



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 04:26 PM UTC

PDB ID : 4OUD / pdb_00004oud
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

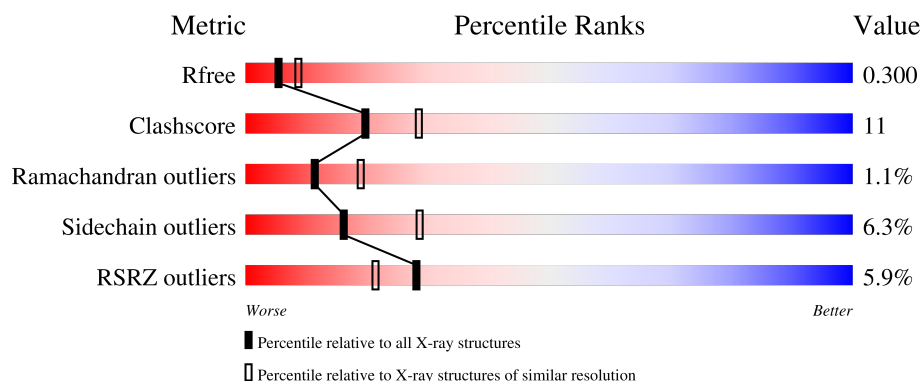
1 Overall quality at a glance

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}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	425	2% 77% 19% ..
2	B	394	9% 63% 23% .. 9%

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:

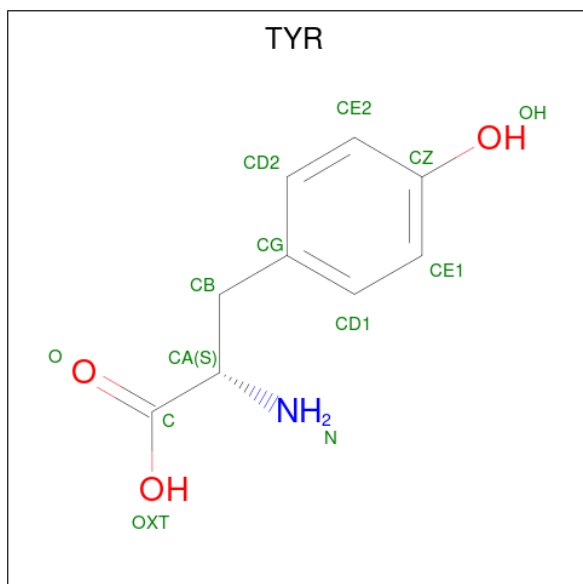
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP U6N9P2
B	1	PRO	-	expression tag	UNP U6N9P2
B	49	ALA	LEU	engineered mutation	UNP U6N9P2
B	236	ALA	PHE	engineered mutation	UNP U6N9P2
B	260	ALA	TRP	engineered mutation	UNP U6N9P2
B	263	ALA	THR	engineered mutation	UNP U6N9P2
B	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 (CCD ID: 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		

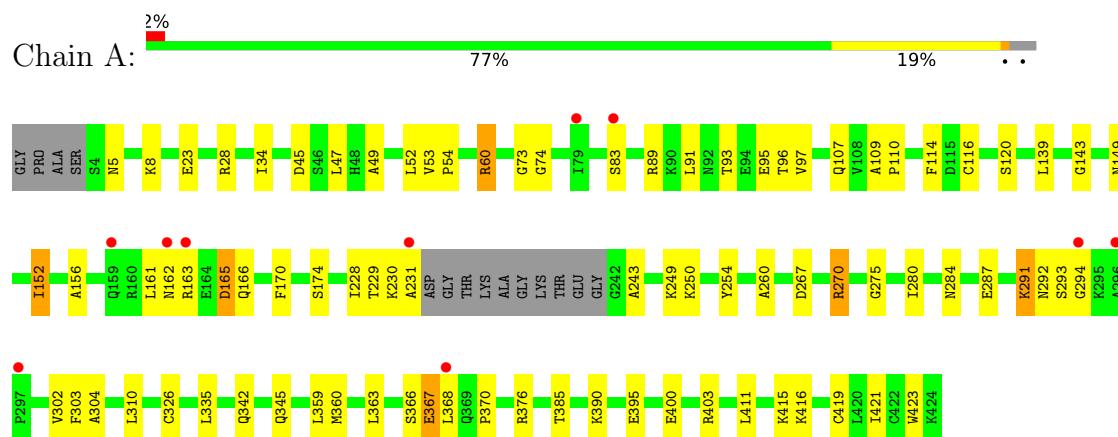
- Molecule 4 is water.

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

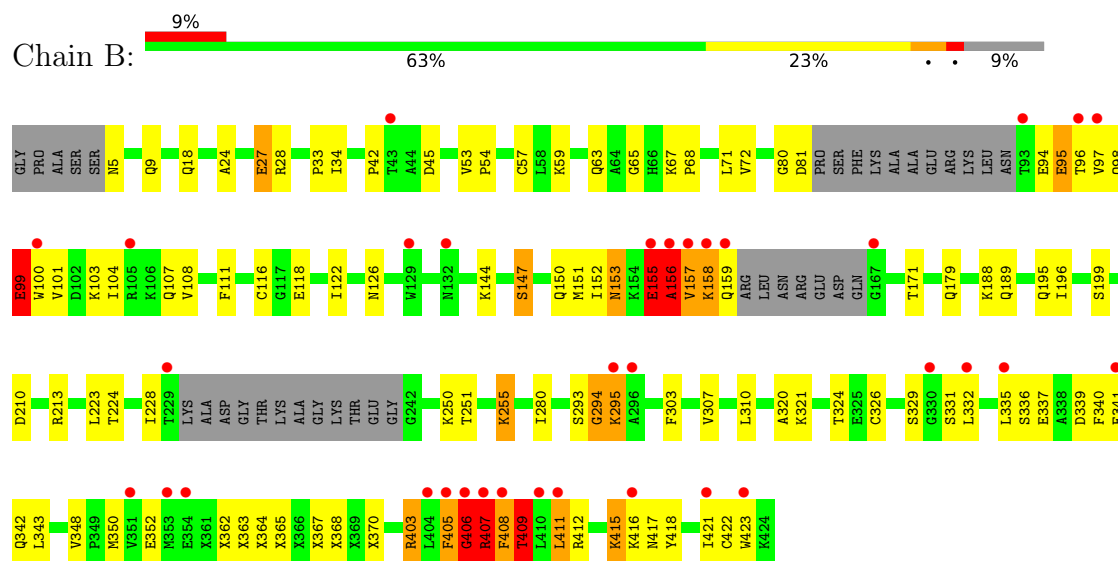
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 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, α , β , γ	81.34Å 67.20Å 90.68Å 90.00° 102.65° 90.00°	Depositor
Resolution (Å)	45.00 – 2.65 45.00 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.9 (45.00-2.65) 99.0 (45.00-2.65)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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	1398 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 32.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6108	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

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	0.82	0/3293	0.99	4/4442 (0.1%)
2	B	0.83	0/2738	1.06	9/3694 (0.2%)
All	All	0.83	0/6031	1.02	13/8136 (0.2%)

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 (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	163	ARG	N-CA-C	12.44	124.57	111.14
2	B	408	PHE	N-CA-C	-8.82	95.44	107.88
2	B	407	ARG	N-CA-C	-8.08	101.55	112.94
2	B	157	VAL	N-CA-C	7.32	118.41	107.80
2	B	409	THR	N-CA-C	6.85	118.20	108.74
2	B	155	GLU	N-CA-C	-6.38	105.12	113.17
1	A	97	VAL	N-CA-C	5.99	116.64	110.36
1	A	143	GLY	N-CA-C	5.97	121.37	113.37
2	B	348	VAL	N-CA-CB	5.75	116.56	111.67
2	B	116	CYS	N-CA-C	-5.47	103.88	110.88
1	A	23	GLU	N-CA-C	-5.42	105.45	111.36
2	B	406	GLY	N-CA-C	-5.01	101.30	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	156	ALA	N-CA-C	5.01	121.47	110.80

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
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	49	0
2	B	2789	0	2674	92	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	137	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 (137) 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:CZ	2:B:407:ARG:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	2:B:407:ARG:NH1	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
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:CZ	2:B:407:ARG:CA	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
1:A:47:LEU:H	1:A:107:GLN:NE2	1.98	0.60
2:B:407:ARG:NE	2:B:407:ARG:O	2.34	0.60
2:B:350:MET:HE2	2:B:422:CYS:SG	2.42	0.59
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CA	2:B:407:ARG:NE	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
1:A:385:THR:HG22	1:A:390:LYS:HG2	1.91	0.51
2:B:99:GLU:HA	2:B:99:GLU:OE2	2.10	0.51
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:407:ARG:NE	2:B:407:ARG:C	2.71	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:O	2:B:415:LYS:HG3	2.14	0.48
2:B:28:ARG:CZ	2:B:34:ILE:HG22	2.44	0.48
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:O	2:B:158:LYS:HG2	2.15	0.47
1:A:49:ALA:O	1:A:52:LEU:HB2	2.15	0.47
1:A:267:ASP:OD1	1:A:270:ARG:NH2	2.48	0.47
2:B:408:PHE:HA	2:B:423:TRP:CE3	2.49	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:170:PHE:O	1:A:174:SER:OG	2.32	0.46
1:A:254:TYR:H	1:A:342:GLN:NE2	2.13	0.46
1:A:403:ARG:HG2	1:A:423:TRP:CD1	2.51	0.46
1:A:260:ALA:HB1	1:A:304:ALA:HA	1.97	0.46
2:B:293:SER:C	2:B:295:LYS:H	2.24	0.45
2:B:412:ARG:HA	2:B:417:ASN:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:GLY:HA3	1:A:303:BIF:H11	1.99	0.45
2:B:303:BIF:CE1	2:B:307:VAL:CG2	2.92	0.45
2:B:340:PHE:CG	2:B:408:PHE:HE1	2.35	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
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
2:B:293:SER:C	2:B:295:LYS:N	2.75	0.44
2:B:408:PHE:HA	2:B:423:TRP:HE3	1.83	0.43
1:A:109:ALA:N	1:A:110:PRO:CD	2.81	0.43
2:B:321:LYS:HA	2:B:324:THR:HG22	2.00	0.43
2:B:71:LEU:HD11	2:B:126:ASN:HB3	1.99	0.43
1:A:359:LEU:O	1:A:360:MET:C	2.61	0.43
2:B:5:ASN:OD1	2:B:9:GLN:NE2	2.52	0.43
2:B:405:PHE:C	2:B:405:PHE:CD1	2.96	0.43
1:A:53:VAL:HB	1:A:54:PRO:CD	2.49	0.43
1:A:249:LYS:HA	1:A:345:GLN:HE22	1.83	0.43
1:A:139:LEU:O	2:B:171:THR:OG1	2.28	0.42
1:A:73:GLY:O	1:A:74:GLY:C	2.61	0.42
2:B:18:GLN:HG3	4:B:517:HOH:O	2.18	0.42
2:B:332:LEU:HD12	2:B:332:LEU:N	2.34	0.42
2:B:155:GLU:HB2	2:B:157:VAL:HG23	2.02	0.42
2:B:196:ILE:HG22	2:B:223:LEU:HB3	2.02	0.42
2:B:210:ASP:O	2:B:213:ARG:HB2	2.20	0.42
2:B:363:UNK:O	2:B:365:UNK:N	2.52	0.42
2:B:331:SER:C	2:B:332:LEU:HD12	2.44	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
1:A:231:ALA:HA	1:A:243:ALA:CB	2.47	0.41
2:B:27:GLU:HG3	2:B:28:ARG:N	2.36	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:114:PHE:C	1:A:120:SER:OG	2.63	0.41
1:A:363:LEU:HD23	1:A:368:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:MET:C	2:B:153:ASN:H	2.28	0.41
2:B:294:GLY:O	2:B:295:LYS:HB2	2.21	0.41
2:B:409:THR:HB	2:B:423:TRP:CZ3	2.56	0.41
1:A:302:VAL:O	1:A:303:BIF:C	2.68	0.40
1:A:366:SER:C	1:A:367:GLU:HG2	2.46	0.40
1:A:403:ARG:NH1	1:A:423:TRP:CD2	2.90	0.40
2:B:339:ASP:O	2:B:342:GLN:N	2.53	0.40
2:B:340:PHE:CB	2:B:408:PHE:HE1	2.29	0.40
2:B:99:GLU:O	2:B:100:TRP:C	2.63	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%)	18	30
2	B	331/394 (84%)	309 (93%)	17 (5%)	5 (2%)	8	13
All	All	737/819 (90%)	697 (95%)	32 (4%)	8 (1%)	11	19

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%)	329 (97%)	11 (3%)	34	55
2	B	282/308 (92%)	254 (90%)	28 (10%)	7	11
All	All	622/656 (95%)	583 (94%)	39 (6%)	16	29

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ARG
1	A	96	THR
1	A	152	ILE
1	A	165	ASP
1	A	166	GLN
1	A	270	ARG
1	A	291	LYS
1	A	310	LEU
1	A	367	GLU
1	A	415	LYS
1	A	416	LYS
2	B	27	GLU
2	B	57	CYS
2	B	63	GLN
2	B	95	GLU
2	B	96	THR
2	B	98	GLN
2	B	99	GLU
2	B	108	VAL
2	B	118	GLU
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	188	LYS

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Mol	Chain	Res	Type
2	B	189	GLN
2	B	228	ILE
2	B	255	LYS
2	B	310	LEU
2	B	336	SER
2	B	352	GLU
2	B	403	ARG
2	B	407	ARG
2	B	409	THR
2	B	411	LEU
2	B	415	LYS
2	B	416	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) 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	149	ASN
1	A	159	GLN
1	A	162	ASN
1	A	179	GLN
1	A	189	GLN
1	A	204	ASN
1	A	258	GLN
1	A	342	GLN
1	A	345	GLN
1	A	369	GLN
1	A	374	GLN
1	A	417	ASN
2	B	9	GLN
2	B	176	ASN
2	B	187	ASN
2	B	189	GLN
2	B	195	GLN
2	B	204	ASN
2	B	216	HIS
2	B	218	ASN
2	B	258	GLN
2	B	306	GLN

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Mol	Chain	Res	Type
2	B	318	GLN
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	$\# Z > 2$
2	BIF	B	303	2	17,18,19	0.49	0	18,23,25	0.45	0
1	BIF	A	303	1	17,18,19	0.61	0	18,23,25	0.76	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
2	BIF	B	303	2	-	0/9/10/12	0/2/2/2
1	BIF	A	303	1	-	1/9/10/12	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	303	BIF	CA-CB-CG-CD1

There are no ring outliers.

2 monomers are involved in 4 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	-	12,13,13	0.82	0	13,17,17	0.99	1 (7%)

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	-	-	0/8/8/8	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	501	TYR	OXT-C-O	-2.89	117.52	124.08

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance ($\text{\AA}$)
1	B	354:GLU	C	361:UNK	N	19.35
1	B	377:UNK	C	403:ARG	N	12.46

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	410/425 (96%)	0.10	10 (2%) 59 53	32, 50, 82, 150	0
2	B	341/394 (86%)	0.51	34 (9%) 12 10	36, 57, 102, 123	0
All	All	751/819 (91%)	0.29	44 (5%) 28 21	32, 53, 101, 150	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	404	LEU	5.5
2	B	132	ASN	4.6
1	A	231	ALA	4.1
2	B	100	TRP	4.0
1	A	297	PRO	4.0
2	B	354	GLU	3.9
1	A	296	ALA	3.8
2	B	158	LYS	3.7
2	B	353	MET	3.5
2	B	406	GLY	3.5
2	B	341	GLU	3.5
1	A	163	ARG	3.5
2	B	159	GLN	3.4
2	B	157	VAL	3.3
2	B	229	THR	3.2
2	B	97	VAL	3.2
2	B	332	LEU	3.1
2	B	411	LEU	3.0
1	A	83	SER	3.0
2	B	96	THR	3.0
2	B	421	ILE	2.9
2	B	295	LYS	2.9
2	B	423	TRP	2.9
2	B	43	THR	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	408	PHE	2.7
1	A	79	ILE	2.6
2	B	93	THR	2.5
2	B	156	ALA	2.4
2	B	405	PHE	2.4
1	A	294	GLY	2.4
1	A	159	GLN	2.4
2	B	105	ARG	2.4
1	A	162	ASN	2.4
2	B	296	ALA	2.2
1	A	368	LEU	2.2
2	B	155	GLU	2.2
2	B	416	LYS	2.2
2	B	167	GLY	2.2
2	B	351	VAL	2.2
2	B	129	TRP	2.1
2	B	335	LEU	2.1
2	B	410	LEU	2.1
2	B	407	ARG	2.1
2	B	330	GLY	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	BIF	A	303	17/18	0.96	0.07	40,42,44,44	0
2	BIF	B	303	17/18	0.97	0.07	41,45,46,47	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	TYR	A	501	13/13	0.94	0.09	38,51,59,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.