
H	115	HIS	-	expression tag	UNP P72761
H	116	HIS	-	expression tag	UNP P72761
I	1	MET	-	initiating methionine	UNP P72761
I	52	GLY	GLU	engineered mutation	UNP P72761
I	104	GLY	-	expression tag	UNP P72761
I	105	VAL	-	expression tag	UNP P72761
I	106	PRO	-	expression tag	UNP P72761
I	107	ARG	-	expression tag	UNP P72761
I	108	GLY	-	expression tag	UNP P72761
I	109	LEU	-	expression tag	UNP P72761
I	110	GLU	-	expression tag	UNP P72761
I	111	HIS	-	expression tag	UNP P72761

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Chain	Residue	Modelled	Actual	Comment	Reference
I	112	HIS	-	expression tag	UNP P72761
I	113	HIS	-	expression tag	UNP P72761
I	114	HIS	-	expression tag	UNP P72761
I	115	HIS	-	expression tag	UNP P72761
I	116	HIS	-	expression tag	UNP P72761
J	1	MET	-	initiating methionine	UNP P72761
J	52	GLY	GLU	engineered mutation	UNP P72761
J	104	GLY	-	expression tag	UNP P72761
J	105	VAL	-	expression tag	UNP P72761
J	106	PRO	-	expression tag	UNP P72761
J	107	ARG	-	expression tag	UNP P72761
J	108	GLY	-	expression tag	UNP P72761
J	109	LEU	-	expression tag	UNP P72761
J	110	GLU	-	expression tag	UNP P72761
J	111	HIS	-	expression tag	UNP P72761
J	112	HIS	-	expression tag	UNP P72761
J	113	HIS	-	expression tag	UNP P72761
J	114	HIS	-	expression tag	UNP P72761
J	115	HIS	-	expression tag	UNP P72761
J	116	HIS	-	expression tag	UNP P72761
K	1	MET	-	initiating methionine	UNP P72761
K	52	GLY	GLU	engineered mutation	UNP P72761
K	104	GLY	-	expression tag	UNP P72761
K	105	VAL	-	expression tag	UNP P72761
K	106	PRO	-	expression tag	UNP P72761
K	107	ARG	-	expression tag	UNP P72761
K	108	GLY	-	expression tag	UNP P72761
K	109	LEU	-	expression tag	UNP P72761
K	110	GLU	-	expression tag	UNP P72761
K	111	HIS	-	expression tag	UNP P72761
K	112	HIS	-	expression tag	UNP P72761
K	113	HIS	-	expression tag	UNP P72761
K	114	HIS	-	expression tag	UNP P72761
K	115	HIS	-	expression tag	UNP P72761
K	116	HIS	-	expression tag	UNP P72761
L	1	MET	-	initiating methionine	UNP P72761
L	52	GLY	GLU	engineered mutation	UNP P72761
L	104	GLY	-	expression tag	UNP P72761
L	105	VAL	-	expression tag	UNP P72761
L	106	PRO	-	expression tag	UNP P72761
L	107	ARG	-	expression tag	UNP P72761
L	108	GLY	-	expression tag	UNP P72761

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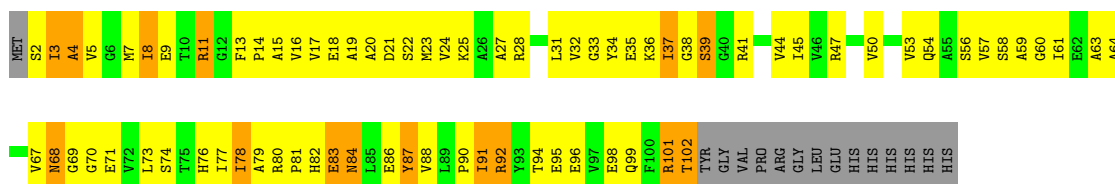
Chain	Residue	Modelled	Actual	Comment	Reference
L	109	LEU	-	expression tag	UNP P72761
L	110	GLU	-	expression tag	UNP P72761
L	111	HIS	-	expression tag	UNP P72761
L	112	HIS	-	expression tag	UNP P72761
L	113	HIS	-	expression tag	UNP P72761
L	114	HIS	-	expression tag	UNP P72761
L	115	HIS	-	expression tag	UNP P72761
L	116	HIS	-	expression tag	UNP P72761

3 Residue-property plots

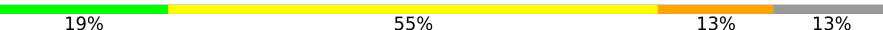
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

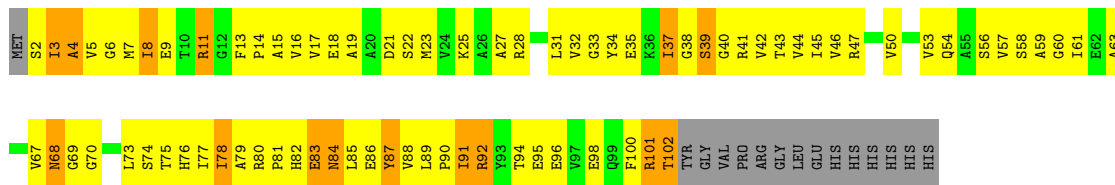
- Molecule 1: Carbon dioxide concentrating mechanism protein ccmK homolog 2

Chain A: 

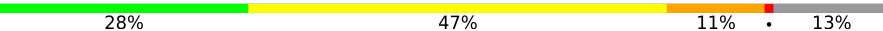


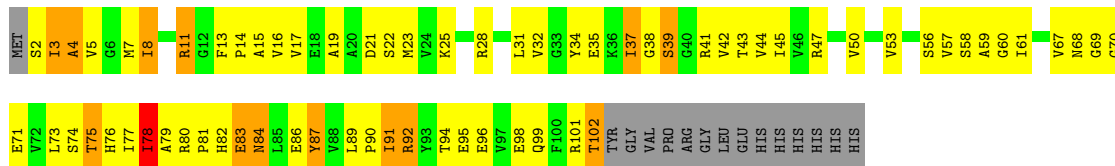
- Molecule 1: Carbon dioxide concentrating mechanism protein ccmK homolog 2

Chain B: 



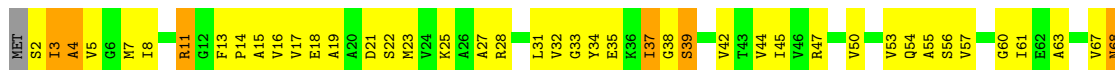
- Molecule 1: Carbon dioxide concentrating mechanism protein ccmK homolog 2

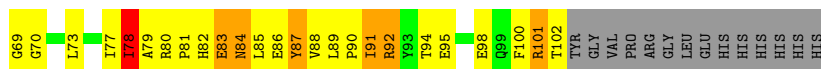
Chain C: 



- Molecule 1: Carbon dioxide concentrating mechanism protein ccmK homolog 2

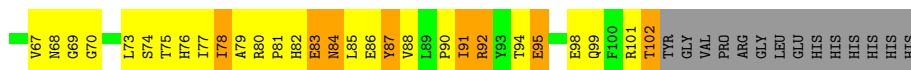
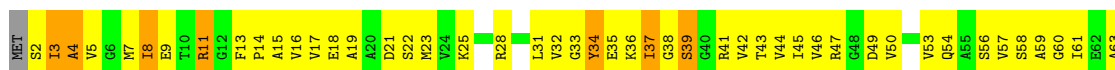
Chain D: 





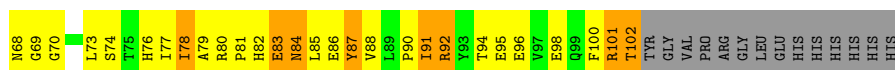
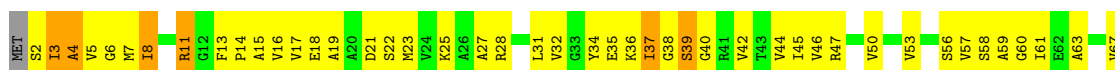
- Molecule 1: Carbon dioxide concentrating mechanism protein ccmK homolog 2

Chain E: 22% 53% 13% 13%



- Molecule 1: Carbon dioxide concentrating mechanism protein ccmK homolog 2

Chain F: 24% 51% 12% 13%



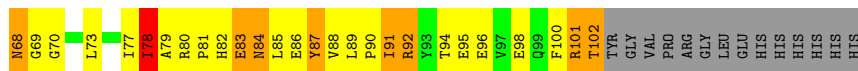
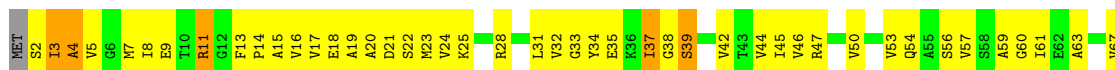
- Molecule 1: Carbon dioxide concentrating mechanism protein ccmK homolog 2

Chain G: 26% 48% 12% 13%



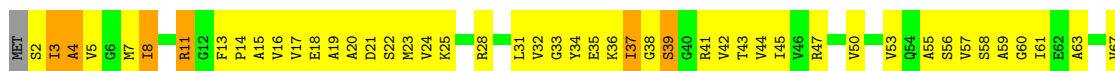
- Molecule 1: Carbon dioxide concentrating mechanism protein ccmK homolog 2

Chain H: 25% 50% 11% 13%



- Molecule 1: Carbon dioxide concentrating mechanism protein ccmK homolog 2

Chain I: 20% 55% 12% 13%



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.74Å 179.99Å 69.77Å 90.00° 119.98° 90.00°	Depositor
Resolution (Å)	89.99 – 2.90 89.99 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.0 (89.99-2.90) 95.8 (89.99-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.86Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.313 , 0.346 0.280 , 0.282	Depositor DCC
R_{free} test set	2881 reflections (9.02%)	wwPDB-VP
Wilson B-factor (Å ²)	38.1	Xtriage
Anisotropy	1.457	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 59.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.420 for -h-l,k,h 0.420 for l,k,-h-l 0.427 for h,-k,-h-l 0.448 for -h-l,-k,l 0.427 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9072	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.66% 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

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	0.60	0/765	1.07	3/1037 (0.3%)
1	B	0.61	0/765	1.05	3/1037 (0.3%)
1	C	0.61	0/765	1.07	4/1037 (0.4%)
1	D	0.62	0/765	1.06	3/1037 (0.3%)
1	E	0.60	0/765	1.05	2/1037 (0.2%)
1	F	0.62	0/765	1.06	3/1037 (0.3%)
1	G	0.60	0/765	1.07	4/1037 (0.4%)
1	H	0.62	0/765	1.06	4/1037 (0.4%)
1	I	0.59	0/765	1.07	3/1037 (0.3%)
1	J	0.62	0/765	1.07	3/1037 (0.3%)
1	K	0.63	0/765	1.05	3/1037 (0.3%)
1	L	0.61	0/765	1.06	3/1037 (0.3%)
All	All	0.61	0/9180	1.06	38/12444 (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
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
1	J	0	1
1	K	0	1
All	All	0	11

There are no bond length outliers.

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	GLU	N-CA-C	7.53	120.20	111.02
1	I	96	GLU	N-CA-C	7.44	120.10	111.02
1	B	96	GLU	N-CA-C	7.42	120.07	111.02
1	G	96	GLU	N-CA-C	7.38	120.03	111.02
1	J	96	GLU	N-CA-C	7.37	120.01	111.02

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	87	TYR	Sidechain
1	B	87	TYR	Sidechain
1	C	87	TYR	Sidechain
1	D	87	TYR	Sidechain
1	E	87	TYR	Sidechain

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	756	0	767	107	1
1	B	756	0	767	116	0
1	C	756	0	767	113	0
1	D	756	0	767	122	0
1	E	756	0	767	115	1
1	F	756	0	767	105	0
1	G	756	0	767	109	1
1	H	756	0	767	128	0
1	I	756	0	767	136	0
1	J	756	0	767	123	0
1	K	756	0	767	107	1
1	L	756	0	767	87	0
All	All	9072	0	9204	1077	2

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 59.

The worst 5 of 1077 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:G:102:THR:HG22	1:H:101:ARG:N	1.42	1.32
1:I:102:THR:HG22	1:J:101:ARG:CA	1.56	1.31
1:I:102:THR:HG22	1:J:101:ARG:N	1.48	1.27
1:C:99:GLN:O	1:D:100:PHE:HE2	1.13	1.24
1:J:99:GLN:O	1:K:100:PHE:HE2	1.18	1.24

All (2) 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)
1:G:28:ARG:NE	1:K:49:ASP:OD2[1_655]	2.00	0.20
1:A:28:ARG:NE	1:E:49:ASP:OD2[1_454]	2.17	0.03

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	99/116 (85%)	75 (76%)	20 (20%)	4 (4%)	2 9
1	B	99/116 (85%)	77 (78%)	18 (18%)	4 (4%)	2 9
1	C	99/116 (85%)	77 (78%)	18 (18%)	4 (4%)	2 9
1	D	99/116 (85%)	76 (77%)	18 (18%)	5 (5%)	1 6
1	E	99/116 (85%)	76 (77%)	18 (18%)	5 (5%)	1 6
1	F	99/116 (85%)	76 (77%)	19 (19%)	4 (4%)	2 9
1	G	99/116 (85%)	75 (76%)	20 (20%)	4 (4%)	2 9
1	H	99/116 (85%)	78 (79%)	17 (17%)	4 (4%)	2 9
1	I	99/116 (85%)	76 (77%)	17 (17%)	6 (6%)	1 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	99/116 (85%)	76 (77%)	18 (18%)	5 (5%)	1	6
1	K	99/116 (85%)	75 (76%)	17 (17%)	7 (7%)	1	2
1	L	99/116 (85%)	76 (77%)	18 (18%)	5 (5%)	1	6
All	All	1188/1392 (85%)	913 (77%)	218 (18%)	57 (5%)	2	7

5 of 57 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	ALA
1	B	4	ALA
1	C	4	ALA
1	D	4	ALA
1	E	4	ALA

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	80/93 (86%)	68 (85%)	12 (15%)	3	10
1	B	80/93 (86%)	69 (86%)	11 (14%)	3	12
1	C	80/93 (86%)	68 (85%)	12 (15%)	3	10
1	D	80/93 (86%)	69 (86%)	11 (14%)	3	12
1	E	80/93 (86%)	69 (86%)	11 (14%)	3	12
1	F	80/93 (86%)	70 (88%)	10 (12%)	4	15
1	G	80/93 (86%)	68 (85%)	12 (15%)	3	10
1	H	80/93 (86%)	69 (86%)	11 (14%)	3	12
1	I	80/93 (86%)	70 (88%)	10 (12%)	4	15
1	J	80/93 (86%)	68 (85%)	12 (15%)	3	10
1	K	80/93 (86%)	68 (85%)	12 (15%)	3	10
1	L	80/93 (86%)	69 (86%)	11 (14%)	3	12
All	All	960/1116 (86%)	825 (86%)	135 (14%)	3	11

5 of 135 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	37	ILE
1	K	78	ILE
1	L	78	ILE
1	E	34	TYR
1	E	11	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	84	ASN
1	H	84	ASN
1	D	84	ASN
1	D	68	ASN
1	H	68	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 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

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	101/116 (87%)	-1.07	0 100 100	30, 53, 89, 99	0
1	B	101/116 (87%)	-1.01	0 100 100	19, 49, 88, 96	0
1	C	101/116 (87%)	-1.10	0 100 100	37, 50, 96, 104	0
1	D	101/116 (87%)	-1.08	0 100 100	13, 47, 87, 98	0
1	E	101/116 (87%)	-1.03	0 100 100	11, 51, 92, 102	0
1	F	101/116 (87%)	-1.07	0 100 100	31, 51, 100, 106	0
1	G	101/116 (87%)	-1.09	0 100 100	23, 54, 92, 99	0
1	H	101/116 (87%)	-1.07	0 100 100	10, 50, 87, 99	0
1	I	101/116 (87%)	-1.01	0 100 100	14, 50, 85, 94	0
1	J	101/116 (87%)	-1.08	0 100 100	24, 51, 102, 108	0
1	K	101/116 (87%)	-1.04	0 100 100	23, 49, 91, 103	0
1	L	101/116 (87%)	-1.09	0 100 100	22, 51, 98, 109	0
All	All	1212/1392 (87%)	-1.06	0 100 100	10, 51, 95, 109	0

There are no RSRZ outliers to report.

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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.