



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 23, 2024 – 09:14 AM EDT

PDB ID : 1YNF
Title : Crystal Structure of N-Succinylarginine Dihydrolase, AstB, bound to Substrate and Product, an Enzyme from the Arginine Catabolic Pathway of Escherichia coli
Authors : Tocilj, A.; Schrag, J.D.; Li, Y.; Schneider, B.L.; Reitzer, L.; Matte, A.; Cygler, M.
Deposited on : 2005-01-24
Resolution : 1.90 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

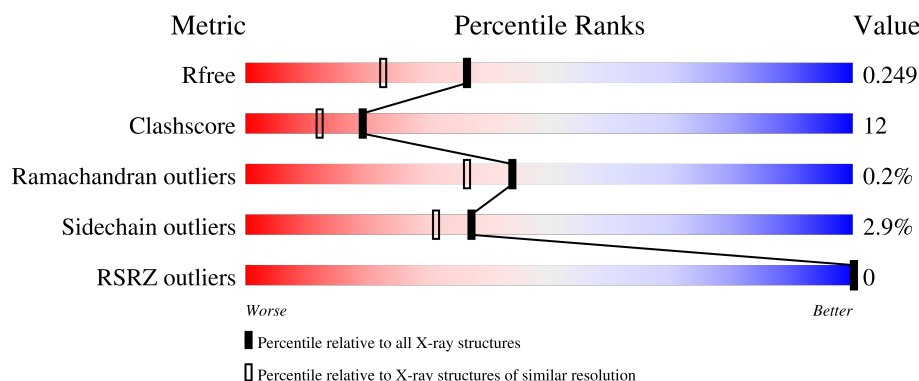
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION




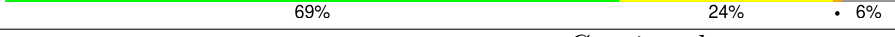
The reported resolution of this entry is 1.90 Å.

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}	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

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	458	
1	B	458	
1	C	458	
1	D	458	

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Mol	Chain	Length	Quality of chain
1	E	458	<div><div></div><div>72%</div><div>21%</div><div>• 6%</div></div>
1	F	458	<div><div></div><div>70%</div><div>22%</div><div>• 6%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21526 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 Succinylarginine dihydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	429	Total	C	N	O	S	Se	0	0	0
			3353	2102	612	627	3	9			
1	B	429	Total	C	N	O	S	Se	0	0	0
			3353	2102	612	627	3	9			
1	C	429	Total	C	N	O	S	Se	0	0	0
			3353	2102	612	627	3	9			
1	D	429	Total	C	N	O	S	Se	0	0	0
			3353	2102	612	627	3	9			
1	E	429	Total	C	N	O	S	Se	0	0	0
			3353	2102	612	627	3	9			
1	F	429	Total	C	N	O	S	Se	0	0	0
			3353	2102	612	627	3	9			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	expression tag	UNP P76216
A	-9	GLY	-	expression tag	UNP P76216
A	-8	SER	-	expression tag	UNP P76216
A	-7	SER	-	expression tag	UNP P76216
A	-6	HIS	-	expression tag	UNP P76216
A	-5	HIS	-	expression tag	UNP P76216
A	-4	HIS	-	expression tag	UNP P76216
A	-3	HIS	-	expression tag	UNP P76216
A	-2	HIS	-	expression tag	UNP P76216
A	-1	HIS	-	expression tag	UNP P76216
A	0	GLY	-	expression tag	UNP P76216
A	1	SER	-	expression tag	UNP P76216
A	49	MSE	MET	modified residue	UNP P76216
A	106	MSE	MET	modified residue	UNP P76216
A	191	MSE	MET	modified residue	UNP P76216
A	285	MSE	MET	modified residue	UNP P76216
A	317	MSE	MET	modified residue	UNP P76216

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Chain	Residue	Modelled	Actual	Comment	Reference
A	318	MSE	MET	modified residue	UNP P76216
A	357	MSE	MET	modified residue	UNP P76216
A	385	MSE	MET	modified residue	UNP P76216
A	386	MSE	MET	modified residue	UNP P76216
B	-10	MET	-	expression tag	UNP P76216
B	-9	GLY	-	expression tag	UNP P76216
B	-8	SER	-	expression tag	UNP P76216
B	-7	SER	-	expression tag	UNP P76216
B	-6	HIS	-	expression tag	UNP P76216
B	-5	HIS	-	expression tag	UNP P76216
B	-4	HIS	-	expression tag	UNP P76216
B	-3	HIS	-	expression tag	UNP P76216
B	-2	HIS	-	expression tag	UNP P76216
B	-1	HIS	-	expression tag	UNP P76216
B	0	GLY	-	expression tag	UNP P76216
B	1	SER	-	expression tag	UNP P76216
B	49	MSE	MET	modified residue	UNP P76216
B	106	MSE	MET	modified residue	UNP P76216
B	191	MSE	MET	modified residue	UNP P76216
B	285	MSE	MET	modified residue	UNP P76216
B	317	MSE	MET	modified residue	UNP P76216
B	318	MSE	MET	modified residue	UNP P76216
B	357	MSE	MET	modified residue	UNP P76216
B	385	MSE	MET	modified residue	UNP P76216
B	386	MSE	MET	modified residue	UNP P76216
C	-10	MET	-	expression tag	UNP P76216
C	-9	GLY	-	expression tag	UNP P76216
C	-8	SER	-	expression tag	UNP P76216
C	-7	SER	-	expression tag	UNP P76216
C	-6	HIS	-	expression tag	UNP P76216
C	-5	HIS	-	expression tag	UNP P76216
C	-4	HIS	-	expression tag	UNP P76216
C	-3	HIS	-	expression tag	UNP P76216
C	-2	HIS	-	expression tag	UNP P76216
C	-1	HIS	-	expression tag	UNP P76216
C	0	GLY	-	expression tag	UNP P76216
C	1	SER	-	expression tag	UNP P76216
C	49	MSE	MET	modified residue	UNP P76216
C	106	MSE	MET	modified residue	UNP P76216
C	191	MSE	MET	modified residue	UNP P76216
C	285	MSE	MET	modified residue	UNP P76216
C	317	MSE	MET	modified residue	UNP P76216

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Chain	Residue	Modelled	Actual	Comment	Reference
C	318	MSE	MET	modified residue	UNP P76216
C	357	MSE	MET	modified residue	UNP P76216
C	385	MSE	MET	modified residue	UNP P76216
C	386	MSE	MET	modified residue	UNP P76216
D	-10	MET	-	expression tag	UNP P76216
D	-9	GLY	-	expression tag	UNP P76216
D	-8	SER	-	expression tag	UNP P76216
D	-7	SER	-	expression tag	UNP P76216
D	-6	HIS	-	expression tag	UNP P76216
D	-5	HIS	-	expression tag	UNP P76216
D	-4	HIS	-	expression tag	UNP P76216
D	-3	HIS	-	expression tag	UNP P76216
D	-2	HIS	-	expression tag	UNP P76216
D	-1	HIS	-	expression tag	UNP P76216
D	0	GLY	-	expression tag	UNP P76216
D	1	SER	-	expression tag	UNP P76216
D	49	MSE	MET	modified residue	UNP P76216
D	106	MSE	MET	modified residue	UNP P76216
D	191	MSE	MET	modified residue	UNP P76216
D	285	MSE	MET	modified residue	UNP P76216
D	317	MSE	MET	modified residue	UNP P76216
D	318	MSE	MET	modified residue	UNP P76216
D	357	MSE	MET	modified residue	UNP P76216
D	385	MSE	MET	modified residue	UNP P76216
D	386	MSE	MET	modified residue	UNP P76216
E	-10	MET	-	expression tag	UNP P76216
E	-9	GLY	-	expression tag	UNP P76216
E	-8	SER	-	expression tag	UNP P76216
E	-7	SER	-	expression tag	UNP P76216
E	-6	HIS	-	expression tag	UNP P76216
E	-5	HIS	-	expression tag	UNP P76216
E	-4	HIS	-	expression tag	UNP P76216
E	-3	HIS	-	expression tag	UNP P76216
E	-2	HIS	-	expression tag	UNP P76216
E	-1	HIS	-	expression tag	UNP P76216
E	0	GLY	-	expression tag	UNP P76216
E	1	SER	-	expression tag	UNP P76216
E	49	MSE	MET	modified residue	UNP P76216
E	106	MSE	MET	modified residue	UNP P76216
E	191	MSE	MET	modified residue	UNP P76216
E	285	MSE	MET	modified residue	UNP P76216
E	317	MSE	MET	modified residue	UNP P76216

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Chain	Residue	Modelled	Actual	Comment	Reference
E	318	MSE	MET	modified residue	UNP P76216
E	357	MSE	MET	modified residue	UNP P76216
E	385	MSE	MET	modified residue	UNP P76216
E	386	MSE	MET	modified residue	UNP P76216
F	-10	MET	-	expression tag	UNP P76216
F	-9	GLY	-	expression tag	UNP P76216
F	-8	SER	-	expression tag	UNP P76216
F	-7	SER	-	expression tag	UNP P76216
F	-6	HIS	-	expression tag	UNP P76216
F	-5	HIS	-	expression tag	UNP P76216
F	-4	HIS	-	expression tag	UNP P76216
F	-3	HIS	-	expression tag	UNP P76216
F	-2	HIS	-	expression tag	UNP P76216
F	-1	HIS	-	expression tag	UNP P76216
F	0	GLY	-	expression tag	UNP P76216
F	1	SER	-	expression tag	UNP P76216
F	49	MSE	MET	modified residue	UNP P76216
F	106	MSE	MET	modified residue	UNP P76216
F	191	MSE	MET	modified residue	UNP P76216
F	285	MSE	MET	modified residue	UNP P76216
F	317	MSE	MET	modified residue	UNP P76216
F	318	MSE	MET	modified residue	UNP P76216
F	357	MSE	MET	modified residue	UNP P76216
F	385	MSE	MET	modified residue	UNP P76216
F	386	MSE	MET	modified residue	UNP P76216

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total K 1 1	0	0
2	B	1	Total K 1 1	0	0
2	C	1	Total K 1 1	0	0
2	D	1	Total K 1 1	0	0
2	E	1	Total K 1 1	0	0
2	F	1	Total K 1 1	0	0


- Molecule 3 is water.

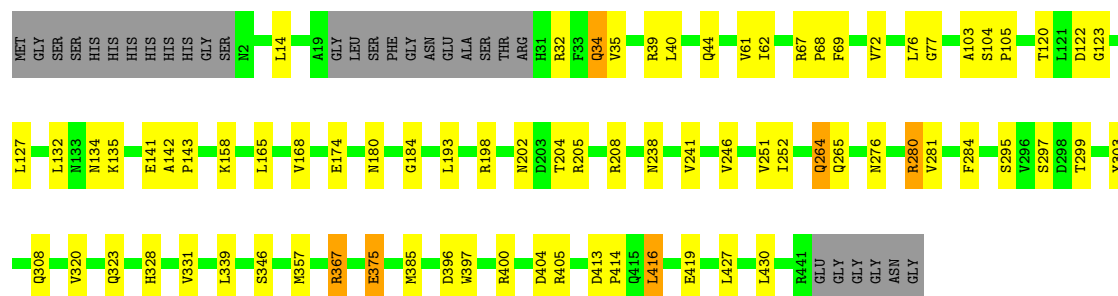
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	260	Total 260	O 260	0	0
3	B	310	Total 310	O 310	0	0
3	C	213	Total 213	O 213	0	0
3	D	192	Total 192	O 192	0	0
3	E	244	Total 244	O 244	0	0
3	F	183	Total 183	O 183	0	0

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.

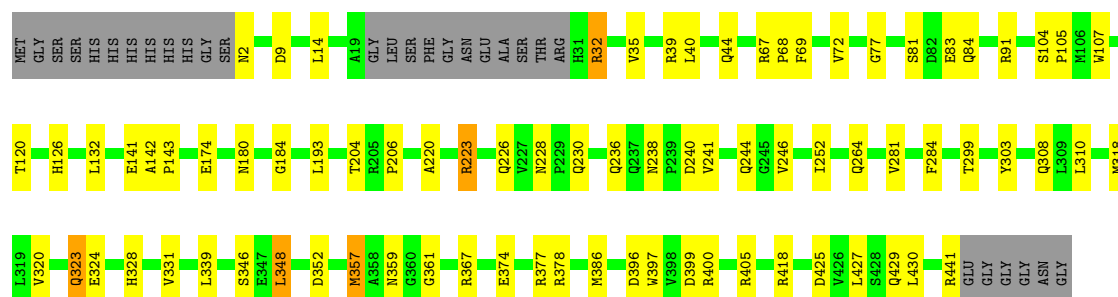
• Molecule 1: Succinylarginine dihydrolase

Chain A: 



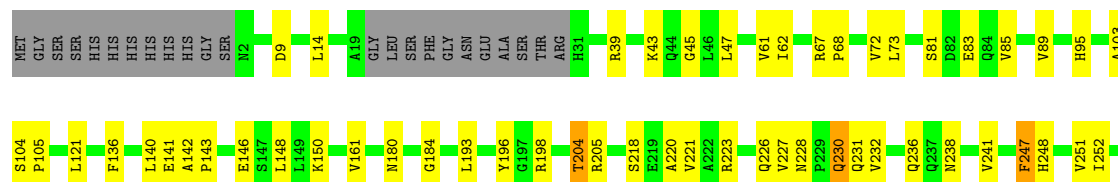
• Molecule 1: Succinylarginine dihydrolase

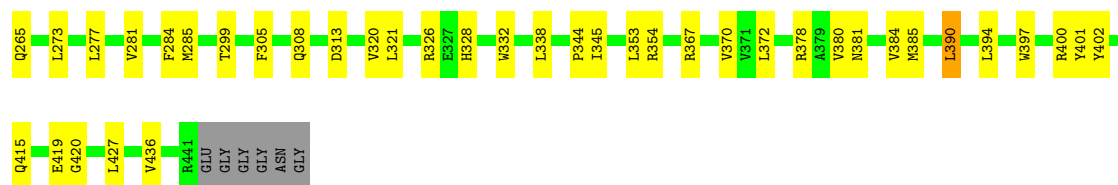
Chain B: 



• Molecule 1: Succinylarginine dihydrolase

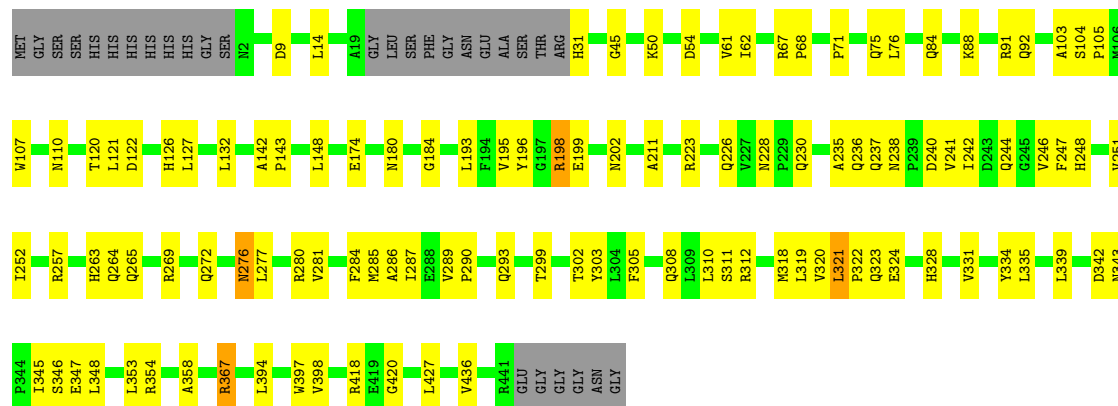
Chain C: 





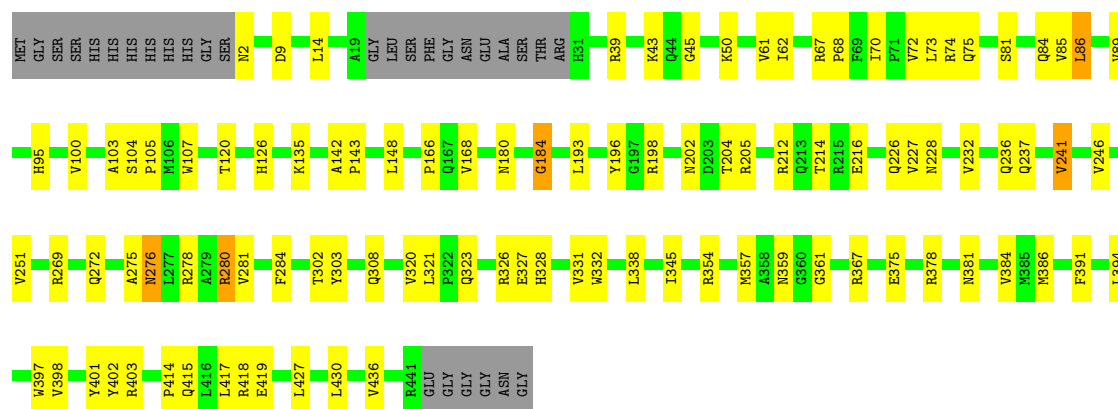
• Molecule 1: Succinylarginine dihydrolase

Chain D: 69% 24% • 6%



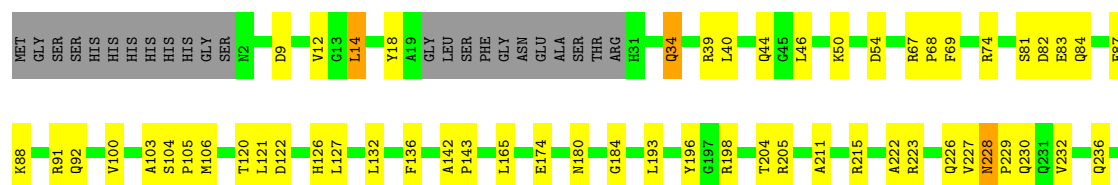
• Molecule 1: Succinylarginine dihydrolase

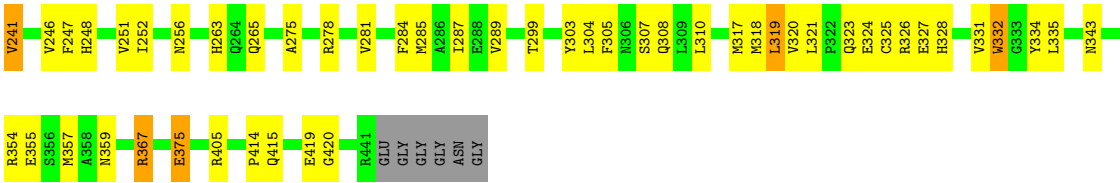
Chain E: 72% 21% • 6%



• Molecule 1: Succinylarginine dihydrolase

Chain F: 70% 22% • 6%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.83Å 94.17Å 139.66Å 75.41° 78.38° 89.74°	Depositor
Resolution (Å)	27.32 – 1.90 27.32 – 1.90	Depositor EDS
% Data completeness (in resolution range)	64.5 (27.32-1.90) 63.8 (27.32-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 1.89Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.214 , 0.252 0.212 , 0.249	Depositor DCC
R_{free} test set	6944 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	21.4	Xtriage
Anisotropy	0.502	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 22.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.468 for h,-k,h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	21526	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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 22.16 % 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 6.0306e-03. 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
K

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	0.36	0/3415	0.58	0/4627
1	B	0.36	0/3415	0.58	0/4627
1	C	0.35	0/3415	0.59	0/4627
1	D	0.33	0/3415	0.57	0/4627
1	E	0.34	0/3415	0.58	0/4627
1	F	0.34	0/3415	0.57	0/4627
All	All	0.35	0/20490	0.58	0/27762

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3353	0	3285	62	0
1	B	3353	0	3285	63	0
1	C	3353	0	3285	66	0
1	D	3353	0	3285	95	0
1	E	3353	0	3285	73	0
1	F	3353	0	3285	108	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	260	0	0	6	0
3	B	310	0	0	7	0
3	C	213	0	0	8	0
3	D	192	0	0	6	0
3	E	244	0	0	10	0
3	F	183	0	0	3	0
All	All	21526	0	19710	459	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 12.

The worst 5 of 459 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:B:220:ALA:HA	1:B:223:ARG:HH12	0.99	1.15
1:B:220:ALA:HA	1:B:223:ARG:NH1	1.68	1.06
1:B:223:ARG:HH11	1:B:223:ARG:HB2	1.35	0.92
1:F:248:HIS:O	1:F:251:VAL:HG12	1.71	0.89
1:F:328:HIS:HB3	1:F:331:VAL:HG12	1.56	0.86

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	425/458 (93%)	411 (97%)	13 (3%)	1 (0%)	44 36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	425/458 (93%)	412 (97%)	12 (3%)	1 (0%)	44	36
1	C	425/458 (93%)	412 (97%)	12 (3%)	1 (0%)	44	36
1	D	425/458 (93%)	411 (97%)	13 (3%)	1 (0%)	44	36
1	E	425/458 (93%)	413 (97%)	11 (3%)	1 (0%)	44	36
1	F	425/458 (93%)	413 (97%)	11 (3%)	1 (0%)	44	36
All	All	2550/2748 (93%)	2472 (97%)	72 (3%)	6 (0%)	44	36

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	GLY
1	B	184	GLY
1	D	184	GLY
1	E	184	GLY
1	C	184	GLY

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	357/368 (97%)	349 (98%)	8 (2%)	47	43
1	B	357/368 (97%)	346 (97%)	11 (3%)	35	29
1	C	357/368 (97%)	347 (97%)	10 (3%)	38	33
1	D	357/368 (97%)	350 (98%)	7 (2%)	50	47
1	E	357/368 (97%)	346 (97%)	11 (3%)	35	29
1	F	357/368 (97%)	342 (96%)	15 (4%)	25	18
All	All	2142/2208 (97%)	2080 (97%)	62 (3%)	37	31

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	390	LEU

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Mol	Chain	Res	Type
1	F	319	LEU
1	D	367	ARG
1	F	241	VAL
1	F	367	ARG

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	D	276	ASN
1	E	226	GLN
1	F	359	ASN
1	D	282	ASN
1	E	2	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	420/458 (91%)	-1.61	0 100 100	10, 22, 37, 50	0
1	B	420/458 (91%)	-1.61	0 100 100	10, 22, 36, 51	0
1	C	420/458 (91%)	-1.57	0 100 100	13, 25, 39, 51	0
1	D	420/458 (91%)	-1.52	0 100 100	12, 27, 42, 52	0
1	E	420/458 (91%)	-1.57	0 100 100	13, 26, 40, 51	0
1	F	420/458 (91%)	-1.52	0 100 100	12, 27, 42, 52	0
All	All	2520/2748 (91%)	-1.57	0 100 100	10, 25, 40, 52	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 monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	K	D	448	1/1	0.98	0.04	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	K	F	448	1/1	0.99	0.04	51,51,51,51	0
2	K	C	448	1/1	1.00	0.01	31,31,31,31	0
2	K	A	448	1/1	1.00	0.03	24,24,24,24	0
2	K	E	448	1/1	1.00	0.01	27,27,27,27	0
2	K	B	448	1/1	1.00	0.01	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.