



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:31 AM GMT

PDB ID : 3B46  
Title : Crystal Structure of Bna3p, a Putative Kynurenine Aminotransferase from *Saccharomyces cerevisiae*  
Authors : Wogulis, M.  
Deposited on : 2007-10-23  
Resolution : 2.00 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

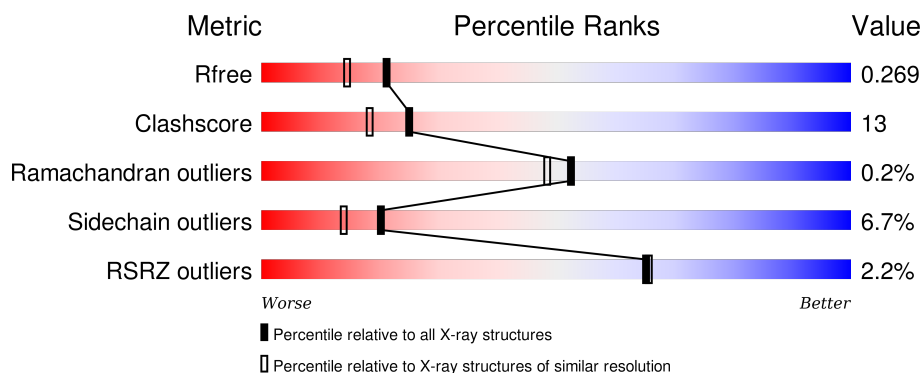
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

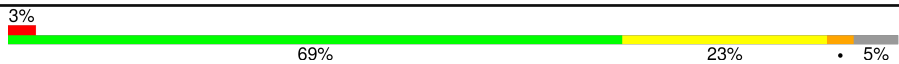
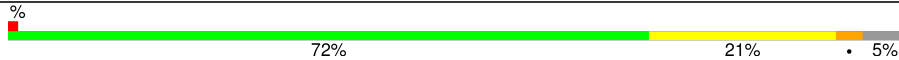
The reported resolution of this entry is 2.00 Å.

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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	447	
1	B	447	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7010 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 Aminotransferase BNA3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	P	S	0	0	0
			3380	2183	549	638	1	9			
1	B	425	Total	C	N	O	P	S	0	0	0
			3388	2187	551	640	1	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	ALA	-	EXPRESSION TAG	UNP P47039
A	-1	GLY	-	EXPRESSION TAG	UNP P47039
A	0	HIS	-	EXPRESSION TAG	UNP P47039
B	-2	ALA	-	EXPRESSION TAG	UNP P47039
B	-1	GLY	-	EXPRESSION TAG	UNP P47039
B	0	HIS	-	EXPRESSION TAG	UNP P47039

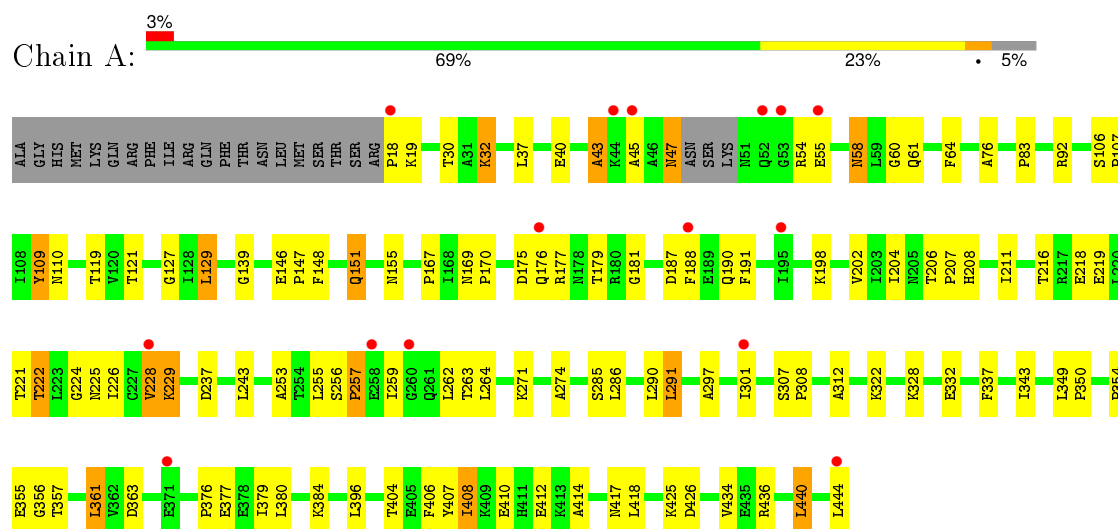
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	94	Total	O	0	0
			94	94		
2	B	148	Total	O	0	0
			148	148		

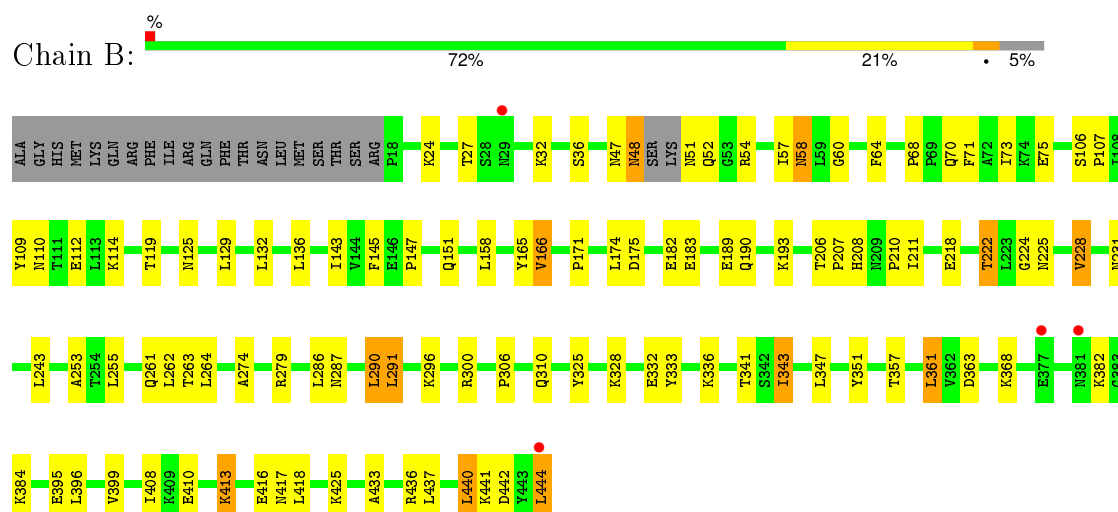
### 3 Residue-property plots

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: Aminotransferase BNA3



#### • Molecule 1: Aminotransferase BNA3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.78Å 66.52Å 115.20Å 90.00° 90.75° 90.00°	Depositor
Resolution (Å)	28.80 – 2.00 43.54 – 1.95	Depositor EDS
% Data completeness (in resolution range)	95.8 (28.80-2.00) 94.3 (43.54-1.95)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.40 (at 1.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.227 , 0.271 0.226 , 0.269	Depositor DCC
$R_{free}$ test set	2211 reflections (4.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.9	Xtriage
Anisotropy	0.535	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 52.1	EDS
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 60594 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7010	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% 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

### 5.1 Standard geometry

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	0.46	1/3435 (0.0%)	0.70	1/4667 (0.0%)
1	B	0.49	0/3443	0.70	1/4678 (0.0%)
All	All	0.47	1/6878 (0.0%)	0.70	2/9345 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	43	ALA	CA-CB	6.46	1.66	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	TYR	N-CA-C	-6.62	93.13	111.00
1	B	112	GLU	N-CA-C	-5.16	97.08	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	333	TYR	Sidechain

## 5.2 Too-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 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	3380	0	3363	89	0
1	B	3388	0	3369	86	0
2	A	94	0	0	3	0
2	B	148	0	0	5	0
All	All	7010	0	6732	172	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 13.

All (172) 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:A:54:ARG:HD3	1:A:436:ARG:CZ	1.99	0.93
1:A:218:GLU:O	1:A:222:THR:HG22	1.70	0.91
1:B:218:GLU:O	1:B:222:THR:HG22	1.83	0.78
1:A:384:LYS:HE2	1:A:417:ASN:ND2	1.97	0.78
1:A:58:ASN:ND2	1:A:60:GLY:H	1.82	0.78
1:A:175:ASP:HB3	1:A:363:ASP:OD2	1.85	0.77
1:B:175:ASP:HB3	1:B:363:ASP:OD2	1.83	0.77
1:A:208:HIS:HD2	1:A:211:ILE:H	1.34	0.75
1:A:377:GLU:HA	1:A:380:LEU:HD11	1.67	0.75
1:A:396:LEU:CD2	1:A:440:LEU:HD13	2.16	0.75
1:A:377:GLU:HA	1:A:380:LEU:CD1	2.15	0.74
1:A:58:ASN:HD22	1:A:60:GLY:H	1.36	0.74
1:B:58:ASN:HD22	1:B:60:GLY:H	1.38	0.71
1:A:396:LEU:HD21	1:A:440:LEU:HD13	1.72	0.71
1:A:343:ILE:HD12	1:A:434:VAL:O	1.92	0.70
1:A:225:ASN:O	1:A:229:LYS:HD3	1.92	0.70
1:B:57:ILE:HD13	1:B:433:ALA:HA	1.75	0.69
1:B:125:ASN:HD21	1:B:279:ARG:NH2	1.91	0.68
1:B:64:PHE:CE1	1:B:274:ALA:HA	2.29	0.68
1:B:165:TYR:CE1	1:B:408:ILE:HD13	2.31	0.66
1:B:211:ILE:HA	1:B:361:LEU:HD22	1.77	0.66
1:B:68:PRO:HG2	1:B:73:ILE:HD11	1.79	0.65
1:A:54:ARG:HD3	1:A:436:ARG:NH1	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:THR:HG23	1:A:219:GLU:OE1	1.97	0.64
1:B:58:ASN:ND2	1:B:60:GLY:H	1.95	0.64
1:A:170:PRO:HG2	1:A:414:ALA:HB1	1.80	0.64
1:A:376:PRO:HD2	1:A:379:ILE:HD11	1.79	0.64
1:B:384:LYS:HD3	1:B:417:ASN:ND2	2.13	0.64
1:B:396:LEU:CD2	1:B:440:LEU:HD13	2.29	0.63
1:B:165:TYR:CZ	1:B:408:ILE:HD13	2.34	0.63
1:B:396:LEU:HD22	1:B:440:LEU:HD13	1.80	0.63
1:A:32:LYS:HD3	1:A:37:LEU:HD21	1.80	0.63
1:A:64:PHE:CE1	1:A:274:ALA:HA	2.35	0.62
1:B:208:HIS:HD2	1:B:211:ILE:H	1.47	0.61
1:A:384:LYS:HE2	1:A:417:ASN:HD21	1.64	0.61
1:A:129:LEU:HD13	1:A:301:ILE:HD13	1.83	0.60
1:B:343:ILE:HD12	1:B:437:LEU:HB2	1.83	0.60
1:B:343:ILE:HD12	1:B:437:LEU:CB	2.32	0.60
1:A:45:ALA:O	1:A:47:ASN:N	2.33	0.60
1:A:181:GLY:HA3	1:A:355:GLU:CD	2.23	0.59
1:B:132:LEU:O	1:B:136:LEU:HG	2.04	0.57
1:B:224:GLY:O	1:B:228:VAL:HG12	2.03	0.57
1:A:225:ASN:HA	1:A:228:VAL:HG13	1.86	0.57
1:A:147:PRO:HG3	1:A:407:TYR:CE2	2.40	0.57
1:B:408:ILE:HG23	1:B:410:GLU:HG2	1.87	0.56
1:B:182:GLU:HG3	2:B:549:HOH:O	2.06	0.56
1:B:343:ILE:CD1	1:B:347:LEU:HD11	2.36	0.56
1:A:404:THR:CG2	1:A:412:GLU:HG3	2.36	0.56
1:A:61:GLN:HE21	1:A:425:LYS:NZ	2.03	0.56
1:A:146:GLU:OE1	1:A:167:PRO:HG3	2.06	0.55
1:A:32:LYS:HD3	1:A:37:LEU:CD2	2.36	0.55
1:A:396:LEU:HD22	1:A:440:LEU:HD13	1.85	0.55
1:A:106:SER:O	1:A:109:TYR:O	2.24	0.55
1:B:190:GLN:NE2	2:B:504:HOH:O	2.39	0.55
1:A:337:PHE:CE2	1:A:354:PRO:HG2	2.42	0.55
1:A:61:GLN:NE2	1:A:425:LYS:NZ	2.55	0.55
1:A:377:GLU:HA	1:A:380:LEU:HD12	1.89	0.55
1:B:384:LYS:HD3	1:B:417:ASN:HD21	1.72	0.54
1:A:208:HIS:CD2	1:A:211:ILE:H	2.20	0.54
1:A:61:GLN:HE21	1:A:425:LYS:HZ1	1.55	0.54
1:A:54:ARG:HG2	1:A:436:ARG:NH2	2.23	0.54
1:B:325:TYR:HA	1:B:328:LYS:HE2	1.90	0.53
1:A:253:ALA:HB2	1:A:263:THR:HG21	1.89	0.53
1:B:413:LYS:O	1:B:416:GLU:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:PHE:CD2	1:B:166:VAL:HG13	2.45	0.52
1:B:287:ASN:CG	1:B:290:LEU:HB2	2.30	0.52
1:A:218:GLU:O	1:A:222:THR:CG2	2.52	0.51
1:B:253:ALA:HB2	1:B:263:THR:HG21	1.93	0.51
1:A:222:THR:O	1:A:226:ILE:HG13	2.11	0.51
1:A:40:GLU:O	1:A:43:ALA:HB3	2.11	0.51
1:B:54:ARG:HD3	1:B:436:ARG:CZ	2.41	0.51
1:A:181:GLY:HA3	1:A:355:GLU:OE1	2.12	0.50
1:A:408:ILE:CG2	1:A:410:GLU:HG3	2.40	0.50
1:A:187:ASP:HB3	1:A:190:GLN:HE21	1.76	0.50
1:A:363:ASP:HA	1:A:418:LEU:HD23	1.93	0.50
1:A:55:GLU:HG3	1:A:55:GLU:O	2.13	0.49
1:B:125:ASN:HD21	1:B:279:ARG:HH22	1.58	0.49
1:B:145:PHE:HA	1:B:166:VAL:O	2.13	0.49
1:B:425:LYS:HE3	2:B:520:HOH:O	2.12	0.49
1:A:139:GLY:O	1:A:198:LYS:HE2	2.13	0.49
1:B:408:ILE:CG2	1:B:410:GLU:HG2	2.43	0.49
1:B:343:ILE:HD13	1:B:347:LEU:HD11	1.92	0.49
1:B:48:ASN:HD22	1:B:51:ASN:N	2.11	0.48
1:A:61:GLN:NE2	1:A:425:LYS:HZ3	2.11	0.48
1:A:54:ARG:HD3	1:A:436:ARG:NE	2.26	0.48
1:B:68:PRO:HG2	1:B:73:ILE:CD1	2.44	0.48
1:B:47:ASN:O	1:B:52:GLN:HG2	2.13	0.48
1:A:18:PRO:HG2	1:B:262:LEU:HG	1.96	0.47
1:B:225:ASN:HA	1:B:228:VAL:CG1	2.45	0.47
1:B:48:ASN:ND2	1:B:51:ASN:N	2.62	0.47
1:B:171:PRO:HG3	1:B:183:GLU:CB	2.44	0.47
1:B:54:ARG:HD2	1:B:436:ARG:NH1	2.30	0.47
1:A:307:SER:HB2	1:A:308:PRO:HD3	1.97	0.47
1:A:204:ILE:HD12	2:A:455:HOH:O	2.14	0.46
1:B:410:GLU:CD	1:B:410:GLU:H	2.18	0.46
1:A:54:ARG:CD	1:A:436:ARG:CZ	2.83	0.46
1:A:92:ARG:HH22	1:A:291:LEU:HD13	1.80	0.46
1:B:109:TYR:HD2	1:B:286:LEU:HD21	1.80	0.46
1:B:54:ARG:CD	1:B:436:ARG:NH1	2.79	0.46
1:A:151:GLN:HE21	1:A:151:GLN:HA	1.81	0.46
1:B:332:GLU:O	1:B:336:LYS:HG3	2.15	0.45
1:A:224:GLY:O	1:A:228:VAL:HG12	2.17	0.45
1:A:404:THR:HB	1:A:412:GLU:HG3	1.98	0.45
1:B:125:ASN:ND2	1:B:279:ARG:HH22	2.14	0.45
1:B:343:ILE:HD13	1:B:347:LEU:CD1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ALA:HA	1:A:312:ALA:HB2	1.97	0.45
1:B:58:ASN:C	1:B:58:ASN:HD22	2.19	0.45
1:B:106:SER:N	1:B:107:PRO:HD2	2.32	0.45
1:A:187:ASP:HB3	1:A:190:GLN:HB3	1.98	0.45
1:B:382:LYS:NZ	2:B:542:HOH:O	2.50	0.45
1:B:306:PRO:O	1:B:310:GLN:HG3	2.16	0.44
1:A:297:ALA:O	1:A:301:ILE:HG13	2.17	0.44
1:A:356:GLY:C	1:A:357:THR:HG23	2.38	0.44
1:B:228:VAL:HA	1:B:262:LEU:CD1	2.47	0.44
1:A:45:ALA:C	1:A:47:ASN:N	2.71	0.44
1:B:109:TYR:CD2	1:B:286:LEU:HD21	2.53	0.44
1:B:444:LEU:O	1:B:444:LEU:HD13	2.17	0.44
1:A:147:PRO:O	1:A:208:HIS:CE1	2.70	0.44
1:B:143:ILE:HG23	1:B:166:VAL:HG12	1.99	0.44
1:A:376:PRO:HD2	1:A:379:ILE:CD1	2.46	0.43
1:B:54:ARG:CD	1:B:436:ARG:CZ	2.95	0.43
1:B:441:LYS:HG3	1:B:442:ASP:N	2.33	0.43
1:B:264:LEU:HD21	1:B:290:LEU:HD13	2.00	0.43
1:A:264:LEU:HD23	1:A:285:SER:HB2	2.00	0.43
1:B:125:ASN:ND2	1:B:279:ARG:NH2	2.62	0.43
1:B:341:THR:HB	1:B:351:TYR:CZ	2.53	0.43
1:A:18:PRO:HB3	1:B:231:ASN:OD1	2.19	0.43
1:B:171:PRO:HG3	1:B:183:GLU:HB3	2.00	0.43
1:A:219:GLU:O	1:A:222:THR:HG23	2.18	0.43
1:A:440:LEU:HA	1:A:440:LEU:HD12	1.91	0.43
1:A:256:SER:O	1:A:259:ILE:N	2.50	0.43
1:B:243:LEU:HD22	1:B:357:THR:N	2.34	0.43
1:B:24:LYS:HA	1:B:27:THR:OG1	2.20	0.42
1:B:343:ILE:CD1	1:B:437:LEU:HB3	2.49	0.42
1:A:425:LYS:HE3	2:A:494:HOH:O	2.19	0.42
1:B:225:ASN:O	1:B:228:VAL:HG13	2.20	0.42
1:A:206:THR:HA	1:A:207:PRO:C	2.40	0.42
1:B:206:THR:HA	1:B:207:PRO:C	2.40	0.42
1:A:410:GLU:HG2	1:A:410:GLU:H	1.43	0.42
1:B:47:ASN:O	1:B:48:ASN:HB2	2.18	0.42
1:B:70:GLN:HA	1:B:70:GLN:NE2	2.35	0.42
1:B:296:LYS:O	1:B:300:ARG:HG2	2.20	0.41
1:A:237:ASP:OD2	1:A:271:LLP:N1	2.52	0.41
1:B:174:LEU:HD21	1:B:418:LEU:HD21	2.01	0.41
1:A:106:SER:HB2	1:A:107:PRO:HD3	2.03	0.41
1:B:158:LEU:HD23	1:B:158:LEU:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:PHE:CD1	1:B:274:ALA:HA	2.55	0.41
1:A:169:ASN:HA	1:A:170:PRO:HD3	1.73	0.41
1:B:343:ILE:HD11	1:B:347:LEU:HD11	2.02	0.41
1:B:147:PRO:O	1:B:208:HIS:CE1	2.74	0.41
1:A:188:PHE:HA	1:A:191:PHE:HB3	2.02	0.41
1:A:361:LEU:HA	1:A:361:LEU:HD12	1.95	0.41
1:A:190:GLN:O	1:A:190:GLN:HG2	2.20	0.41
1:A:218:GLU:HA	1:A:221:THR:HB	2.03	0.41
1:A:175:ASP:N	1:A:175:ASP:OD1	2.53	0.41
1:A:148:PHE:O	1:A:406:PHE:HB3	2.20	0.41
1:A:349:LEU:HA	1:A:350:PRO:HD3	1.93	0.41
1:A:224:GLY:O	1:A:228:VAL:CG1	2.69	0.41
1:B:425:LYS:HE2	2:B:503:HOH:O	2.21	0.41
1:A:121:THR:HG21	1:A:127:GLY:HA2	2.02	0.41
1:B:291:LEU:HD23	1:B:291:LEU:HA	1.92	0.41
1:B:218:GLU:O	1:B:222:THR:CG2	2.60	0.41
1:B:343:ILE:HD12	1:B:437:LEU:HB3	2.02	0.41
1:B:71:PHE:O	1:B:75:GLU:HG2	2.21	0.41
1:A:328:LYS:O	1:A:332:GLU:HG3	2.21	0.41
1:A:155:ASN:ND2	2:A:479:HOH:O	2.53	0.41
1:A:176:GLN:HG3	1:A:177:ARG:N	2.35	0.41
1:A:202:VAL:O	1:A:202:VAL:HG13	2.20	0.41
1:B:300:ARG:HH21	1:B:300:ARG:HG2	1.86	0.40
1:B:189:GLU:O	1:B:193:LYS:HB2	2.20	0.40
1:B:58:ASN:HA	1:B:399:VAL:HB	2.02	0.40
1:A:18:PRO:HD3	1:B:261:GLN:HB3	2.03	0.40

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	419/447 (94%)	393 (94%)	24 (6%)	2 (0%)	34	26
1	B	420/447 (94%)	405 (96%)	15 (4%)	0	100	100
All	All	839/894 (94%)	798 (95%)	39 (5%)	2 (0%)	52	48

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	257	PRO
1	A	83	PRO

### 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	366/387 (95%)	340 (93%)	26 (7%)	18	12
1	B	367/387 (95%)	344 (94%)	23 (6%)	22	16
All	All	733/774 (95%)	684 (93%)	49 (7%)	20	14

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LYS
1	A	30	THR
1	A	32	LYS
1	A	47	ASN
1	A	58	ASN
1	A	110	ASN
1	A	119	THR
1	A	129	LEU
1	A	151	GLN
1	A	179	THR
1	A	222	THR
1	A	228	VAL
1	A	229	LYS
1	A	243	LEU

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Mol	Chain	Res	Type
1	A	255	LEU
1	A	257	PRO
1	A	262	LEU
1	A	286	LEU
1	A	290	LEU
1	A	291	LEU
1	A	322	LYS
1	A	361	LEU
1	A	408	ILE
1	A	426	ASP
1	A	440	LEU
1	A	444	LEU
1	B	32	LYS
1	B	36	SER
1	B	48	ASN
1	B	58	ASN
1	B	110	ASN
1	B	114	LYS
1	B	119	THR
1	B	129	LEU
1	B	151	GLN
1	B	166	VAL
1	B	210	PRO
1	B	222	THR
1	B	228	VAL
1	B	255	LEU
1	B	290	LEU
1	B	291	LEU
1	B	343	ILE
1	B	361	LEU
1	B	368	LYS
1	B	395	GLU
1	B	413	LYS
1	B	440	LEU
1	B	444	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	61	GLN
1	A	70	GLN

*Continued on next page...*

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Mol	Chain	Res	Type
1	A	151	GLN
1	A	155	ASN
1	A	190	GLN
1	A	208	HIS
1	A	242	HIS
1	A	261	GLN
1	A	417	ASN
1	B	47	ASN
1	B	58	ASN
1	B	61	GLN
1	B	151	GLN
1	B	190	GLN
1	B	208	HIS
1	B	417	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	271	1	23,24,25	1.35	1 (4%)	28,32,34	1.69	8 (28%)
1	LLP	B	271	1	23,24,25	1.32	1 (4%)	28,32,34	1.95	11 (39%)

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	271	1	-	0/15/17/19	0/1/1/1
1	LLP	B	271	1	-	0/15/17/19	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	271	LLP	C4-C4'	-4.08	1.39	1.46
1	B	271	LLP	C4-C4'	-3.96	1.39	1.46

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	271	LLP	C5-C4-C4'	-2.85	117.41	121.52
1	B	271	LLP	O-C-CA	-2.54	118.87	125.49
1	A	271	LLP	O-C-CA	-2.26	119.60	125.49
1	B	271	LLP	OP4-P-OP1	-2.26	101.39	107.14
1	A	271	LLP	OP3-P-OP1	-2.19	103.52	110.58
1	B	271	LLP	OP3-P-OP1	-2.16	103.64	110.58
1	B	271	LLP	C5-C4-C4'	-2.11	118.48	121.52
1	A	271	LLP	OP2-P-OP1	-2.06	103.94	110.58
1	B	271	LLP	OP2-P-OP1	-2.03	104.05	110.58
1	A	271	LLP	C5'-C5-C4	2.06	124.94	121.47
1	B	271	LLP	C5'-C5-C4	2.06	124.94	121.47
1	B	271	LLP	OP4-C5'-C5	2.11	112.48	108.99
1	B	271	LLP	OP3-P-OP2	2.83	118.15	107.38
1	B	271	LLP	CG-CD-CE	2.98	126.13	113.97
1	A	271	LLP	OP3-P-OP2	3.00	118.82	107.38
1	A	271	LLP	CD-CE-NZ	3.06	116.00	110.98
1	A	271	LLP	OP2-P-OP4	3.39	116.32	106.56
1	B	271	LLP	OP2-P-OP4	3.86	117.69	106.56
1	B	271	LLP	CD-CG-CB	4.84	130.87	113.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	271	LLP	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 [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, 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	423/447 (94%)	0.36	15 (3%) 48 49	22, 45, 71, 80	0
1	B	424/447 (94%)	0.02	4 (0%) 85 86	24, 39, 58, 74	0
All	All	847/894 (94%)	0.19	19 (2%) 65 66	22, 41, 66, 80	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	371	GLU	3.7
1	A	52	GLN	3.5
1	A	176	GLN	3.4
1	A	444	LEU	3.4
1	A	53	GLY	3.3
1	A	45	ALA	3.1
1	A	228	VAL	2.8
1	B	444	LEU	2.8
1	B	29	ASN	2.8
1	A	18	PRO	2.7
1	A	260	GLY	2.7
1	B	381	ASN	2.6
1	A	301	ILE	2.5
1	B	377	GLU	2.4
1	A	188	PHE	2.4
1	A	195	ILE	2.3
1	A	44	LYS	2.3
1	A	55	GLU	2.1
1	A	258	GLU	2.1

### 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. 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	LLP	B	271	24/25	0.96	0.15	-	24,28,32,37	0
1	LLP	A	271	24/25	0.96	0.16	-	24,30,35,39	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.