



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:24 PM GMT

PDB ID : 4OUD  
Title : Engineered tyrosyl-tRNA synthetase with the nonstandard amino acid L-4,4-biphenylalanine  
Authors : Takeuchi, R.; Mandell, D.J.; Lajoie, M.J.; Church, G.M.; Stoddard, B.L.  
Deposited on : 2014-02-16  
Resolution : 2.65 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

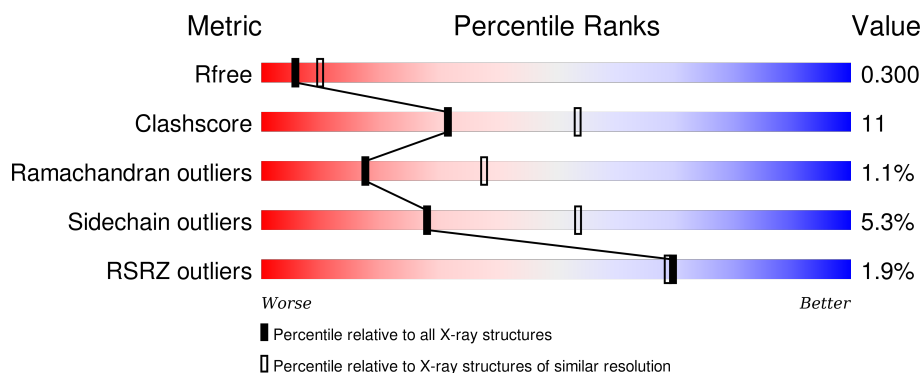
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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	425	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 16%, green 80%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>80%</span> <span>16%</span> <span>• •</span> </div> </div>
2	B	394	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 2%, yellow 23%, green 64%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>64%</span> <span>23%</span> <span>• • 9%</span> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6108 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 Tyrosyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	0	0
			3249	2060	562	614	13			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	EXPRESSION TAG	UNP U6N9P2
A	1	PRO	-	EXPRESSION TAG	UNP U6N9P2
A	49	ALA	LEU	ENGINEERED MUTATION	UNP U6N9P2
A	236	ALA	PHE	ENGINEERED MUTATION	UNP U6N9P2
A	260	ALA	TRP	ENGINEERED MUTATION	UNP U6N9P2
A	263	ALA	THR	ENGINEERED MUTATION	UNP U6N9P2
A	271	TRP	PHE	ENGINEERED MUTATION	UNP U6N9P2
A	275	GLY	PHE	ENGINEERED MUTATION	UNP U6N9P2
A	303	BIF	LEU	ENGINEERED MUTATION	UNP U6N9P2

- Molecule 2 is a protein called Tyrosyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	359	Total	C	N	O	S	0	0	0
			2789	1778	479	520	12			

There are 9 discrepancies between the modelled and reference sequences:

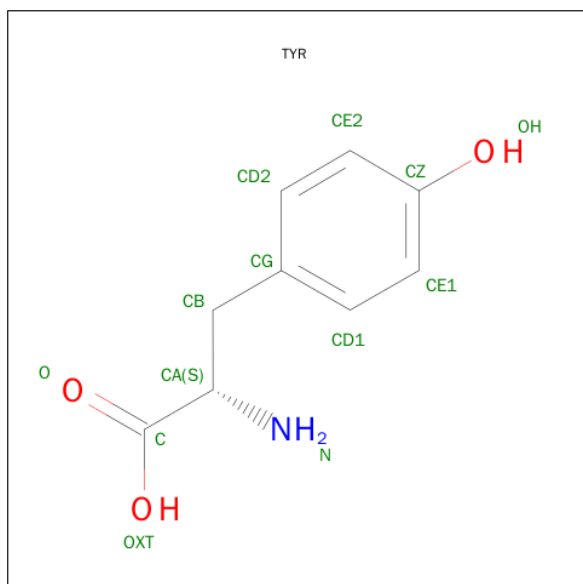
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	EXPRESSION TAG	UNP U6N9P2
B	1	PRO	-	EXPRESSION TAG	UNP U6N9P2
B	49	ALA	LEU	ENGINEERED MUTATION	UNP U6N9P2
B	236	ALA	PHE	ENGINEERED MUTATION	UNP U6N9P2
B	260	ALA	TRP	ENGINEERED MUTATION	UNP U6N9P2
B	263	ALA	THR	ENGINEERED MUTATION	UNP U6N9P2
B	271	TRP	PHE	ENGINEERED MUTATION	UNP U6N9P2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	275	GLY	PHE	ENGINEERED MUTATION	UNP U6N9P2
B	303	BIF	LEU	ENGINEERED MUTATION	UNP U6N9P2

- Molecule 3 is TYROSINE (three-letter code: TYR) (formula:  $C_9H_{11}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			13	9	1	3		

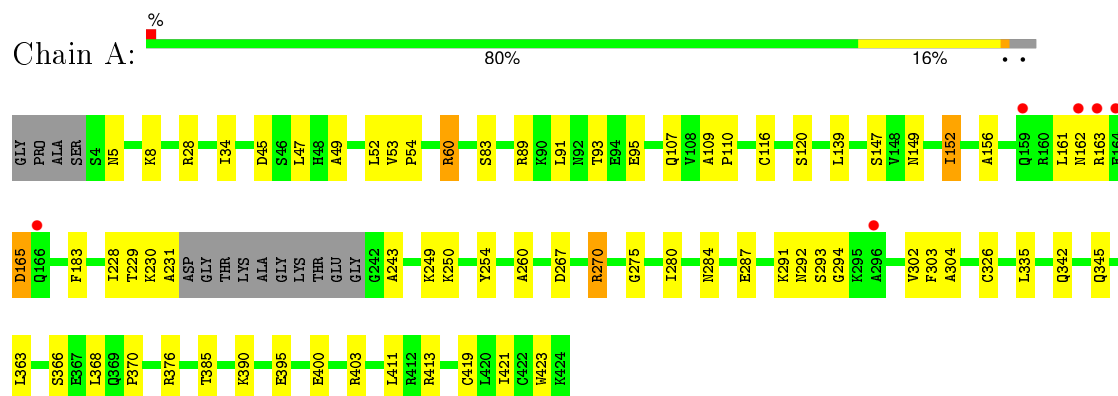
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	37	Total	O	0	0
			37	37		
4	B	20	Total	O	0	0
			20	20		

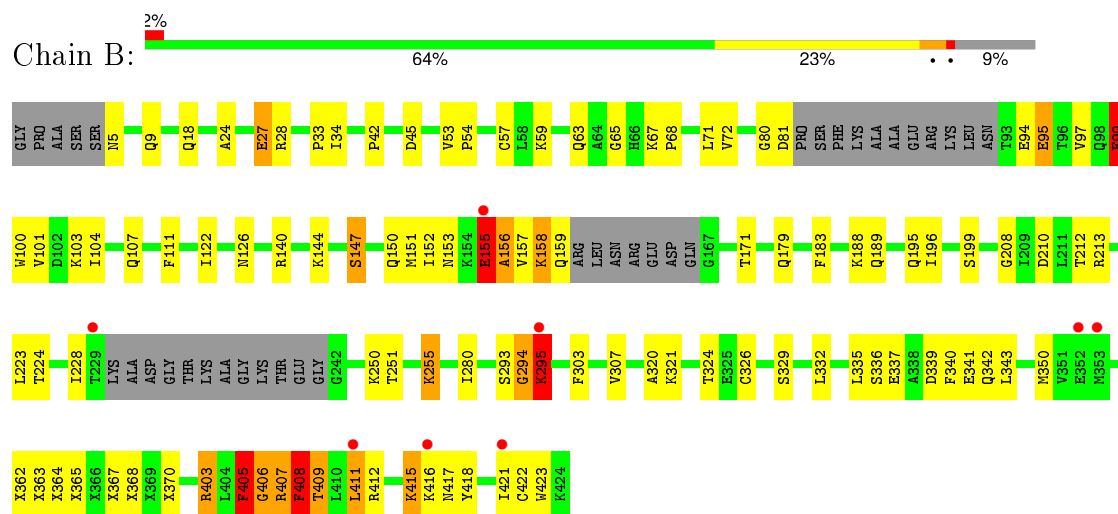
### 3 Residue-property plots [i](#)

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: Tyrosyl-tRNA synthetase



#### • Molecule 2: Tyrosyl-tRNA synthetase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.34Å 67.20Å 90.68Å 90.00° 102.65° 90.00°	Depositor
Resolution (Å)	45.00 – 2.65 44.24 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.9 (45.00-2.65) 98.9 (44.24-2.65)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.54 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.222 , 0.306 0.226 , 0.300	Depositor DCC
$R_{free}$ test set	1394 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.7	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 33.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 27806 reflections (0.007%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6108	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.55 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.0057e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: BIF

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	0.61	0/3293	0.75	2/4442 (0.0%)
2	B	0.62	0/2738	0.81	1/3694 (0.0%)
All	All	0.61	0/6031	0.78	3/8136 (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	A	0	1
2	B	0	5
All	All	0	6

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	413	ARG	NE-CZ-NH1	7.09	123.84	120.30
2	B	408	PHE	N-CA-C	-5.76	95.44	111.00
1	A	163	ARG	N-CA-C	5.03	124.57	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	162	ASN	Peptide
2	B	155	GLU	Peptide
2	B	329	SER	Peptide

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Mol	Chain	Res	Type	Group
2	B	403	ARG	Peptide
2	B	405	PHE	Peptide
2	B	406	GLY	Peptide

## 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	3249	0	3196	44	0
2	B	2789	0	2674	88	0
3	A	13	0	8	0	0
4	A	37	0	0	2	0
4	B	20	0	0	3	0
All	All	6108	0	5878	128	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 11.

All (128) 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)
2:B:407:ARG:HA	2:B:407:ARG:CZ	1.99	0.92
2:B:408:PHE:HB2	2:B:422:CYS:HA	1.51	0.88
2:B:320:ALA:O	2:B:324:THR:HG22	1.78	0.83
2:B:251:THR:HG23	2:B:255:LYS:HD2	1.62	0.81
1:A:45:ASP:OD1	1:A:250:LYS:HE3	1.82	0.79
2:B:250:LYS:NZ	4:B:514:HOH:O	2.15	0.79
2:B:72:VAL:HG21	2:B:101:VAL:HG13	1.64	0.79
2:B:337:GLU:O	2:B:341:GLU:HG2	1.82	0.79
2:B:340:PHE:HB3	2:B:408:PHE:CE1	2.20	0.77
2:B:367:UNK:O	2:B:370:UNK:N	2.20	0.74
2:B:407:ARG:NH1	2:B:407:ARG:HA	2.04	0.73
1:A:280:ILE:O	1:A:284:ASN:ND2	2.21	0.72
1:A:89:ARG:O	2:B:144:LYS:NZ	2.25	0.69
1:A:149:ASN:O	1:A:152:ILE:HG13	1.92	0.69
2:B:409:THR:O	2:B:421:ILE:N	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:ALA:HA	2:B:27:GLU:HG2	1.74	0.67
1:A:91:LEU:HD11	2:B:144:LYS:HG3	1.77	0.67
2:B:280:ILE:HG22	4:B:501:HOH:O	1.94	0.66
2:B:408:PHE:CB	2:B:422:CYS:HA	2.23	0.66
2:B:409:THR:HG22	2:B:423:TRP:CH2	2.31	0.66
2:B:407:ARG:CA	2:B:407:ARG:CZ	2.74	0.65
1:A:152:ILE:HG22	1:A:161:LEU:CD1	2.27	0.65
1:A:116:CYS:O	4:A:603:HOH:O	2.14	0.65
1:A:47:LEU:H	1:A:107:GLN:HE22	1.44	0.65
2:B:303:BIF:CE1	2:B:307:VAL:HG21	2.28	0.64
1:A:326:CYS:SG	1:A:335:LEU:CD1	2.86	0.63
1:A:231:ALA:HA	1:A:243:ALA:HB2	1.81	0.62
2:B:340:PHE:HB3	2:B:408:PHE:CZ	2.35	0.62
2:B:59:LYS:HD3	2:B:111:PHE:O	1.99	0.61
2:B:409:THR:CG2	2:B:423:TRP:CH2	2.83	0.61
2:B:407:ARG:NE	2:B:407:ARG:O	2.34	0.60
1:A:47:LEU:H	1:A:107:GLN:NE2	1.98	0.60
2:B:80:GLY:O	2:B:81:ASP:HB2	2.02	0.59
1:A:60:ARG:NH1	4:A:632:HOH:O	2.35	0.59
2:B:340:PHE:HB3	2:B:408:PHE:HE1	1.63	0.59
2:B:339:ASP:O	2:B:342:GLN:HB2	2.03	0.57
1:A:152:ILE:HG22	1:A:161:LEU:HD13	1.87	0.57
2:B:409:THR:N	2:B:421:ILE:O	2.33	0.57
1:A:28:ARG:CZ	1:A:34:ILE:HG22	2.35	0.57
1:A:5:ASN:HD22	1:A:8:LYS:HB2	1.70	0.56
2:B:406:GLY:HA3	2:B:408:PHE:O	2.06	0.55
2:B:412:ARG:HB3	2:B:418:TYR:CE1	2.41	0.55
2:B:100:TRP:O	2:B:104:ILE:HG12	2.07	0.54
1:A:83:SER:HA	1:A:156:ALA:HB1	1.88	0.54
2:B:367:UNK:O	2:B:370:UNK:CB	2.55	0.54
2:B:95:GLU:HB2	2:B:97:VAL:HG22	1.89	0.54
2:B:179:GLN:HE21	2:B:195:GLN:HE22	1.56	0.54
2:B:405:PHE:O	2:B:423:TRP:CZ3	2.61	0.54
2:B:411:LEU:HD11	2:B:421:ILE:CD1	2.37	0.53
2:B:350:MET:CE	2:B:422:CYS:SG	2.98	0.52
2:B:407:ARG:NE	2:B:407:ARG:CA	2.73	0.52
1:A:400:GLU:OE2	1:A:403:ARG:HD2	2.10	0.52
1:A:366:SER:HB2	1:A:419:CYS:SG	2.50	0.52
2:B:199:SER:HA	2:B:224:THR:HB	1.92	0.51
2:B:99:GLU:OE2	2:B:99:GLU:HA	2.10	0.51
1:A:385:THR:HG22	1:A:390:LYS:HG2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:ILE:O	1:A:230:LYS:N	2.45	0.50
1:A:91:LEU:CD1	2:B:144:LYS:HG3	2.40	0.50
1:A:287:GLU:O	1:A:291:LYS:HG2	2.11	0.50
1:A:292:ASN:O	1:A:294:GLY:N	2.46	0.49
1:A:376:ARG:NH1	1:A:395:GLU:OE2	2.31	0.49
2:B:340:PHE:CB	2:B:408:PHE:CE1	2.94	0.49
2:B:53:VAL:HB	2:B:54:PRO:CD	2.43	0.48
2:B:412:ARG:HB3	2:B:418:TYR:CD1	2.48	0.48
2:B:364:UNK:O	2:B:368:UNK:N	2.47	0.48
2:B:415:LYS:HG3	2:B:415:LYS:O	2.14	0.48
2:B:28:ARG:CZ	2:B:34:ILE:HG22	2.44	0.48
2:B:350:MET:HE1	2:B:422:CYS:SG	2.54	0.47
2:B:103:LYS:O	2:B:107:GLN:HG3	2.15	0.47
2:B:45:ASP:OD1	2:B:250:LYS:HD2	2.14	0.47
2:B:158:LYS:HG2	2:B:158:LYS:O	2.15	0.47
2:B:408:PHE:HA	2:B:423:TRP:CE3	2.49	0.47
1:A:267:ASP:OD1	1:A:270:ARG:NH2	2.48	0.47
1:A:49:ALA:O	1:A:52:LEU:HB2	2.15	0.47
2:B:42:PRO:HB2	2:B:100:TRP:HB3	1.95	0.47
2:B:147:SER:O	2:B:151:MET:HG3	2.15	0.47
1:A:165:ASP:OD1	1:A:165:ASP:N	2.48	0.47
1:A:326:CYS:SG	1:A:335:LEU:HD13	2.55	0.46
2:B:24:ALA:O	2:B:27:GLU:HG3	2.16	0.46
2:B:33:PRO:HB3	2:B:65:GLY:O	2.15	0.46
1:A:403:ARG:HG2	1:A:423:TRP:CD1	2.51	0.46
1:A:254:TYR:H	1:A:342:GLN:NE2	2.13	0.46
1:A:260:ALA:HB1	1:A:304:ALA:HA	1.97	0.46
2:B:412:ARG:HA	2:B:417:ASN:O	2.16	0.45
1:A:275:GLY:HA3	1:A:303:BIF:H11	1.99	0.45
2:B:208:GLY:O	2:B:212:THR:OG1	2.27	0.45
2:B:340:PHE:CG	2:B:408:PHE:HE1	2.35	0.45
2:B:303:BIF:CE1	2:B:307:VAL:CG2	2.92	0.45
2:B:326:CYS:SG	2:B:335:LEU:CD1	3.05	0.45
1:A:45:ASP:OD1	1:A:45:ASP:N	2.44	0.45
1:A:116:CYS:SG	1:A:120:SER:HA	2.57	0.45
1:A:93:THR:HG22	1:A:95:GLU:H	1.82	0.44
2:B:152:ILE:O	2:B:156:ALA:CB	2.65	0.44
2:B:67:LYS:CE	2:B:122:ILE:HD11	2.48	0.44
2:B:407:ARG:C	2:B:407:ARG:NE	2.71	0.44
1:A:411:LEU:HD11	1:A:421:ILE:HD11	1.99	0.44
2:B:152:ILE:O	2:B:156:ALA:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:408:PHE:HA	2:B:423:TRP:HE3	1.83	0.43
2:B:321:LYS:HA	2:B:324:THR:HG22	2.00	0.43
1:A:109:ALA:N	1:A:110:PRO:CD	2.81	0.43
2:B:71:LEU:HD11	2:B:126:ASN:HB3	1.99	0.43
2:B:5:ASN:OD1	2:B:9:GLN:NE2	2.52	0.43
1:A:249:LYS:HA	1:A:345:GLN:HE22	1.83	0.43
1:A:53:VAL:HB	1:A:54:PRO:CD	2.49	0.43
1:A:139:LEU:O	2:B:171:THR:OG1	2.28	0.42
2:B:18:GLN:HG3	4:B:517:HOH:O	2.18	0.42
2:B:332:LEU:N	2:B:332:LEU:HD12	2.34	0.42
2:B:363:UNK:O	2:B:365:UNK:N	2.52	0.42
2:B:210:ASP:O	2:B:213:ARG:HB2	2.20	0.42
2:B:196:ILE:HG22	2:B:223:LEU:HB3	2.02	0.42
2:B:155:GLU:HB2	2:B:157:VAL:HG23	2.02	0.42
2:B:364:UNK:O	2:B:365:UNK:C	2.67	0.42
2:B:196:ILE:HA	2:B:223:LEU:O	2.20	0.42
2:B:94:GLU:O	2:B:94:GLU:HG2	2.21	0.41
2:B:362:UNK:O	2:B:363:UNK:C	2.67	0.41
2:B:340:PHE:HA	2:B:343:LEU:HD13	2.03	0.41
2:B:27:GLU:HG3	2:B:28:ARG:N	2.36	0.41
1:A:231:ALA:HA	1:A:243:ALA:CB	2.47	0.41
2:B:99:GLU:O	2:B:103:LYS:N	2.34	0.41
2:B:67:LYS:HE3	2:B:122:ILE:HD11	2.03	0.41
1:A:363:LEU:HD23	1:A:368:LEU:HD12	2.03	0.41
2:B:409:THR:HB	2:B:423:TRP:CZ3	2.56	0.41
2:B:293:SER:C	2:B:295:LYS:H	2.24	0.41
2:B:294:GLY:O	2:B:295:LYS:HB2	2.21	0.41
1:A:302:VAL:O	1:A:303:BIF:C	2.68	0.40
2:B:340:PHE:CB	2:B:408:PHE:HE1	2.29	0.40
2:B:339:ASP:O	2:B:342:GLN:N	2.53	0.40
1:A:403:ARG:NH1	1:A:423:TRP:CD2	2.90	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	406/425 (96%)	388 (96%)	15 (4%)	3 (1%)	26	51
2	B	331/394 (84%)	309 (93%)	17 (5%)	5 (2%)	13	28
All	All	737/819 (90%)	697 (95%)	32 (4%)	8 (1%)	17	38

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	293	SER
2	B	156	ALA
2	B	294	GLY
1	A	229	THR
2	B	295	LYS
2	B	99	GLU
2	B	68	PRO
1	A	370	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	340/348 (98%)	334 (98%)	6 (2%)	66	88
2	B	282/308 (92%)	255 (90%)	27 (10%)	10	21
All	All	622/656 (95%)	589 (95%)	33 (5%)	28	54

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ARG
1	A	147	SER
1	A	152	ILE
1	A	165	ASP
1	A	183	PHE

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Mol	Chain	Res	Type
1	A	270	ARG
2	B	27	GLU
2	B	57	CYS
2	B	63	GLN
2	B	95	GLU
2	B	99	GLU
2	B	140	ARG
2	B	147	SER
2	B	150	GLN
2	B	153	ASN
2	B	155	GLU
2	B	158	LYS
2	B	159	GLN
2	B	183	PHE
2	B	188	LYS
2	B	189	GLN
2	B	228	ILE
2	B	255	LYS
2	B	295	LYS
2	B	336	SER
2	B	403	ARG
2	B	405	PHE
2	B	407	ARG
2	B	408	PHE
2	B	409	THR
2	B	411	LEU
2	B	415	LYS
2	B	416	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	31	GLN
1	A	107	GLN
1	A	134	ASN
1	A	159	GLN
1	A	176	ASN
1	A	179	GLN
1	A	187	ASN
1	A	204	ASN
1	A	284	ASN

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Mol	Chain	Res	Type
1	A	342	GLN
1	A	345	GLN
1	A	369	GLN
1	A	391	GLN
1	A	417	ASN
2	B	9	GLN
2	B	176	ASN
2	B	179	GLN
2	B	187	ASN
2	B	204	ASN
2	B	218	ASN
2	B	342	GLN
2	B	345	GLN

### 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	BIF	A	303	1	17,18,19	0.53	0	20,23,25	0.99	1 (5%)
2	BIF	B	303	2	17,18,19	0.45	0	20,23,25	0.70	0

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	BIF	A	303	1	-	0/8/10/12	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BIF	B	303	2	-	0/8/10/12	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	303	BIF	CG-CB-CA	-2.86	107.75	114.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	303	BIF	2	0
2	B	303	BIF	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z  > 2$
3	TYR	A	501	-	10,13,13	0.61	0	11,17,17	0.59	0

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
3	TYR	A	501	-	-	0/4/8/8	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 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	410/425 (96%)	-0.32	6 (1%) 76 75	32, 50, 82, 150	0
2	B	341/394 (86%)	-0.18	8 (2%) 64 62	36, 57, 102, 123	0
All	All	751/819 (91%)	-0.26	14 (1%) 70 69	32, 53, 101, 150	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	163	ARG	3.9
2	B	421	ILE	3.7
1	A	162	ASN	3.5
2	B	411	LEU	3.0
1	A	166	GLN	2.8
2	B	353	MET	2.7
2	B	155	GLU	2.6
1	A	164	GLU	2.5
1	A	296	ALA	2.4
1	A	159	GLN	2.2
2	B	352	GLU	2.2
2	B	416	LYS	2.2
2	B	229	THR	2.1
2	B	295	LYS	2.1

### 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( $\text{\AA}^2$ )	Q<0.9
2	BIF	B	303	17/18	0.97	0.13	-	41,45,46,47	0
1	BIF	A	303	17/18	0.97	0.13	-	40,42,44,44	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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( $\text{\AA}^2$ )	Q<0.9
3	TYR	A	501	13/13	0.94	0.13	-0.13	38,51,59,61	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.