



# wwPDB X-ray Structure Validation Summary Report

Mar 31, 2014 – 05:48 PM BST

PDB ID : 3IFG  
Title : Crystal structure of succinate-semialdehydedehydrogenase from Burkholderia pseudomallei, part 1 of 2  
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)  
Deposited on : 2009-07-24  
Resolution : 2.70 Å(reported)

This is a wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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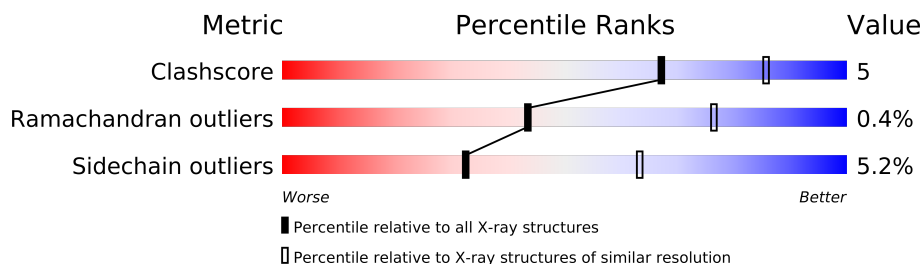
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23004

# 1 Overall quality at a glance

The reported resolution of this entry is 2.70 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))
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	484	
1	B	484	
1	C	484	
1	D	484	
1	E	484	
1	F	484	
1	G	484	
1	H	484	
1	I	484	
1	J	484	
1	K	484	
1	L	484	
1	M	484	
1	N	484	
1	O	484	
1	P	484	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 57595 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Succinate-semialdehydedehydrogenase (NADP+).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	0	0
			3549	2259	607	669	14			
1	B	482	Total	C	N	O	S	0	0	0
			3553	2261	607	671	14			
1	C	482	Total	C	N	O	S	0	0	0
			3549	2259	607	669	14			
1	D	482	Total	C	N	O	S	0	0	0
			3549	2259	607	669	14			
1	E	482	Total	C	N	O	S	0	0	0
			3549	2259	607	669	14			
1	F	482	Total	C	N	O	S	0	0	0
			3549	2259	607	669	14			
1	G	482	Total	C	N	O	S	0	0	0
			3549	2259	607	669	14			
1	H	482	Total	C	N	O	S	0	0	0
			3549	2259	607	669	14			
1	I	482	Total	C	N	O	S	0	0	0
			3520	2242	597	667	14			
1	J	482	Total	C	N	O	S	0	0	0
			3549	2259	607	669	14			
1	K	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			
1	L	482	Total	C	N	O	S	0	0	0
			3543	2255	607	667	14			
1	M	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			
1	N	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			
1	O	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			
1	P	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
A	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
A	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
A	4	SER	-	EXPRESSION TAG	UNP Q3JS51
B	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
B	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
B	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
B	4	SER	-	EXPRESSION TAG	UNP Q3JS51
C	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
C	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
C	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
C	4	SER	-	EXPRESSION TAG	UNP Q3JS51
D	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
D	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
D	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
D	4	SER	-	EXPRESSION TAG	UNP Q3JS51
E	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
E	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
E	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
E	4	SER	-	EXPRESSION TAG	UNP Q3JS51
F	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
F	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
F	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
F	4	SER	-	EXPRESSION TAG	UNP Q3JS51
G	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
G	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
G	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
G	4	SER	-	EXPRESSION TAG	UNP Q3JS51
H	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
H	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
H	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
H	4	SER	-	EXPRESSION TAG	UNP Q3JS51
I	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
I	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
I	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
I	4	SER	-	EXPRESSION TAG	UNP Q3JS51
J	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
J	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
J	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
J	4	SER	-	EXPRESSION TAG	UNP Q3JS51
K	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
K	2	PRO	-	EXPRESSION TAG	UNP Q3JS51

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Chain	Residue	Modelled	Actual	Comment	Reference
K	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
K	4	SER	-	EXPRESSION TAG	UNP Q3JS51
L	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
L	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
L	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
L	4	SER	-	EXPRESSION TAG	UNP Q3JS51
M	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
M	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
M	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
M	4	SER	-	EXPRESSION TAG	UNP Q3JS51
N	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
N	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
N	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
N	4	SER	-	EXPRESSION TAG	UNP Q3JS51
O	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
O	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
O	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
O	4	SER	-	EXPRESSION TAG	UNP Q3JS51
P	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
P	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
P	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
P	4	SER	-	EXPRESSION TAG	UNP Q3JS51

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	45	Total O 45 45	0	0
2	B	59	Total O 59 59	0	0
2	C	56	Total O 56 56	0	0
2	D	61	Total O 61 61	0	0
2	E	72	Total O 72 72	0	0
2	F	75	Total O 75 75	0	0
2	G	66	Total O 66 66	0	0
2	H	58	Total O 58 58	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	I	24	Total 24	O 24	0	0
2	J	35	Total 35	O 35	0	0
2	K	55	Total 55	O 55	0	0
2	L	57	Total 57	O 57	0	0
2	M	40	Total 40	O 40	0	0
2	N	47	Total 47	O 47	0	0
2	O	38	Total 38	O 38	0	0
2	P	74	Total 74	O 74	0	0

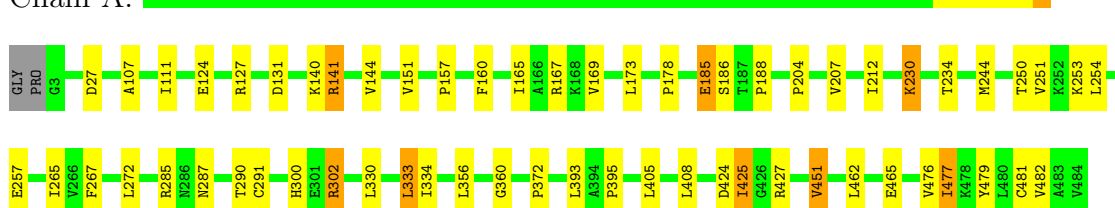
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

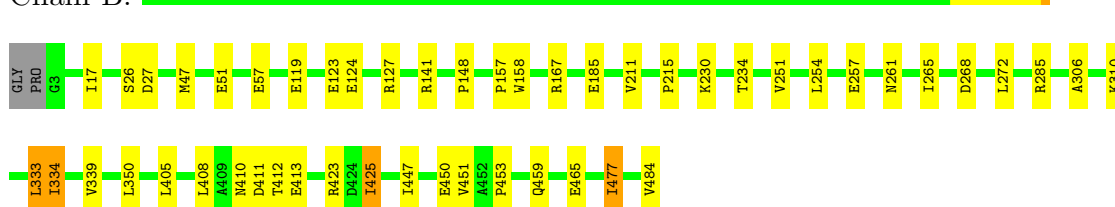
- Molecule 1: Succinate-semialdehydedehydrogenase (NADP+)

Chain A:



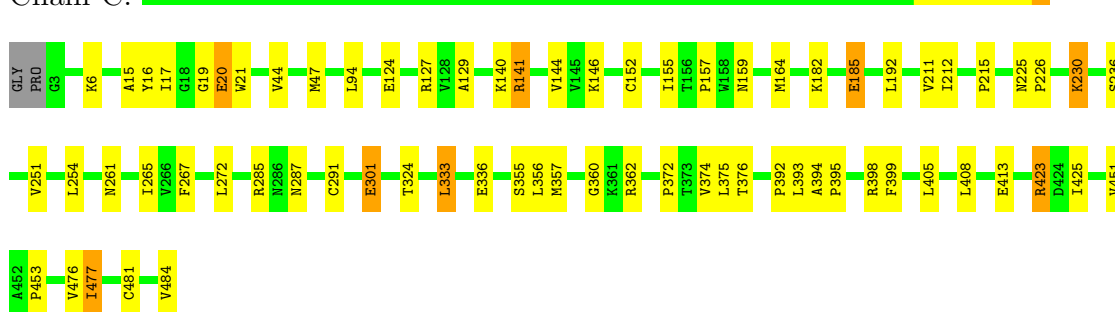
- Molecule 1: Succinate-semialdehydedehydrogenase (NADP+)

Chain B:



- Molecule 1: Succinate-semialdehydedehydrogenase (NADP+)

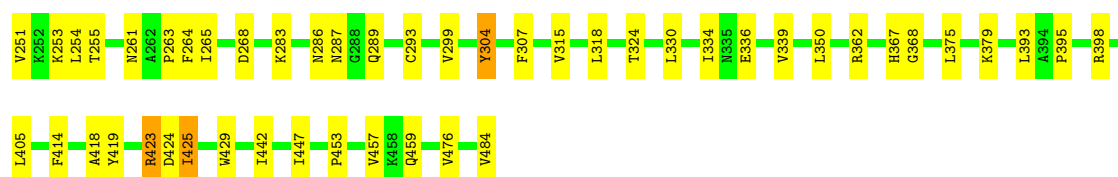
Chain C:



- Molecule 1: Succinate-semialdehydedehydrogenase (NADP+)

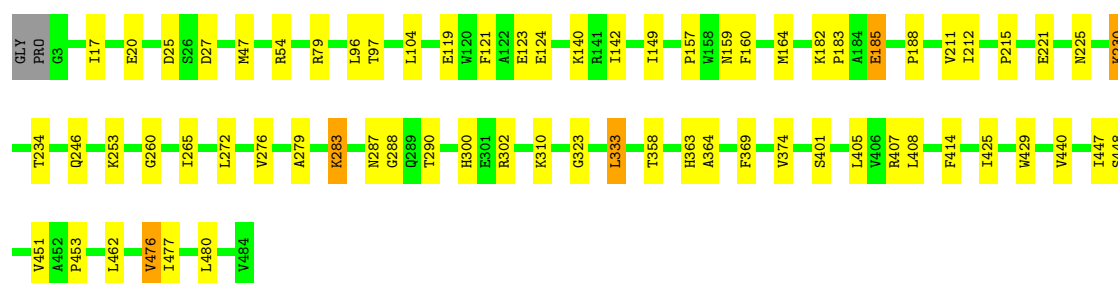
Chain D:





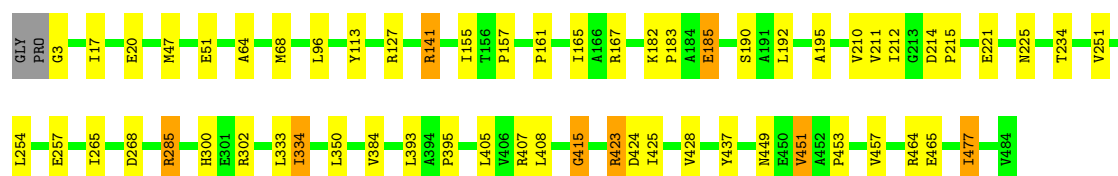
- Molecule 1: Succinate-semialdehydedehydrogenase (NADP+)

Chain E:



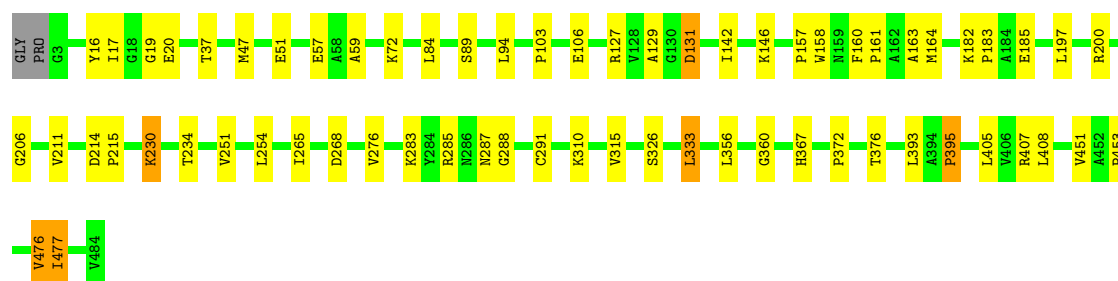
- Molecule 1: Succinate-semialdehydedehydrogenase (NADP+)

Chain F:



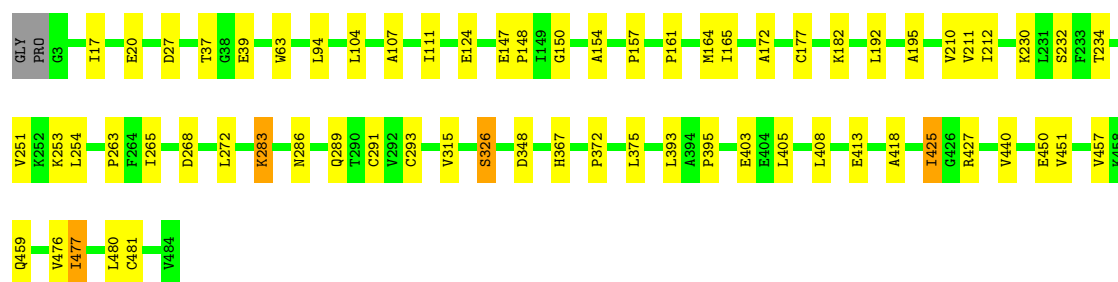
- Molecule 1: Succinate-semialdehydedehydrogenase (NADP+)

Chain G:



- Molecule 1: Succinate-semialdehydedehydrogenase (NADP+)

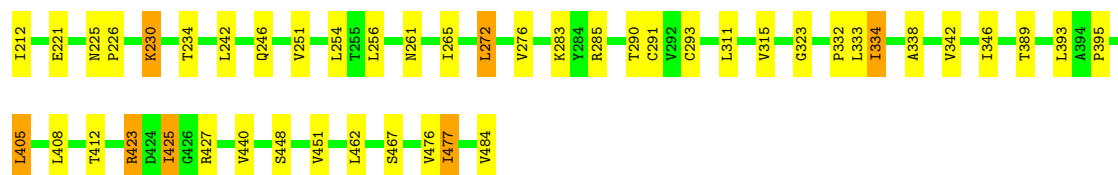
Chain H:





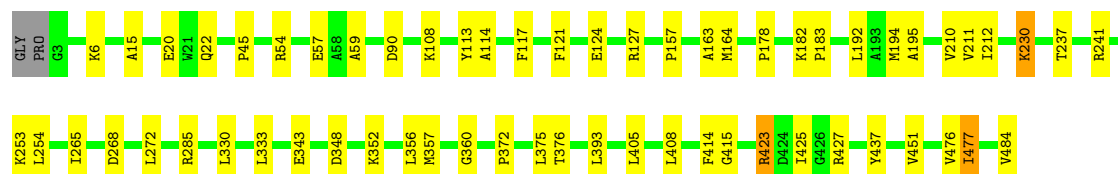
Chain I:





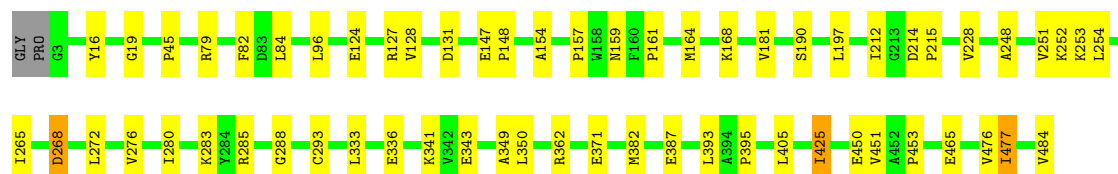
- Molecule 1: Succinate-semialdehydedehydrogenase (NADP+)

Chain N:



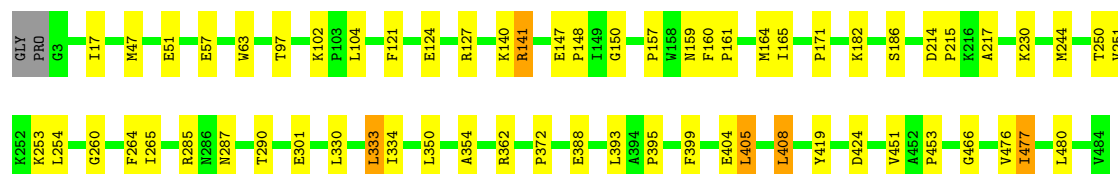
- Molecule 1: Succinate-semialdehydedehydrogenase (NADP+)

Chain O:



- Molecule 1: Succinate-semialdehydedehydrogenase (NADP+)

Chain P:



## 4 Data and refinement statistics i

EDS was not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	185.66Å 164.87Å 278.90Å 90.00° 92.01° 90.00°	Depositor
Resolution (Å)	49.47 – 2.70	Depositor
% Data completeness (in resolution range)	98.3 (49.47-2.70)	Depositor
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.83 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, $R_{free}$	0.236 , 0.282	Depositor
Wilson B-factor (Å <sup>2</sup> )	47.8	Xtriage
Anisotropy	0.054	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	4 of 453146 reflections (0.001%)	Xtriage
Total number of atoms	57595	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	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 43.06 % 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 1.8625e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

## 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	0.39	0/3623	0.55	0/4930
1	B	0.40	0/3627	0.55	0/4935
1	C	0.41	0/3623	0.56	0/4930
1	D	0.41	0/3623	0.56	0/4930
1	E	0.40	0/3623	0.56	0/4930
1	F	0.41	0/3623	0.55	0/4930
1	G	0.41	0/3623	0.56	0/4930
1	H	0.41	0/3623	0.56	0/4930
1	I	0.44	0/3594	0.54	0/4896
1	J	0.41	0/3623	0.55	0/4930
1	K	0.41	0/3619	0.53	0/4925
1	L	0.40	0/3617	0.56	0/4922
1	M	0.41	0/3619	0.54	0/4925
1	N	0.39	0/3619	0.53	0/4925
1	O	0.41	0/3619	0.54	0/4925
1	P	0.39	0/3619	0.55	0/4925
All	All	0.41	0/57917	0.55	0/78818

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3549	0	3507	37	0
1	B	3553	0	3511	34	0
1	C	3549	0	3507	41	0
1	D	3549	0	3507	45	0
1	E	3549	0	3507	44	0
1	F	3549	0	3507	47	0
1	G	3549	0	3507	36	0
1	H	3549	0	3507	38	0
1	I	3520	0	3450	49	0
1	J	3549	0	3507	50	0
1	K	3545	0	3503	34	0
1	L	3543	0	3496	34	0
1	M	3545	0	3503	46	0
1	N	3545	0	3503	26	0
1	O	3545	0	3503	28	0
1	P	3545	0	3503	38	0
2	A	45	0	0	0	0
2	B	59	0	0	1	0
2	C	56	0	0	1	0
2	D	61	0	0	3	0
2	E	72	0	0	2	0
2	F	75	0	0	4	0
2	G	66	0	0	1	0
2	H	58	0	0	1	0
2	I	24	0	0	1	0
2	J	35	0	0	2	0
2	K	55	0	0	2	0
2	L	57	0	0	2	0
2	M	40	0	0	1	0
2	N	47	0	0	0	0
2	O	38	0	0	0	0
2	P	74	0	0	1	0
All	All	57595	0	56028	559	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

The worst 5 of 559 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:265:ILE:HG21	1:H:405:LEU:HD21	1.51	0.91
1:J:160:PHE:HE2	1:J:290:THR:HG22	1.42	0.85
1:C:375:LEU:HD12	1:C:393:LEU:HD11	1.58	0.84
1:M:138:ALA:O	1:M:139:ASN:HB2	1.77	0.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:251:VAL:HG12	1:H:251:VAL:O	1.83	0.79

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	480/484 (99%)	457 (95%)	21 (4%)	2 (0%)	43	76
1	B	480/484 (99%)	464 (97%)	13 (3%)	3 (1%)	33	66
1	C	480/484 (99%)	465 (97%)	14 (3%)	1 (0%)	56	86
1	D	480/484 (99%)	450 (94%)	27 (6%)	3 (1%)	33	66
1	E	480/484 (99%)	456 (95%)	24 (5%)	0	100	100
1	F	480/484 (99%)	463 (96%)	15 (3%)	2 (0%)	43	76
1	G	480/484 (99%)	462 (96%)	16 (3%)	2 (0%)	43	76
1	H	480/484 (99%)	454 (95%)	24 (5%)	2 (0%)	43	76
1	I	480/484 (99%)	445 (93%)	32 (7%)	3 (1%)	33	66
1	J	480/484 (99%)	451 (94%)	27 (6%)	2 (0%)	43	76
1	K	480/484 (99%)	459 (96%)	19 (4%)	2 (0%)	43	76
1	L	480/484 (99%)	460 (96%)	19 (4%)	1 (0%)	56	86
1	M	480/484 (99%)	458 (95%)	19 (4%)	3 (1%)	33	66
1	N	480/484 (99%)	463 (96%)	16 (3%)	1 (0%)	56	86
1	O	480/484 (99%)	460 (96%)	19 (4%)	1 (0%)	56	86
1	P	480/484 (99%)	458 (95%)	22 (5%)	0	100	100
All	All	7680/7744 (99%)	7325 (95%)	327 (4%)	28 (0%)	43	76

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	268	ASP

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Mol	Chain	Res	Type
1	D	261	ASN
1	D	268	ASP
1	G	268	ASP
1	H	268	ASP

### 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	350/363 (96%)	334 (95%)	16 (5%)	37	70
1	B	351/363 (97%)	337 (96%)	14 (4%)	42	75
1	C	350/363 (96%)	325 (93%)	25 (7%)	21	46
1	D	350/363 (96%)	333 (95%)	17 (5%)	35	67
1	E	350/363 (96%)	332 (95%)	18 (5%)	33	64
1	F	350/363 (96%)	337 (96%)	13 (4%)	45	78
1	G	350/363 (96%)	332 (95%)	18 (5%)	33	64
1	H	350/363 (96%)	331 (95%)	19 (5%)	31	61
1	I	344/363 (95%)	319 (93%)	25 (7%)	20	44
1	J	350/363 (96%)	332 (95%)	18 (5%)	33	64
1	K	349/363 (96%)	336 (96%)	13 (4%)	45	78
1	L	348/363 (96%)	328 (94%)	20 (6%)	29	58
1	M	349/363 (96%)	327 (94%)	22 (6%)	25	53
1	N	349/363 (96%)	330 (95%)	19 (5%)	31	61
1	O	349/363 (96%)	332 (95%)	17 (5%)	35	67
1	P	349/363 (96%)	334 (96%)	15 (4%)	40	72
All	All	5588/5808 (96%)	5299 (95%)	289 (5%)	32	63

5 of 289 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	283	LYS
1	I	427	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	O	350	LEU
1	H	348	ASP
1	I	159	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	287	ASN
1	J	159	ASN
1	J	287	ASN
1	J	443	ASN
1	J	468	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.