



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:02 PM GMT

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 Full wwPDB X-ray Structure Validation 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/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

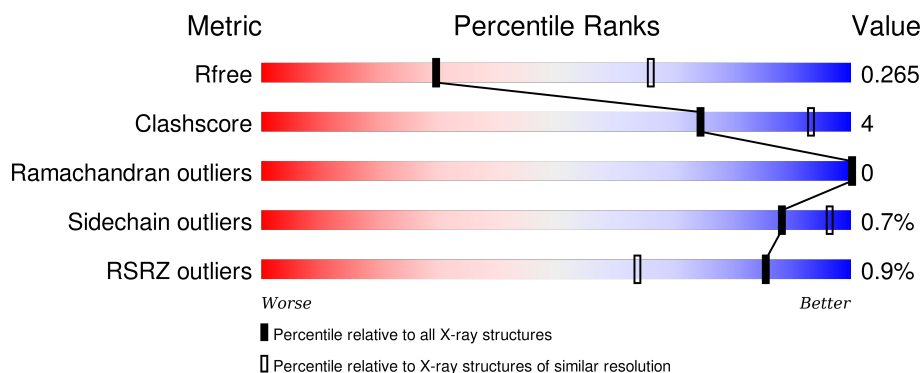
# 1 Overall quality at a glance

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))
$R_{free}$	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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. 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	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>11%</div> <div>12%</div> </div> </div>
1	B	472	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>10%</div> <div>13%</div> </div> </div>
1	C	472	<div> <div></div> <div> <div></div> <div>77%</div> <div>11%</div> <div>12%</div> </div> </div>
1	D	472	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>12%</div> <div>12%</div> </div> </div>

## 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

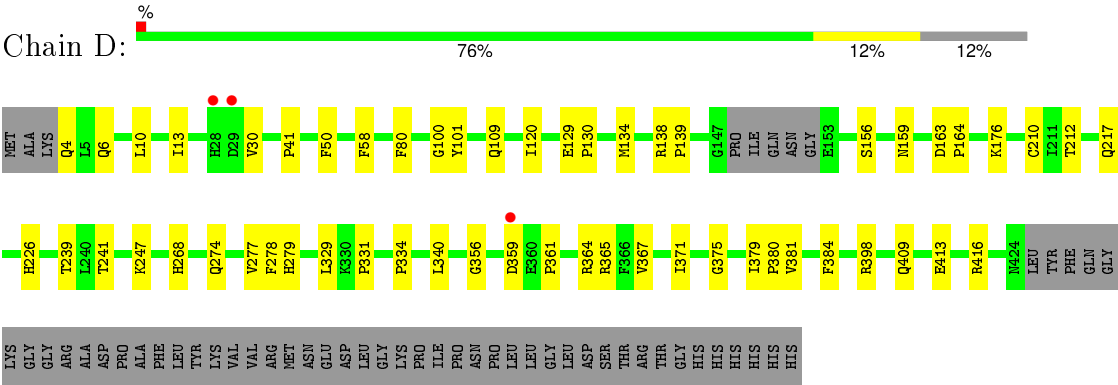
- Molecule 2 is water.

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





● Molecule 1: Kynurenine--oxoglutarate transaminase 1



## 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 0.235 , 0.265	Depositor DCC
$R_{free}$ test set	1665 reflections (5.31%)	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 , 19.4	EDS
Estimated twinning fraction	0.047 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	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.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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 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	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
All	All	13483	0	13070	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.

All (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: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
1:A:416:ARG:NH1	2:A:501:HOH:O	2.26	0.64
1:B:18:TRP:NE1	1:B:126:ASP:OD2	2.30	0.64
1:D:30:VAL:HG11	1:D:371:ILE:HG23	1.81	0.63
1:D:356:GLY:HA3	1:D:365:ARG:HD3	1.79	0.63
1:A:268:HIS:NE2	1:B:6:GLN:OE1	2.32	0.63
1:A:30:VAL:HG11	1:A:371:ILE:HG23	1.82	0.61
1:C:6:GLN:OE1	1:D:268:HIS:NE2	2.34	0.61
1:D:30:VAL:HG12	1:D:375:GLY:HA2	1.83	0.61
1:A:30:VAL:HG12	1:A:375:GLY:HA2	1.83	0.61
1:D:210:CYS:HB3	1:D:239:THR:HG22	1.83	0.60
1:D:409:GLN:NE2	2:D:502:HOH:O	2.34	0.60
1:A:6:GLN:OE1	1:B:268:HIS:NE2	2.35	0.59
1:A:210:CYS:HB3	1:A:239:THR:HG22	1.83	0.59
1:D:367:VAL:HG21	1:D:380:PRO:HD3	1.85	0.57
1:B:416:ARG:NH1	2:B:514:HOH:O	2.39	0.56
1:C:210:CYS:HB3	1:C:239:THR:HG22	1.87	0.56
1:B:30:VAL:HG11	1:B:371:ILE:HG23	1.88	0.56
1:C:30:VAL:HG12	1:C:375:GLY:HA2	1.88	0.55
1:D:100:GLY:N	1:D:247:IT1:OP1	2.28	0.55
1:B:367:VAL:HG21	1:B:380:PRO:HD3	1.88	0.55
1:B:329:LEU:O	1:B:331:PRO:HD3	2.07	0.54
1:B:381:VAL:HA	1:B:384:PHE:HD2	1.72	0.54
1:D:361:PRO:HG2	1:D:364:ARG:HG3	1.90	0.54
1:C:100:GLY:N	1:C:247:IT1:OP1	2.30	0.53
1:B:210:CYS:HB3	1:B:239:THR:HG22	1.90	0.53
1:C:417:LYS:O	1:C:421:GLU:HG2	2.09	0.52
1:B:351:MET:SD	2:B:517:HOH:O	2.59	0.52
1:C:154:LEU:HD13	1:C:333:ILE:HD11	1.90	0.51
1:D:4:GLN:N	2:D:503:HOH:O	2.44	0.50
1:C:274:GLN:HA	1:C:278:PHE:HA	1.93	0.50
1:A:202:LEU:HD23	2:A:516:HOH:O	2.10	0.50
1:C:30:VAL:HG11	1:C:371:ILE:HG23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:VAL:HG21	1:A:415:LEU:HD22	1.93	0.50
1:A:274:GLN:HA	1:A:278:PHE:HA	1.94	0.49
1:C:367:VAL:HG21	1:C:380:PRO:HD3	1.94	0.49
1:C:5:LEU:HA	1:D:176:LYS:HE3	1.94	0.49
1:A:5:LEU:HA	1:B:176:LYS:HE3	1.93	0.49
1:B:153:GLU:OE2	1:B:330:LYS:HG2	2.13	0.49
1:B:129:GLU:HB3	1:B:130:PRO:HD3	1.95	0.49
1:D:381:VAL:HA	1:D:384:PHE:HD2	1.78	0.48
1:A:381:VAL:HA	1:A:384:PHE:HD2	1.77	0.48
1:A:10:LEU:HD11	1:B:110:ALA:HA	1.95	0.48
1:A:329:LEU:O	1:A:331:PRO:HD3	2.13	0.48
1:C:129:GLU:HB3	1:C:130:PRO:HD3	1.95	0.48
1:B:100:GLY:N	1:B:247:IT1:OP1	2.36	0.48
1:C:268:HIS:NE2	1:D:6:GLN:OE1	2.47	0.48
1:A:129:GLU:HB3	1:A:130:PRO:HD3	1.95	0.48
1:C:9:ARG:NH1	1:D:109:GLN:O	2.45	0.48
1:D:379:ILE:O	1:D:398:ARG:N	2.38	0.48
1:D:413:GLU:HG2	2:D:501:HOH:O	2.14	0.48
1:C:381:VAL:HA	1:C:384:PHE:HD2	1.79	0.47
1:C:329:LEU:O	1:C:331:PRO:HD3	2.14	0.47
1:C:294:ARG:NH1	1:C:295:GLU:OE2	2.48	0.47
1:D:329:LEU:O	1:D:331:PRO:HD3	2.15	0.47
1:D:156:SER:H	1:D:159:ASN:HD21	1.61	0.47
1:B:166:GLU:O	1:B:170:LYS:HG2	2.15	0.47
1:B:274:GLN:HA	1:B:278:PHE:HA	1.97	0.47
1:A:17:PRO:O	1:A:20:GLU:HG2	2.16	0.46
1:A:367:VAL:HG21	1:A:380:PRO:HD3	1.97	0.46
1:A:356:GLY:HA3	1:A:365:ARG:HD3	1.96	0.46
1:A:18:TRP:NE1	1:A:126:ASP:OD2	2.48	0.46
1:D:129:GLU:HB3	1:D:130:PRO:HD3	1.97	0.46
1:D:80:PHE:HE1	1:D:217:GLN:HE22	1.65	0.45
1:D:217:GLN:HB2	1:D:226:HIS:CD2	2.52	0.45
1:D:274:GLN:HA	1:D:278:PHE:HA	1.98	0.44
1:C:41:PRO:HG3	1:D:58:PHE:CG	2.52	0.44
1:D:163:ASP:HA	1:D:164:PRO:HD3	1.85	0.44
1:D:120:ILE:HD12	1:D:139:PRO:HB3	1.99	0.44
1:A:16:ASN:OD1	1:A:19:VAL:HG23	2.17	0.44
1:A:242:ILE:HG12	1:A:259:VAL:HG22	1.99	0.44
1:C:277:VAL:O	1:C:279:HIS:N	2.49	0.44
1:D:138:ARG:HA	1:D:139:PRO:HD3	1.82	0.43
1:B:212:THR:HG23	1:B:241:THR:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ARG:NH1	1:A:295:GLU:OE2	2.50	0.43
1:A:338:TYR:CD1	1:A:402:VAL:HG21	2.54	0.43
1:A:205:GLN:HB3	2:A:516:HOH:O	2.17	0.43
1:B:138:ARG:HA	1:B:139:PRO:HD3	1.78	0.43
1:D:334:PRO:HG3	1:D:340:LEU:HB3	2.01	0.42
1:C:110:ALA:HA	1:D:10:LEU:HD11	2.01	0.42
1:D:13:ILE:HD13	1:D:134:MET:HB2	2.00	0.42
1:B:324:LEU:HD13	1:B:342:THR:HG21	2.01	0.42
1:A:212:THR:HG23	1:A:241:THR:HA	2.02	0.42
1:C:327:VAL:HG11	1:C:418:TRP:CD2	2.54	0.42
1:D:212:THR:HG23	1:D:241:THR:HA	2.02	0.42
1:A:176:LYS:HE3	1:B:5:LEU:HA	2.00	0.42
1:C:163:ASP:HA	1:C:164:PRO:HD3	1.87	0.41
1:D:277:VAL:O	1:D:279:HIS:N	2.50	0.41
1:C:58:PHE:CG	1:D:41:PRO:HG3	2.55	0.41
1:B:360:GLU:HA	1:B:361:PRO:HD2	1.85	0.41
1:B:277:VAL:O	1:B:279:HIS:N	2.50	0.41
1:B:145:LYS:HA	1:B:146:PRO:HD3	1.86	0.41
1:A:110:ALA:HA	1:B:10:LEU:HD11	2.03	0.41
1:C:212:THR:HG23	1:C:241:THR:HA	2.02	0.41
1:C:360:GLU:HA	1:C:361:PRO:HD2	1.90	0.41
1:A:54:VAL:HG21	1:B:54:VAL:HG21	2.03	0.41
1:A:334:PRO:HG3	1:A:340:LEU:HB3	2.03	0.41
1:C:38:PRO:HB3	1:C:40:PHE:CZ	2.56	0.40
1:C:334:PRO:HG3	1:C:340:LEU:HB3	2.03	0.40
1:A:38:PRO:HB3	1:A:40:PHE:CZ	2.57	0.40
1:B:154:LEU:HD21	1:B:331:PRO:HD2	2.03	0.40

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

### 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%)	90	97
1	B	361/409 (88%)	359 (99%)	2 (1%)	90	97
1	C	362/409 (88%)	358 (99%)	4 (1%)	80	94
1	D	363/409 (89%)	361 (99%)	2 (1%)	90	97
All	All	1449/1636 (89%)	1439 (99%)	10 (1%)	88	96

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	PHE
1	A	101	TYR

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

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 molecules 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	23,24,25	1.21	1 (4%)	28,32,34	1.42	4 (14%)
1	IT1	B	247	1	23,24,25	1.17	1 (4%)	28,32,34	1.49	6 (21%)
1	IT1	C	247	1	23,24,25	1.16	1 (4%)	28,32,34	1.44	4 (14%)
1	IT1	D	247	1	23,24,25	1.17	1 (4%)	28,32,34	1.42	4 (14%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	247	IT1	C3-C2	4.11	1.43	1.40
1	B	247	IT1	C3-C2	4.14	1.43	1.40
1	D	247	IT1	C3-C2	4.19	1.43	1.40
1	A	247	IT1	C3-C2	4.37	1.43	1.40

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	247	IT1	C2A-C2-C3	-2.63	117.87	121.04
1	D	247	IT1	C2A-C2-C3	-2.59	117.92	121.04
1	A	247	IT1	C2A-C2-C3	-2.59	117.92	121.04
1	B	247	IT1	C2A-C2-C3	-2.56	117.95	121.04
1	B	247	IT1	OP3-P-OP2	-2.27	98.74	107.38
1	C	247	IT1	OP3-P-OP2	-2.25	98.82	107.38
1	D	247	IT1	OP3-P-OP2	-2.20	98.99	107.38
1	A	247	IT1	OP3-P-OP2	-2.15	99.19	107.38
1	B	247	IT1	OP4-C5A-C5	2.04	112.36	108.99
1	B	247	IT1	C5A-C5-C4	2.17	125.11	121.47
1	A	247	IT1	OP4-P-OP1	2.56	113.65	107.14
1	B	247	IT1	OP4-P-OP1	2.58	113.71	107.14
1	C	247	IT1	OP4-P-OP1	2.59	113.73	107.14
1	D	247	IT1	OP4-P-OP1	2.60	113.76	107.14
1	A	247	IT1	OP2-P-OP1	3.12	120.62	110.58
1	C	247	IT1	OP2-P-OP1	3.14	120.69	110.58
1	D	247	IT1	OP2-P-OP1	3.20	120.87	110.58
1	B	247	IT1	OP2-P-OP1	3.26	121.06	110.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	247	IT1	1	0
1	B	247	IT1	1	0
1	C	247	IT1	1	0
1	D	247	IT1	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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

### 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	415/472 (87%)	-0.17	4 (0%) 84 60	39, 51, 80, 93	4 (0%)
1	B	412/472 (87%)	-0.14	6 (1%) 76 49	38, 54, 83, 102	6 (1%)
1	C	414/472 (87%)	-0.25	2 (0%) 91 76	38, 48, 75, 94	4 (0%)
1	D	415/472 (87%)	-0.27	3 (0%) 89 70	37, 47, 69, 100	5 (1%)
All	All	1656/1888 (87%)	-0.21	15 (0%) 85 64	37, 50, 81, 102	19 (1%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	376	LEU	2.9
1	B	326	SER	2.9
1	A	29	ASP	2.5
1	B	373	ASN	2.4
1	C	29	ASP	2.3
1	B	29	ASP	2.3
1	A	353	ASP	2.3
1	D	29	ASP	2.1
1	D	28	HIS	2.1
1	C	353	ASP	2.1
1	B	21	PHE	2.1
1	B	225	GLN	2.1
1	A	26	SER	2.1
1	D	359	ASP	2.0
1	A	424	ASN	2.0

### 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	IT1	B	247	24/25	0.94	0.18	-	40,44,46,49	0
1	IT1	C	247	24/25	0.95	0.16	-	41,43,46,47	0
1	IT1	A	247	24/25	0.95	0.16	-	41,43,45,52	0
1	IT1	D	247	24/25	0.95	0.15	-	38,43,49,55	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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.