



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 12:58 AM BST

PDB ID : 4WP0
Title : Crystal structure of human kynurenine aminotransferase-I with a C-terminal V5-hexahistidine tag
Authors : Nadvi, N.A.; Salam, N.K.; Park, J.; Akladios, F.N.; Kapoor, V.; Collyer, C.A.; Gorrell, M.D.; Church, W.B.
Deposited on : 2014-10-17
Resolution : 3.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
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)	:	2.13.1

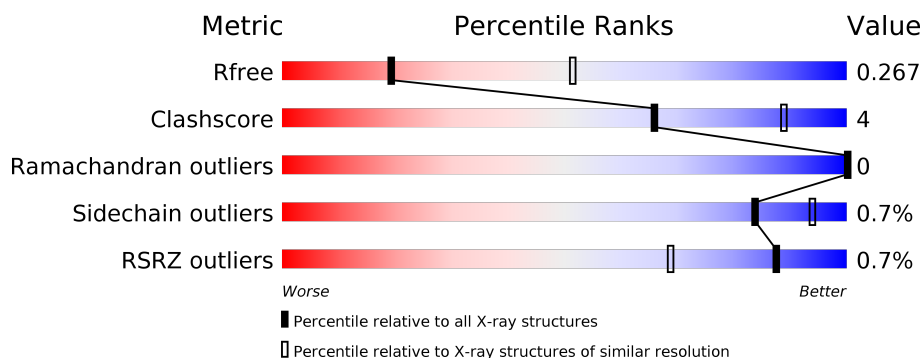
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 ≥ 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	472	
1	B	472	
1	C	472	
1	D	472	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13483 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 Kynurenine--oxoglutarate transaminase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	P	S	0	0	0
			3349	2163	561	605	1	19			
1	B	413	Total	C	N	O	P	S	0	0	0
			3330	2150	558	602	1	19			
1	C	415	Total	C	N	O	P	S	0	0	0
			3339	2159	559	601	1	19			
1	D	416	Total	C	N	O	P	S	0	0	0
			3350	2162	561	607	1	19			

There are 200 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	423	GLU	-	expression tag	UNP Q16773
A	424	ASN	-	expression tag	UNP Q16773
A	425	LEU	-	expression tag	UNP Q16773
A	426	TYR	-	expression tag	UNP Q16773
A	427	PHE	-	expression tag	UNP Q16773
A	428	GLN	-	expression tag	UNP Q16773
A	429	GLY	-	expression tag	UNP Q16773
A	430	LYS	-	expression tag	UNP Q16773
A	431	GLY	-	expression tag	UNP Q16773
A	432	GLY	-	expression tag	UNP Q16773
A	433	ARG	-	expression tag	UNP Q16773
A	434	ALA	-	expression tag	UNP Q16773
A	435	ASP	-	expression tag	UNP Q16773
A	436	PRO	-	expression tag	UNP Q16773
A	437	ALA	-	expression tag	UNP Q16773
A	438	PHE	-	expression tag	UNP Q16773
A	439	LEU	-	expression tag	UNP Q16773
A	440	TYR	-	expression tag	UNP Q16773
A	441	LYS	-	expression tag	UNP Q16773
A	442	VAL	-	expression tag	UNP Q16773
A	443	VAL	-	expression tag	UNP Q16773

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Chain	Residue	Modelled	Actual	Comment	Reference
A	444	ARG	-	expression tag	UNP Q16773
A	445	MET	-	expression tag	UNP Q16773
A	446	ASN	-	expression tag	UNP Q16773
A	447	GLU	-	expression tag	UNP Q16773
A	448	ASP	-	expression tag	UNP Q16773
A	449	LEU	-	expression tag	UNP Q16773
A	450	GLY	-	expression tag	UNP Q16773
A	451	LYS	-	expression tag	UNP Q16773
A	452	PRO	-	expression tag	UNP Q16773
A	453	ILE	-	expression tag	UNP Q16773
A	454	PRO	-	expression tag	UNP Q16773
A	455	ASN	-	expression tag	UNP Q16773
A	456	PRO	-	expression tag	UNP Q16773
A	457	LEU	-	expression tag	UNP Q16773
A	458	LEU	-	expression tag	UNP Q16773
A	459	GLY	-	expression tag	UNP Q16773
A	460	LEU	-	expression tag	UNP Q16773
A	461	ASP	-	expression tag	UNP Q16773
A	462	SER	-	expression tag	UNP Q16773
A	463	THR	-	expression tag	UNP Q16773
A	464	ARG	-	expression tag	UNP Q16773
A	465	THR	-	expression tag	UNP Q16773
A	466	GLY	-	expression tag	UNP Q16773
A	467	HIS	-	expression tag	UNP Q16773
A	468	HIS	-	expression tag	UNP Q16773
A	469	HIS	-	expression tag	UNP Q16773
A	470	HIS	-	expression tag	UNP Q16773
A	471	HIS	-	expression tag	UNP Q16773
A	472	HIS	-	expression tag	UNP Q16773
B	423	GLU	-	expression tag	UNP Q16773
B	424	ASN	-	expression tag	UNP Q16773
B	425	LEU	-	expression tag	UNP Q16773
B	426	TYR	-	expression tag	UNP Q16773
B	427	PHE	-	expression tag	UNP Q16773
B	428	GLN	-	expression tag	UNP Q16773
B	429	GLY	-	expression tag	UNP Q16773
B	430	LYS	-	expression tag	UNP Q16773
B	431	GLY	-	expression tag	UNP Q16773
B	432	GLY	-	expression tag	UNP Q16773
B	433	ARG	-	expression tag	UNP Q16773
B	434	ALA	-	expression tag	UNP Q16773
B	435	ASP	-	expression tag	UNP Q16773

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Chain	Residue	Modelled	Actual	Comment	Reference
B	436	PRO	-	expression tag	UNP Q16773
B	437	ALA	-	expression tag	UNP Q16773
B	438	PHE	-	expression tag	UNP Q16773
B	439	LEU	-	expression tag	UNP Q16773
B	440	TYR	-	expression tag	UNP Q16773
B	441	LYS	-	expression tag	UNP Q16773
B	442	VAL	-	expression tag	UNP Q16773
B	443	VAL	-	expression tag	UNP Q16773
B	444	ARG	-	expression tag	UNP Q16773
B	445	MET	-	expression tag	UNP Q16773
B	446	ASN	-	expression tag	UNP Q16773
B	447	GLU	-	expression tag	UNP Q16773
B	448	ASP	-	expression tag	UNP Q16773
B	449	LEU	-	expression tag	UNP Q16773
B	450	GLY	-	expression tag	UNP Q16773
B	451	LYS	-	expression tag	UNP Q16773
B	452	PRO	-	expression tag	UNP Q16773
B	453	ILE	-	expression tag	UNP Q16773
B	454	PRO	-	expression tag	UNP Q16773
B	455	ASN	-	expression tag	UNP Q16773
B	456	PRO	-	expression tag	UNP Q16773
B	457	LEU	-	expression tag	UNP Q16773
B	458	LEU	-	expression tag	UNP Q16773
B	459	GLY	-	expression tag	UNP Q16773
B	460	LEU	-	expression tag	UNP Q16773
B	461	ASP	-	expression tag	UNP Q16773
B	462	SER	-	expression tag	UNP Q16773
B	463	THR	-	expression tag	UNP Q16773
B	464	ARG	-	expression tag	UNP Q16773
B	465	THR	-	expression tag	UNP Q16773
B	466	GLY	-	expression tag	UNP Q16773
B	467	HIS	-	expression tag	UNP Q16773
B	468	HIS	-	expression tag	UNP Q16773
B	469	HIS	-	expression tag	UNP Q16773
B	470	HIS	-	expression tag	UNP Q16773
B	471	HIS	-	expression tag	UNP Q16773
B	472	HIS	-	expression tag	UNP Q16773
C	423	GLU	-	expression tag	UNP Q16773
C	424	ASN	-	expression tag	UNP Q16773
C	425	LEU	-	expression tag	UNP Q16773
C	426	TYR	-	expression tag	UNP Q16773
C	427	PHE	-	expression tag	UNP Q16773

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Chain	Residue	Modelled	Actual	Comment	Reference
C	428	GLN	-	expression tag	UNP Q16773
C	429	GLY	-	expression tag	UNP Q16773
C	430	LYS	-	expression tag	UNP Q16773
C	431	GLY	-	expression tag	UNP Q16773
C	432	GLY	-	expression tag	UNP Q16773
C	433	ARG	-	expression tag	UNP Q16773
C	434	ALA	-	expression tag	UNP Q16773
C	435	ASP	-	expression tag	UNP Q16773
C	436	PRO	-	expression tag	UNP Q16773
C	437	ALA	-	expression tag	UNP Q16773
C	438	PHE	-	expression tag	UNP Q16773
C	439	LEU	-	expression tag	UNP Q16773
C	440	TYR	-	expression tag	UNP Q16773
C	441	LYS	-	expression tag	UNP Q16773
C	442	VAL	-	expression tag	UNP Q16773
C	443	VAL	-	expression tag	UNP Q16773
C	444	ARG	-	expression tag	UNP Q16773
C	445	MET	-	expression tag	UNP Q16773
C	446	ASN	-	expression tag	UNP Q16773
C	447	GLU	-	expression tag	UNP Q16773
C	448	ASP	-	expression tag	UNP Q16773
C	449	LEU	-	expression tag	UNP Q16773
C	450	GLY	-	expression tag	UNP Q16773
C	451	LYS	-	expression tag	UNP Q16773
C	452	PRO	-	expression tag	UNP Q16773
C	453	ILE	-	expression tag	UNP Q16773
C	454	PRO	-	expression tag	UNP Q16773
C	455	ASN	-	expression tag	UNP Q16773
C	456	PRO	-	expression tag	UNP Q16773
C	457	LEU	-	expression tag	UNP Q16773
C	458	LEU	-	expression tag	UNP Q16773
C	459	GLY	-	expression tag	UNP Q16773
C	460	LEU	-	expression tag	UNP Q16773
C	461	ASP	-	expression tag	UNP Q16773
C	462	SER	-	expression tag	UNP Q16773
C	463	THR	-	expression tag	UNP Q16773
C	464	ARG	-	expression tag	UNP Q16773
C	465	THR	-	expression tag	UNP Q16773
C	466	GLY	-	expression tag	UNP Q16773
C	467	HIS	-	expression tag	UNP Q16773
C	468	HIS	-	expression tag	UNP Q16773
C	469	HIS	-	expression tag	UNP Q16773

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Chain	Residue	Modelled	Actual	Comment	Reference
C	470	HIS	-	expression tag	UNP Q16773
C	471	HIS	-	expression tag	UNP Q16773
C	472	HIS	-	expression tag	UNP Q16773
D	423	GLU	-	expression tag	UNP Q16773
D	424	ASN	-	expression tag	UNP Q16773
D	425	LEU	-	expression tag	UNP Q16773
D	426	TYR	-	expression tag	UNP Q16773
D	427	PHE	-	expression tag	UNP Q16773
D	428	GLN	-	expression tag	UNP Q16773
D	429	GLY	-	expression tag	UNP Q16773
D	430	LYS	-	expression tag	UNP Q16773
D	431	GLY	-	expression tag	UNP Q16773
D	432	GLY	-	expression tag	UNP Q16773
D	433	ARG	-	expression tag	UNP Q16773
D	434	ALA	-	expression tag	UNP Q16773
D	435	ASP	-	expression tag	UNP Q16773
D	436	PRO	-	expression tag	UNP Q16773
D	437	ALA	-	expression tag	UNP Q16773
D	438	PHE	-	expression tag	UNP Q16773
D	439	LEU	-	expression tag	UNP Q16773
D	440	TYR	-	expression tag	UNP Q16773
D	441	LYS	-	expression tag	UNP Q16773
D	442	VAL	-	expression tag	UNP Q16773
D	443	VAL	-	expression tag	UNP Q16773
D	444	ARG	-	expression tag	UNP Q16773
D	445	MET	-	expression tag	UNP Q16773
D	446	ASN	-	expression tag	UNP Q16773
D	447	GLU	-	expression tag	UNP Q16773
D	448	ASP	-	expression tag	UNP Q16773
D	449	LEU	-	expression tag	UNP Q16773
D	450	GLY	-	expression tag	UNP Q16773
D	451	LYS	-	expression tag	UNP Q16773
D	452	PRO	-	expression tag	UNP Q16773
D	453	ILE	-	expression tag	UNP Q16773
D	454	PRO	-	expression tag	UNP Q16773
D	455	ASN	-	expression tag	UNP Q16773
D	456	PRO	-	expression tag	UNP Q16773
D	457	LEU	-	expression tag	UNP Q16773
D	458	LEU	-	expression tag	UNP Q16773
D	459	GLY	-	expression tag	UNP Q16773
D	460	LEU	-	expression tag	UNP Q16773
D	461	ASP	-	expression tag	UNP Q16773

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Chain	Residue	Modelled	Actual	Comment	Reference
D	462	SER	-	expression tag	UNP Q16773
D	463	THR	-	expression tag	UNP Q16773
D	464	ARG	-	expression tag	UNP Q16773
D	465	THR	-	expression tag	UNP Q16773
D	466	GLY	-	expression tag	UNP Q16773
D	467	HIS	-	expression tag	UNP Q16773
D	468	HIS	-	expression tag	UNP Q16773
D	469	HIS	-	expression tag	UNP Q16773
D	470	HIS	-	expression tag	UNP Q16773
D	471	HIS	-	expression tag	UNP Q16773
D	472	HIS	-	expression tag	UNP Q16773

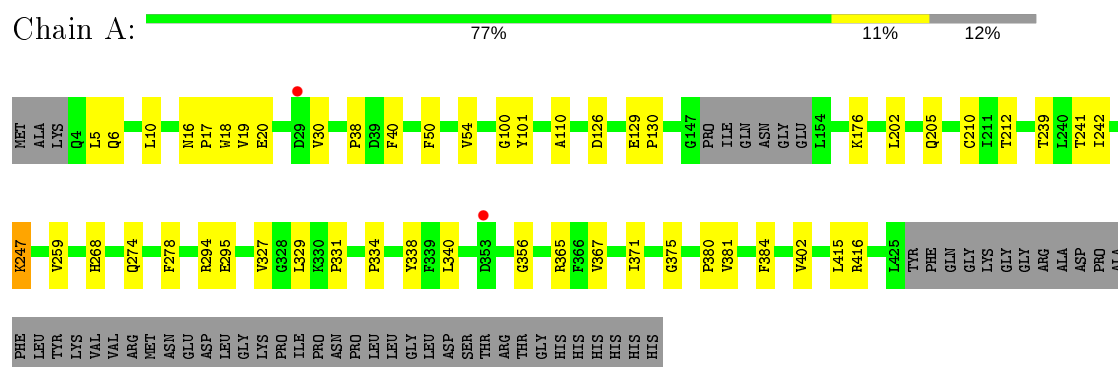
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	26	Total O 26 26	0	0
2	B	24	Total O 24 24	0	0
2	C	32	Total O 32 32	0	0
2	D	33	Total O 33 33	0	0

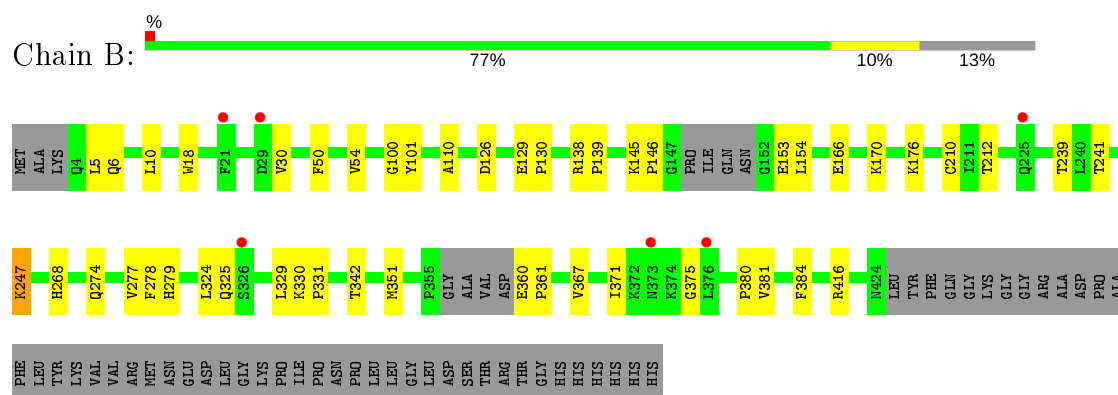
3 Residue-property plots

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.

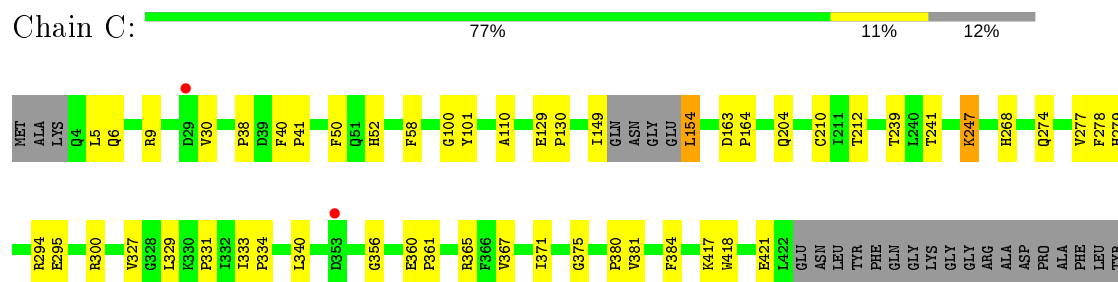
- Molecule 1: Kynurenine--oxoglutarate transaminase 1



- Molecule 1: Kynurenine--oxoglutarate transaminase 1



- Molecule 1: Kynurenine--oxoglutarate transaminase 1



LYS
VAL
VAL
VAL
ARG
MET
ASN
GLU
ASP
LEU
GLY
LYS
PRO
ILE
PRO
ASN
PRO
LEU
LEU
GLY
LEU
ASP
SER
THR
ARG
THR
GLY
HIS
HIS
HIS
HIS
HIS

● Molecule 1: Kynurenine-oxoglutarate transaminase 1

Chain D:

76%

11%

12%

MET
ALA
LYS
Q4
L5
Q6
L10
I13
H28
D28
V30
P41
F50
F88
F80
G100
Y101
Q109
I120
E129
P130
M134
R138
P139
G147
PRO
ILE
GLN
ASN
GLY
E153
S156
M159
D163
P164
K176
C210
E211
T212
Q217

H226
T239
L240
T241
K247
H268
Q274
V277
F278
H279
L329
K330
P331
P334
L340
G356
D359
E360
P361
R364
R365
F366
V367
I371
G375
I379
P380
V381
F384
R398
Q409
E413
R416
R424
LEU
TYR
PHE
GLN
GLY

LYS
GLY
GLY
ARG
ALA
ASP
PRO
ALA
PHE
LEU
TYR
LYS
VAL
VAL
ARG
MET
ASN
GLU
ASP
LEU
GLY
LYS
PRO
ILE
PRO
ASN
PRO
LEU
LEU
GLY
LEU
ASP
SER
THR
ARG
THR
GLY
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	231.15Å 231.15Å 56.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.94 – 3.00 48.94 – 2.99	Depositor EDS
% Data completeness (in resolution range)	93.8 (48.94-3.00) 93.8 (48.94-2.99)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.234 , 0.267 0.241 , 0.267	Depositor DCC
R_{free} test set	1680 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	59.3	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 19.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.047 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13483	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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](#)

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

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	0.22	0/3419	0.40	0/4639
1	B	0.22	0/3399	0.40	0/4609
1	C	0.22	0/3410	0.41	0/4628
1	D	0.22	0/3420	0.41	0/4640
All	All	0.22	0/13648	0.41	0/18516

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	3349	0	3277	30	0
1	B	3330	0	3253	29	0
1	C	3339	0	3272	27	2
1	D	3350	0	3272	33	1
2	A	26	0	0	3	0
2	B	24	0	0	2	0
2	C	32	0	0	0	0
2	D	33	0	0	4	0
All	All	13483	0	13074	105	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 4.

The worst 5 of 105 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:153:GLU:OE1	1:B:325:GLN:NE2	2.13	0.80
1:D:416:ARG:NH1	2:D:501:HOH:O	2.19	0.74
1:A:100:GLY:N	1:A:247:LLP:OP1	2.24	0.68
1:B:30:VAL:HG12	1:B:375:GLY:HA2	1.74	0.68
1:C:356:GLY:HA3	1:C:365:ARG:HD3	1.78	0.66

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:C:52:HIS:NE2	1:D:359:ASP:OD1[1_554]	2.16	0.04
1:C:204:GLN:O	1:C:300:ARG:NH1[4_545]	2.19	0.01

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	411/472 (87%)	399 (97%)	12 (3%)	0	100	100
1	B	406/472 (86%)	393 (97%)	13 (3%)	0	100	100
1	C	410/472 (87%)	399 (97%)	11 (3%)	0	100	100
1	D	411/472 (87%)	399 (97%)	12 (3%)	0	100	100
All	All	1638/1888 (87%)	1590 (97%)	48 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	363/409 (89%)	361 (99%)	2 (1%)	86	95
1	B	361/409 (88%)	359 (99%)	2 (1%)	86	95
1	C	362/409 (88%)	358 (99%)	4 (1%)	73	90
1	D	363/409 (89%)	361 (99%)	2 (1%)	86	95
All	All	1449/1636 (89%)	1439 (99%)	10 (1%)	84	94

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	50	PHE
1	C	101	TYR
1	C	154	LEU
1	B	101	TYR
1	C	149	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	51	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	LLP	A	247	1	23,24,25	0.99	1 (4%)	25,32,34	1.36	4 (16%)
1	LLP	D	247	1	23,24,25	0.96	1 (4%)	25,32,34	1.36	4 (16%)
1	LLP	B	247	1	23,24,25	0.96	1 (4%)	25,32,34	1.41	4 (16%)
1	LLP	C	247	1	23,24,25	0.96	1 (4%)	25,32,34	1.38	4 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	A	247	1	-	6/16/17/19	0/1/1/1
1	LLP	D	247	1	-	5/16/17/19	0/1/1/1
1	LLP	B	247	1	-	5/16/17/19	0/1/1/1
1	LLP	C	247	1	-	8/16/17/19	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	247	LLP	C3-C2	2.89	1.43	1.40
1	D	247	LLP	C3-C2	2.77	1.43	1.40
1	B	247	LLP	C3-C2	2.73	1.43	1.40
1	C	247	LLP	C3-C2	2.71	1.43	1.40

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	247	LLP	OP2-P-OP1	2.65	121.06	110.68
1	D	247	LLP	OP2-P-OP1	2.60	120.87	110.68
1	D	247	LLP	OP4-P-OP1	2.60	113.76	106.47
1	C	247	LLP	OP4-P-OP1	2.59	113.73	106.47
1	B	247	LLP	OP4-P-OP1	2.58	113.71	106.47

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	247	LLP	C5'-OP4-P-OP1
1	A	247	LLP	C5'-OP4-P-OP2
1	D	247	LLP	C5'-OP4-P-OP1
1	D	247	LLP	C5'-OP4-P-OP2
1	D	247	LLP	C5'-OP4-P-OP3

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	247	LLP	1	0
1	D	247	LLP	1	0
1	B	247	LLP	1	0
1	C	247	LLP	1	0

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, 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	415/472 (87%)	-0.19	2 (0%) 91 75	39, 51, 80, 93	4 (0%)
1	B	412/472 (87%)	-0.16	6 (1%) 73 46	38, 54, 83, 102	6 (1%)
1	C	414/472 (87%)	-0.27	2 (0%) 91 75	38, 48, 75, 94	4 (0%)
1	D	415/472 (87%)	-0.28	2 (0%) 91 75	37, 47, 69, 100	5 (1%)
All	All	1656/1888 (87%)	-0.22	12 (0%) 87 69	37, 50, 81, 102	19 (1%)

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	376	LEU	2.8
1	B	326	SER	2.8
1	A	29	ASP	2.4
1	B	373	ASN	2.4
1	C	29	ASP	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	LLP	B	247	24/25	0.94	0.18	40,44,46,49	0
1	LLP	D	247	24/25	0.95	0.15	38,43,49,55	0
1	LLP	A	247	24/25	0.95	0.16	41,43,45,52	0
1	LLP	C	247	24/25	0.95	0.16	41,43,46,47	0

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.