



# wwPDB X-ray Structure Validation Summary Report

Nov 12, 2014 – 05:26 PM EST

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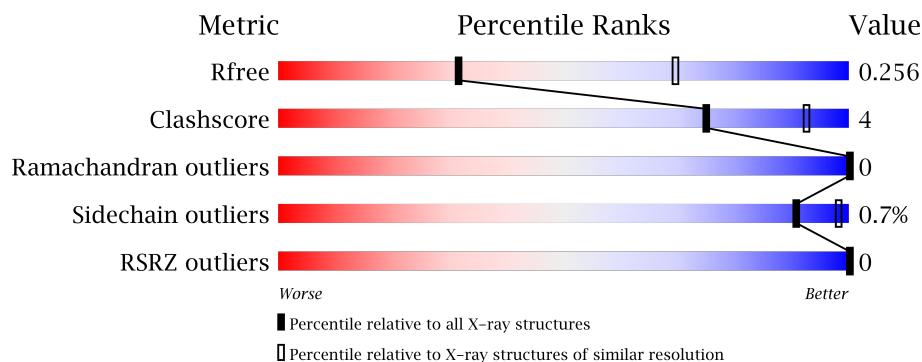
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable24195  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.1.3  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable24195

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (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  $\geq 3$ , 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.

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 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 Kynurenine--oxoglutaratetransaminase 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

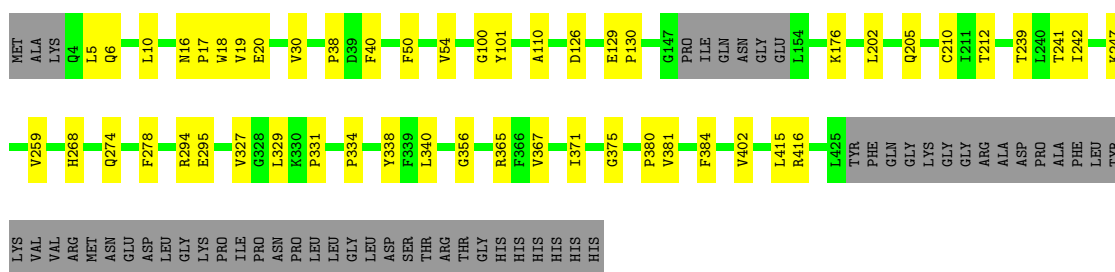


### 3 Residue-property plots

These plots are drawn for all protein, RNA 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.

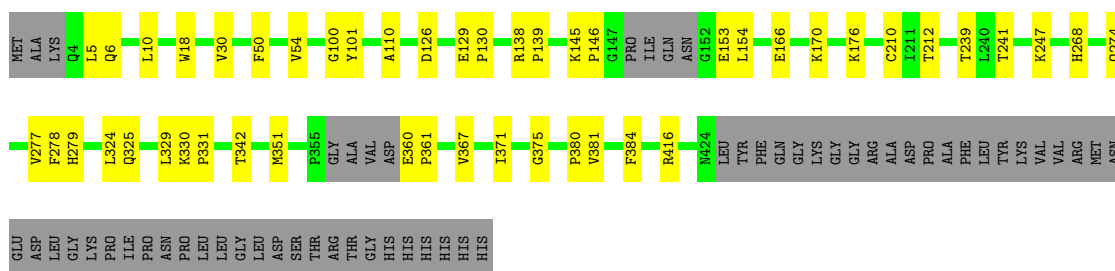
#### • Molecule 1: Kynurenine--oxoglutaratetransaminase 1

Chain A:



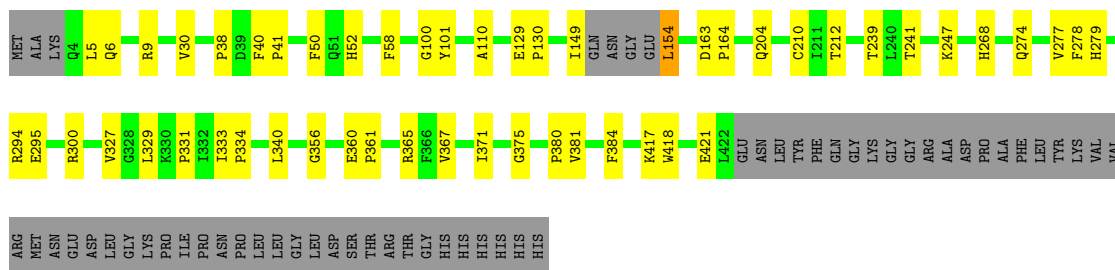
#### • Molecule 1: Kynurenine--oxoglutaratetransaminase 1

Chain B:



#### • Molecule 1: Kynurenine--oxoglutaratetransaminase 1

Chain C:



#### • Molecule 1: Kynurenine--oxoglutaratetransaminase 1

Chain D:

GLY	ARG	T239	MET
ALA	ALA	L240	ALA
ASP	ASP	T241	LYS
PRO	PRO	K247	Q4
PHE	PHE	H288	L5
LEU	LEU	H288	Q6
TYR	TYR	Q274	L10
LYS	LYS	V277	I13
VAL	VAL	F278	V30
ARG	ARG	H279	P41
MET	MET	L329	F50
ASN	ASN	K330	F58
GLU	GLU	P331	F80
ASP	ASP	P334	G100
LEU	LEU	L340	Y101
GLY	GLY	G356	Q109
LYS	LYS	D359	I120
PRO	PRO	E360	E129
ILE	ILE	P361	P130
PRO	PRO	R364	M134
ASN	ASN	R365	R138
PRO	PRO	F366	P139
LEU	LEU	V367	G147
LEU	LEU	I371	PRO
GLY	GLY	G375	ILE
HIS	HIS	I379	GLN
HIS	HIS	P380	ASN
HIS	HIS	V381	GLY
HIS	HIS	F384	E153
		R398	S156
		Q409	N159
		E413	D163
		R416	P164
		N424	K176
		LEU	C210
		TYR	T211
		PHE	T212
		GLN	Q217
		GLY	LYS
		LYS	H226

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.42 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.234 , 0.267 0.229 , 0.256	Depositor DCC
$R_{free}$ test set	1652 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	59.3	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 18.4	EDS
Estimated twinning fraction	0.047 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 33359 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	13483	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IT1

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 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	3349	0	3276	30	0
1	B	3330	0	3252	29	0
1	C	3339	0	3271	27	2
1	D	3350	0	3271	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13483	0	13070	105	2

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 4.

The worst 5 of 105 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:IT1: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	Distance(Å)	Clash(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

### 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	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 ⓘ

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%)	92	98
1	B	361/409 (88%)	359 (99%)	2 (1%)	92	98
1	C	362/409 (88%)	358 (99%)	4 (1%)	84	97
1	D	363/409 (89%)	361 (99%)	2 (1%)	92	98
All	All	1449/1636 (89%)	1439 (99%)	10 (1%)	91	98

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 ⓘ

There are no RNA chains in this entry.

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

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	IT1	A	247	1	24,24,25	3.91	2 (8%)	30,32,34	1.37	4 (13%)
1	IT1	B	247	1	24,24,25	3.90	2 (8%)	30,32,34	1.43	5 (16%)
1	IT1	C	247	1	24,24,25	3.91	2 (8%)	30,32,34	1.39	4 (13%)
1	IT1	D	247	1	24,24,25	3.89	2 (8%)	30,32,34	1.37	4 (13%)

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	IT1	A	247	1	-	0/15/17/19	0/1/1/1
1	IT1	B	247	1	-	0/15/17/19	0/1/1/1
1	IT1	C	247	1	-	0/15/17/19	0/1/1/1
1	IT1	D	247	1	-	0/15/17/19	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	247	IT1	O-C	18.26	1.24	1.11
1	B	247	IT1	O-C	18.20	1.23	1.11
1	A	247	IT1	O-C	18.19	1.23	1.11
1	D	247	IT1	O-C	18.16	1.23	1.11
1	A	247	IT1	C3-C2	4.29	1.43	1.40

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	247	IT1	OP2-P-OP1	3.27	121.06	110.36
1	D	247	IT1	OP2-P-OP1	3.21	120.87	110.36
1	C	247	IT1	OP2-P-OP1	3.16	120.69	110.36
1	A	247	IT1	OP2-P-OP1	3.14	120.62	110.36
1	C	247	IT1	C2A-C2-C3	-2.64	117.87	121.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	416/472 (88%)	-0.15	0 100 100	39, 51, 80, 93	4 (0%)
1	B	413/472 (87%)	-0.13	0 100 100	38, 54, 83, 102	6 (1%)
1	C	415/472 (87%)	-0.21	0 100 100	38, 48, 75, 94	4 (0%)
1	D	416/472 (88%)	-0.22	0 100 100	37, 47, 69, 100	5 (1%)
All	All	1660/1888 (87%)	-0.18	0 100 100	37, 50, 81, 102	19 (1%)

There are no RSRZ outliers to report.

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	IT1	C	247	24/25	0.17	0.01	41,43,46,47	0
1	IT1	B	247	24/25	0.19	-0.23	40,44,46,49	0
1	IT1	A	247	24/25	0.16	-1.00	41,43,45,52	0
1	IT1	D	247	24/25	0.16	-1.06	38,43,49,55	0

### 6.3 Carbohydrates ⓘ

There are no carbohydrates 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.