WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:35 PM GMT

PDB ID : 3ZXI
Title : CRYSTAL STRUCTURE OF HUMAN MITOCHONDRIAL TYROSYL-TRNA SYNTHETASE IN COMPLEX WITH A TYROSYL-ADENYLATE ANALOG
Authors : Bonnefond, L.; Frugier, M.; Rudinger-Thirion, J.; Balg, C.; Chenevert, R.; Lorber, B.; Giege, R.; Sauter, C.
Deposited on : 2011-08-11
Resolution : 2.75 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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.
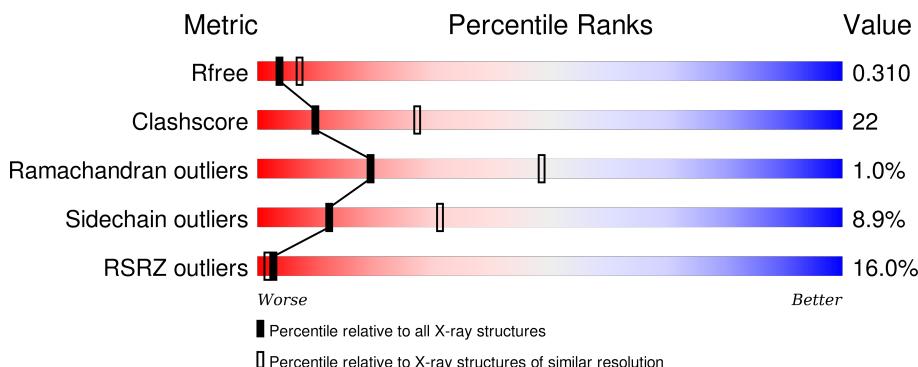
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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 >=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 <=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	356	10% / 49% 33% • 14%
1	B	356	17% / 47% 35% • 14%
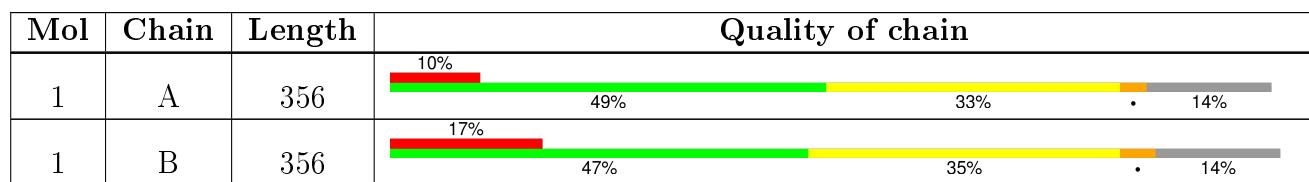
2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4928 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, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total 2430	C 1555	N 436	O 432	S 7	0	0	1
1	B	306	Total 2430	C 1555	N 436	O 432	S 7	0	0	1

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	MET	-	EXPRESSION TAG	UNP Q9Y2Z4
A	29	ARG	-	EXPRESSION TAG	UNP Q9Y2Z4
A	30	GLY	-	EXPRESSION TAG	UNP Q9Y2Z4
A	31	SER	-	EXPRESSION TAG	UNP Q9Y2Z4
A	376	ARG	-	EXPRESSION TAG	UNP Q9Y2Z4
A	377	SER	-	EXPRESSION TAG	UNP Q9Y2Z4
A	378	HIS	-	EXPRESSION TAG	UNP Q9Y2Z4
A	379	HIS	-	EXPRESSION TAG	UNP Q9Y2Z4
A	380	HIS	-	EXPRESSION TAG	UNP Q9Y2Z4
A	381	HIS	-	EXPRESSION TAG	UNP Q9Y2Z4
A	382	HIS	-	EXPRESSION TAG	UNP Q9Y2Z4
A	383	HIS	-	EXPRESSION TAG	UNP Q9Y2Z4
B	28	MET	-	EXPRESSION TAG	UNP Q9Y2Z4
B	29	ARG	-	EXPRESSION TAG	UNP Q9Y2Z4
B	30	GLY	-	EXPRESSION TAG	UNP Q9Y2Z4
B	31	SER	-	EXPRESSION TAG	UNP Q9Y2Z4
B	376	ARG	-	EXPRESSION TAG	UNP Q9Y2Z4
B	377	SER	-	EXPRESSION TAG	UNP Q9Y2Z4
B	378	HIS	-	EXPRESSION TAG	UNP Q9Y2Z4
B	379	HIS	-	EXPRESSION TAG	UNP Q9Y2Z4
B	380	HIS	-	EXPRESSION TAG	UNP Q9Y2Z4
B	381	HIS	-	EXPRESSION TAG	UNP Q9Y2Z4
B	382	HIS	-	EXPRESSION TAG	UNP Q9Y2Z4
B	383	HIS	-	EXPRESSION TAG	UNP Q9Y2Z4

- Molecule 2 is PHOSPHORIC ACID 2-AMINO-3-(4-HYDROXY-PHENYL)-PROPYL ESTER ADENOSIN-5'YL ESTER (three-letter code: TYA) (formula: $C_{19}H_{24}N_6O_8P$).
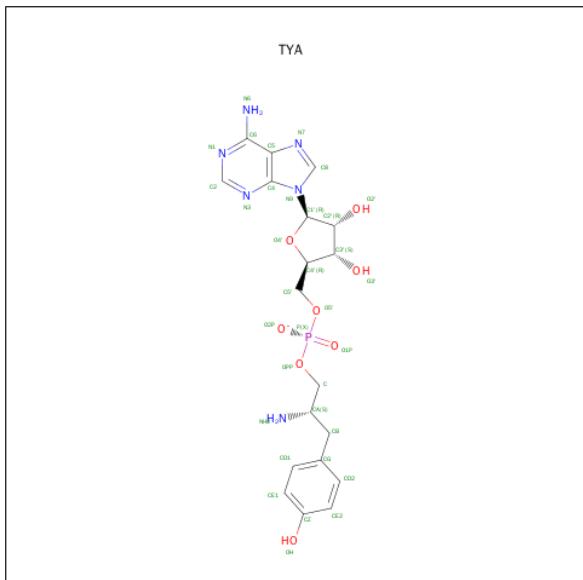
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			34	19	6	8	1		
2	B	1	Total	C	N	O	P	0	0
			34	19	6	8	1		

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: TYROSYL-TRNA SYNTHETASE, MITOCHONDRIAL
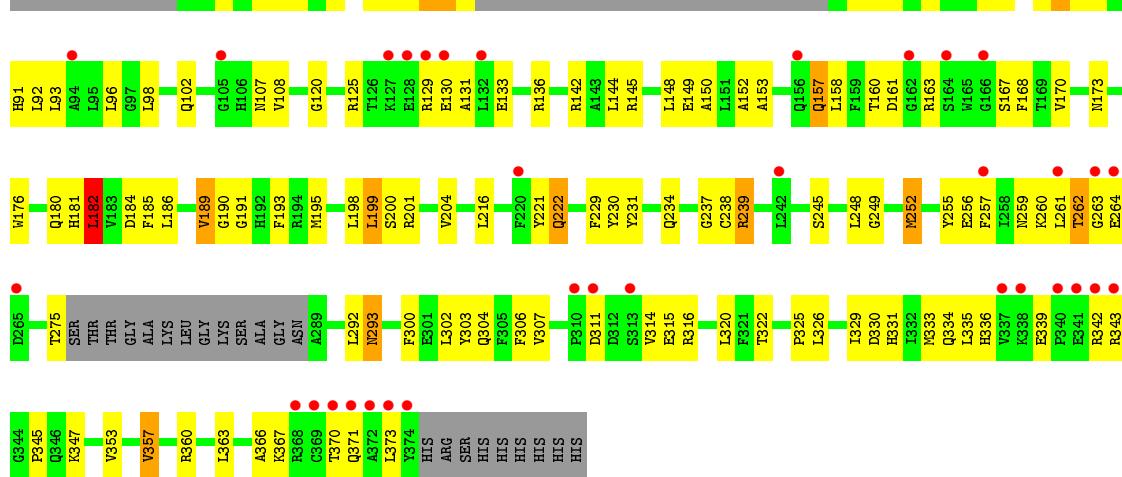
- Molecule 1: TYROSYL-TRNA SYNTHETASE, MITOCHONDRIAL
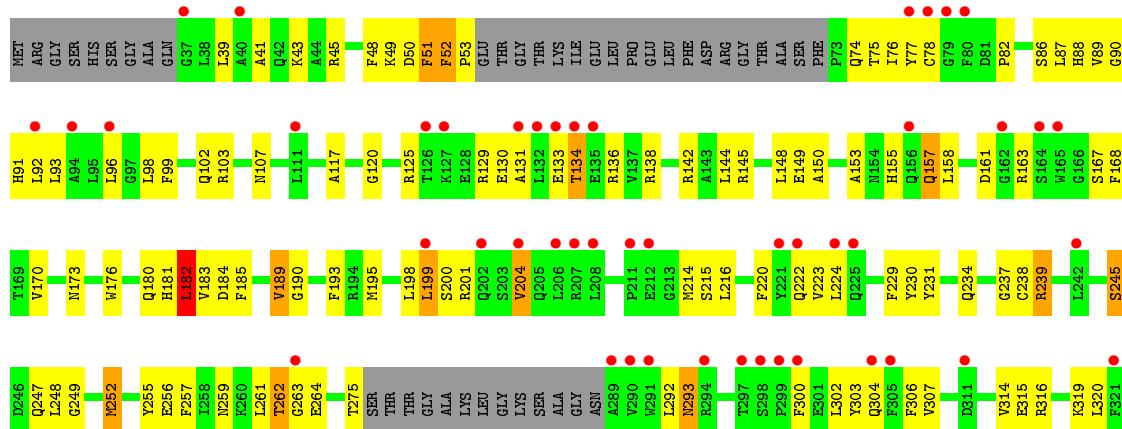
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	53.14Å 62.87Å 196.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.94 – 2.75 29.94 – 2.75	Depositor EDS
% Data completeness (in resolution range)	94.0 (29.94-2.75) 94.0 (29.94-2.75)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.63 (at 2.76Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.224 , 0.307 0.225 , 0.310	Depositor DCC
R_{free} test set	859 reflections (5.41%)	DCC
Wilson B-factor (Å^2)	65.5	Xtriage
Anisotropy	0.973	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 93.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.47, <L^2> = 0.30$	Xtriage
Outliers	0 of 16786 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4928	wwPDB-VP
Average B, all atoms (Å^2)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.99% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ 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: TYA

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	0.42	0/2485	0.55	0/3355
1	B	0.42	0/2485	0.56	0/3355
All	All	0.42	0/4970	0.55	0/6710

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	2430	0	2417	113	1
1	B	2430	0	2417	113	1
2	A	34	0	23	1	0
2	B	34	0	23	2	0
All	All	4928	0	4880	217	1

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 22.

All (217) 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:102:GLN:HE22	1:B:168:PHE:HB2	1.01	1.08
1:A:102:GLN:HE22	1:A:168:PHE:HB2	0.99	1.06
1:A:102:GLN:NE2	1:A:168:PHE:HB2	1.76	0.98
1:B:102:GLN:NE2	1:B:168:PHE:HB2	1.81	0.94
1:A:193:PHE:HB3	1:A:198:LEU:HD21	1.54	0.90
1:B:193:PHE:HB3	1:B:198:LEU:HD21	1.56	0.87
1:A:191:GLY:HA2	1:B:215:SER:HB2	1.57	0.85
1:B:41:ALA:O	1:B:45:ARG:HG3	1.79	0.83
1:A:314:VAL:HG21	1:A:345:PRO:HB2	1.62	0.82
1:A:50:ASP:OD2	1:A:52:PHE:HE2	1.62	0.82
1:B:50:ASP:OD2	1:B:52:PHE:HE2	1.63	0.81
1:B:314:VAL:HG21	1:B:345:PRO:HB2	1.64	0.80
1:B:145:ARG:HG2	1:B:149:GLU:OE2	1.82	0.79
1:A:326:LEU:HD12	1:A:326:LEU:H	1.47	0.79
1:B:257:PHE:O	1:B:261:LEU:HD13	1.84	0.78
1:A:201:ARG:O	1:A:204:VAL:HG12	1.84	0.76
1:A:51:PHE:HD1	1:A:51:PHE:N	1.83	0.75
1:A:257:PHE:O	1:A:261:LEU:HD13	1.87	0.74
1:A:75:THR:HB	1:A:238:CYS:HA	1.69	0.74
1:B:75:THR:HB	1:B:238:CYS:HA	1.70	0.74
1:A:50:ASP:OD2	1:A:52:PHE:CE2	2.41	0.74
1:A:145:ARG:HG2	1:A:149:GLU:OE2	1.87	0.74
1:A:51:PHE:N	1:A:51:PHE:CD1	2.54	0.73
1:A:88:HIS:H	1:A:91:HIS:CD2	2.07	0.72
1:B:51:PHE:CD1	1:B:51:PHE:N	2.58	0.71
1:B:50:ASP:OD2	1:B:52:PHE:CE2	2.43	0.71
1:A:41:ALA:O	1:A:45:ARG:HG3	1.90	0.71
1:B:51:PHE:N	1:B:51:PHE:HD1	1.88	0.70
1:A:262:THR:C	1:A:264:GLU:H	1.92	0.70
2:B:1374:TYA:H5'1	2:B:1374:TYA:H8	1.74	0.70
1:B:262:THR:C	1:B:264:GLU:H	1.94	0.70
1:A:88:HIS:H	1:A:91:HIS:HD2	1.40	0.69
1:B:201:ARG:O	1:B:204:VAL:HG12	1.94	0.68
1:B:252:MET:HE2	1:B:255:TYR:HE2	1.59	0.68
1:A:102:GLN:HE22	1:A:168:PHE:CB	1.92	0.68
1:B:326:LEU:HD12	1:B:326:LEU:H	1.58	0.67
1:A:158:LEU:HD12	1:A:158:LEU:N	2.11	0.66
1:B:339:GLU:HB3	1:B:342:ARG:HG3	1.77	0.65
1:A:339:GLU:HB3	1:A:342:ARG:HG3	1.77	0.65
1:A:252:MET:HE2	1:A:255:TYR:HE2	1.61	0.65
1:A:150:ALA:O	1:A:153:ALA:HB3	1.98	0.64
1:B:331:HIS:HA	1:B:334:GLN:HG2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:LEU:HD13	1:A:51:PHE:CE2	2.33	0.62
1:B:300:PHE:CE1	1:B:370:THR:HG22	2.34	0.62
1:B:39:LEU:HD13	1:B:51:PHE:CE2	2.35	0.62
1:A:182:LEU:HD13	1:B:185:PHE:CD2	2.36	0.61
1:B:325:PRO:O	1:B:329:ILE:HG13	2.00	0.60
1:A:182:LEU:HD21	1:B:224:LEU:HD21	1.82	0.60
1:A:325:PRO:O	1:A:329:ILE:HG13	2.01	0.60
1:A:300:PHE:CE1	1:A:370:THR:HG22	2.36	0.60
1:B:88:HIS:H	1:B:91:HIS:CD2	2.19	0.59
1:B:252:MET:HE2	1:B:255:TYR:CE2	2.37	0.59
1:A:331:HIS:HA	1:A:334:GLN:HG2	1.85	0.58
1:B:173:ASN:HB3	1:B:176:TRP:CZ2	2.38	0.58
1:B:158:LEU:N	1:B:158:LEU:HD12	2.18	0.58
1:B:102:GLN:HE22	1:B:168:PHE:CB	1.95	0.57
1:B:249:GLY:O	1:B:252:MET:HB2	2.05	0.57
1:A:252:MET:HE2	1:A:255:TYR:CE2	2.38	0.57
1:A:262:THR:C	1:A:264:GLU:N	2.58	0.57
1:B:150:ALA:O	1:B:153:ALA:HB3	2.04	0.57
1:B:252:MET:O	1:B:256:GLU:HG3	2.05	0.57
1:B:300:PHE:HE1	1:B:370:THR:HG22	1.68	0.57
1:A:262:THR:O	1:A:264:GLU:N	2.38	0.56
1:A:173:ASN:HB3	1:A:176:TRP:CZ2	2.40	0.56
1:A:87:LEU:HB2	1:A:292:LEU:HD22	1.87	0.56
1:A:300:PHE:HE1	1:A:370:THR:HG22	1.70	0.55
1:A:43:LYS:HE2	1:A:49:LYS:O	2.06	0.55
1:A:191:GLY:HA2	1:B:215:SER:CB	2.35	0.55
1:A:249:GLY:O	1:A:252:MET:HB2	2.07	0.55
1:B:92:LEU:O	1:B:96:LEU:HG	2.06	0.55
1:B:89:VAL:O	1:B:92:LEU:HB3	2.07	0.55
1:B:343:ARG:O	1:B:347:LYS:HG3	2.06	0.55
1:A:182:LEU:HD13	1:B:185:PHE:CG	2.42	0.55
1:A:314:VAL:CG2	1:A:345:PRO:HB2	2.36	0.54
1:B:88:HIS:H	1:B:91:HIS:HD2	1.55	0.54
1:B:262:THR:O	1:B:264:GLU:N	2.40	0.54
1:A:145:ARG:HG3	1:A:170:VAL:HG11	1.89	0.54
1:A:39:LEU:HD13	1:A:51:PHE:HE2	1.73	0.54
1:B:252:MET:HA	1:B:255:TYR:CE2	2.42	0.54
1:A:86:SER:OG	1:A:293:ASN:HB2	2.08	0.54
1:B:52:PHE:CZ	1:B:248:LEU:HD13	2.43	0.53
1:A:176:TRP:CE3	1:A:231:TYR:CE2	2.97	0.53
1:B:262:THR:C	1:B:264:GLU:N	2.60	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:ARG:O	1:A:347:LYS:HG3	2.08	0.53
1:A:252:MET:HA	1:A:255:TYR:CE2	2.43	0.53
1:B:314:VAL:CG2	1:B:345:PRO:HB2	2.38	0.53
1:B:82:PRO:HA	1:B:144:LEU:HD22	1.91	0.53
1:B:145:ARG:HG3	1:B:170:VAL:HG11	1.91	0.53
1:A:92:LEU:O	1:A:96:LEU:HG	2.08	0.53
1:A:306:PHE:CE2	1:A:353:VAL:HG11	2.45	0.52
1:B:237:GLY:O	1:B:239:ARG:HG2	2.08	0.52
1:A:230:TYR:O	1:A:234:GLN:HG2	2.09	0.52
1:A:181:HIS:HB2	1:A:184:ASP:OD2	2.10	0.52
1:A:89:VAL:O	1:A:92:LEU:HB3	2.09	0.52
1:A:53:PRO:HG3	1:A:255:TYR:CE1	2.46	0.51
1:A:87:LEU:HD21	1:A:148:LEU:HD21	1.92	0.51
1:A:186:LEU:HD11	1:B:220:PHE:CD1	2.45	0.51
1:A:93:LEU:HD11	1:A:320:LEU:HG	1.92	0.51
1:B:39:LEU:HD13	1:B:51:PHE:HE2	1.75	0.51
1:A:81:ASP:HB2	2:A:1374:TYA:O2P	2.11	0.51
1:B:230:TYR:O	1:B:234:GLN:HG2	2.11	0.51
1:A:133:GLU:CD	1:A:133:GLU:H	2.14	0.51
1:A:252:MET:O	1:A:256:GLU:HG3	2.11	0.51
1:B:43:LYS:HE2	1:B:49:LYS:O	2.11	0.50
1:B:306:PHE:CE2	1:B:353:VAL:HG11	2.47	0.50
1:A:52:PHE:CZ	1:A:248:LEU:HD13	2.47	0.50
1:B:78:CYS:HB3	1:B:98:LEU:HD11	1.94	0.49
1:B:93:LEU:HD11	1:B:320:LEU:HG	1.95	0.49
1:B:87:LEU:HB2	1:B:292:LEU:HD22	1.93	0.49
1:A:161:ASP:OD2	1:A:163:ARG:HD3	2.12	0.49
1:A:185:PHE:CD2	1:B:182:LEU:HD13	2.47	0.49
1:B:176:TRP:CE3	1:B:231:TYR:CE2	3.01	0.49
1:B:261:LEU:HD12	1:B:261:LEU:N	2.28	0.48
1:B:90:GLY:HA3	2:B:1374:TYA:C6	2.43	0.48
1:A:304:GLN:NE2	1:A:304:GLN:HA	2.28	0.48
1:B:363:LEU:HG	1:B:367:LYS:HE2	1.96	0.48
1:B:201:ARG:HH22	1:B:256:GLU:CD	2.17	0.48
1:A:363:LEU:HG	1:A:367:LYS:HE2	1.96	0.48
1:B:239:ARG:NH2	1:B:264:GLU:HG3	2.28	0.48
1:A:158:LEU:HD12	1:A:158:LEU:H	1.80	0.47
1:A:78:CYS:HB3	1:A:98:LEU:HD11	1.96	0.47
1:B:353:VAL:O	1:B:357:VAL:HG12	2.14	0.47
1:A:316:ARG:O	1:A:320:LEU:HB2	2.13	0.47
1:A:82:PRO:HA	1:A:144:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ARG:HH22	1:A:256:GLU:CD	2.17	0.47
1:A:256:GLU:O	1:A:260:LYS:HG3	2.15	0.47
1:A:237:GLY:O	1:A:239:ARG:HG2	2.14	0.47
1:B:86:SER:OG	1:B:293:ASN:HB2	2.13	0.47
1:A:102:GLN:HE21	1:A:108:VAL:HG22	1.79	0.47
1:B:326:LEU:HD12	1:B:326:LEU:N	2.29	0.47
1:B:316:ARG:O	1:B:320:LEU:HB2	2.15	0.47
1:A:239:ARG:HB3	1:A:239:ARG:CZ	2.45	0.46
1:B:181:HIS:HB2	1:B:184:ASP:OD2	2.14	0.46
1:A:326:LEU:N	1:A:326:LEU:HD12	2.23	0.46
1:B:39:LEU:HD23	1:B:48:PHE:CD2	2.50	0.46
1:B:130:GLU:O	1:B:131:ALA:C	2.54	0.46
1:B:304:GLN:HA	1:B:304:GLN:NE2	2.30	0.46
1:B:303:TYR:CE2	1:B:307:VAL:HG21	2.51	0.46
1:A:216:LEU:HB3	1:B:190:GLY:O	2.16	0.46
1:B:193:PHE:HE1	1:B:257:PHE:CE1	2.34	0.46
1:B:107:ASN:HD22	1:B:167:SER:H	1.64	0.46
1:B:248:LEU:O	1:B:252:MET:HG3	2.15	0.46
1:A:125:ARG:HD2	1:A:129:ARG:NH2	2.31	0.46
1:A:262:THR:HB	1:A:264:GLU:HB2	1.98	0.45
1:A:303:TYR:CE2	1:A:307:VAL:HG21	2.51	0.45
1:B:39:LEU:HD23	1:B:48:PHE:HD2	1.81	0.45
1:B:326:LEU:N	1:B:327:PRO:CD	2.80	0.45
1:B:133:GLU:CD	1:B:133:GLU:H	2.18	0.45
1:A:239:ARG:NH2	1:A:264:GLU:HG3	2.31	0.45
1:B:134:THR:O	1:B:138:ARG:HG2	2.17	0.45
1:A:130:GLU:O	1:A:131:ALA:C	2.55	0.45
1:B:161:ASP:OD2	1:B:163:ARG:HD3	2.16	0.45
1:B:367:LYS:O	1:B:371:GLN:HG3	2.17	0.45
1:A:42:GLN:HB2	1:A:48:PHE:CD2	2.52	0.45
1:A:88:HIS:N	1:A:91:HIS:HD2	2.12	0.45
1:A:193:PHE:HE1	1:A:257:PHE:CE1	2.35	0.45
1:B:262:THR:HB	1:B:264:GLU:HB2	1.98	0.44
1:A:87:LEU:CB	1:A:292:LEU:HD22	2.46	0.44
1:A:302:LEU:HD21	1:A:357:VAL:HG11	1.99	0.44
1:A:333:MET:O	1:A:336:HIS:N	2.50	0.44
1:B:99:PHE:O	1:B:103:ARG:HG3	2.17	0.44
1:B:248:LEU:O	1:B:252:MET:CG	2.66	0.44
1:A:367:LYS:O	1:A:371:GLN:HG3	2.17	0.44
1:A:120:GLY:HA3	1:A:129:ARG:HD2	1.98	0.44
1:A:76:ILE:HD12	1:A:76:ILE:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:PHE:CD2	1:B:223:VAL:HG22	2.53	0.44
1:B:125:ARG:HD2	1:B:129:ARG:NH2	2.33	0.44
1:B:239:ARG:HB3	1:B:239:ARG:CZ	2.48	0.44
1:B:245:SER:C	1:B:247:GLN:H	2.21	0.43
1:A:39:LEU:HD23	1:A:48:PHE:CD2	2.54	0.43
1:A:161:ASP:CG	1:A:163:ARG:HD3	2.37	0.43
1:B:74:GLN:HA	1:B:74:GLN:OE1	2.19	0.43
1:A:193:PHE:HB2	1:B:216:LEU:HB2	2.00	0.43
1:A:50:ASP:OD1	1:A:51:PHE:N	2.51	0.43
1:A:198:LEU:HD12	1:A:222:GLN:OE1	2.19	0.42
1:B:198:LEU:H	1:B:198:LEU:HD22	1.84	0.42
1:B:53:PRO:HG3	1:B:255:TYR:CE1	2.54	0.42
1:B:185:PHE:CE1	1:B:189:VAL:HG21	2.53	0.42
1:B:87:LEU:HD21	1:B:148:LEU:HD21	2.00	0.42
1:A:315:GLU:OE1	1:A:333:MET:HG3	2.19	0.42
1:B:348:ARG:HA	1:B:348:ARG:HD2	1.79	0.42
1:A:161:ASP:C	1:A:163:ARG:H	2.23	0.42
1:A:136:ARG:HD3	1:A:136:ARG:HA	1.82	0.42
1:A:120:GLY:O	1:A:221:TYR:CD2	2.72	0.42
1:B:136:ARG:HA	1:B:136:ARG:HD3	1.83	0.42
1:A:96:LEU:HA	1:A:96:LEU:HD23	1.85	0.42
1:A:42:GLN:NE2	1:A:42:GLN:HA	2.35	0.42
1:A:255:TYR:O	1:A:259:ASN:HB2	2.19	0.42
1:A:190:GLY:O	1:B:216:LEU:HB3	2.20	0.42
1:B:214:MET:HB2	1:B:214:MET:HE2	1.96	0.42
1:A:261:LEU:N	1:A:261:LEU:HD12	2.35	0.42
1:B:120:GLY:HA3	1:B:129:ARG:HD2	2.02	0.42
1:B:315:GLU:O	1:B:319:LYS:HG3	2.20	0.42
1:B:157:GLN:HE21	1:B:157:GLN:HB3	1.50	0.42
1:B:182:LEU:HD23	1:B:183:VAL:HG23	2.02	0.41
1:A:311:ASP:HA	1:A:314:VAL:HG12	2.02	0.41
1:B:315:GLU:OE1	1:B:333:MET:HG3	2.20	0.41
1:B:185:PHE:C	1:B:185:PHE:CD1	2.94	0.41
1:B:302:LEU:HD21	1:B:357:VAL:HG11	2.02	0.41
1:B:93:LEU:HD12	1:B:93:LEU:HA	1.82	0.41
1:A:195:MET:O	1:A:199:LEU:HG	2.20	0.41
1:A:160:THR:HG22	1:A:161:ASP:N	2.35	0.41
1:B:333:MET:O	1:B:336:HIS:N	2.53	0.41
1:B:173:ASN:CB	1:B:176:TRP:CZ2	3.03	0.41
1:A:185:PHE:CE1	1:A:189:VAL:HG21	2.55	0.41
1:B:195:MET:HE3	1:B:199:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:GLN:HA	1:A:74:GLN:OE1	2.21	0.41
1:B:255:TYR:O	1:B:259:ASN:HB2	2.20	0.41
1:A:366:ALA:O	1:A:370:THR:HG23	2.21	0.41
1:A:107:ASN:HD22	1:A:167:SER:H	1.69	0.41
1:A:157:GLN:HB3	1:A:157:GLN:HE21	1.52	0.41
1:A:161:ASP:OD1	1:A:163:ARG:HB2	2.20	0.41
1:A:152:ALA:HB2	1:A:168:PHE:CE2	2.55	0.40
1:B:155:HIS:HB2	1:B:356:LEU:HD11	2.02	0.40
1:A:158:LEU:HD23	1:A:360:ARG:HG2	2.03	0.40
1:B:82:PRO:HD2	1:B:117:ALA:HB2	2.03	0.40
1:B:76:ILE:N	1:B:76:ILE:HD12	2.37	0.40

All (1) 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:A:157:GLN:O	1:B:331:HIS:NE2[2_554]	2.08	0.12

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	300/356 (84%)	282 (94%)	15 (5%)	3 (1%)	19	48
1	B	300/356 (84%)	282 (94%)	15 (5%)	3 (1%)	19	48
All	All	600/712 (84%)	564 (94%)	30 (5%)	6 (1%)	19	48

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	373	LEU
1	B	373	LEU

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Mol	Chain	Res	Type
1	A	263	GLY
1	B	263	GLY
1	B	182	LEU
1	A	182	LEU

5.3.2 Protein sidechains (i)

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	252/292 (86%)	230 (91%)	22 (9%)	13	32
1	B	252/292 (86%)	229 (91%)	23 (9%)	12	30
All	All	504/584 (86%)	459 (91%)	45 (9%)	12	31

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	PHE
1	A	52	PHE
1	A	87	LEU
1	A	142	ARG
1	A	157	GLN
1	A	180	GLN
1	A	182	LEU
1	A	189	VAL
1	A	199	LEU
1	A	200	SER
1	A	222	GLN
1	A	229	PHE
1	A	239	ARG
1	A	245	SER
1	A	252	MET
1	A	262	THR
1	A	275	THR
1	A	293	ASN
1	A	322	THR

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Mol	Chain	Res	Type
1	A	330	ASP
1	A	335	LEU
1	A	357	VAL
1	B	51	PHE
1	B	52	PHE
1	B	77	TYR
1	B	134	THR
1	B	142	ARG
1	B	157	GLN
1	B	180	GLN
1	B	182	LEU
1	B	189	VAL
1	B	199	LEU
1	B	200	SER
1	B	204	VAL
1	B	222	GLN
1	B	229	PHE
1	B	239	ARG
1	B	245	SER
1	B	252	MET
1	B	262	THR
1	B	275	THR
1	B	293	ASN
1	B	322	THR
1	B	335	LEU
1	B	357	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	91	HIS
1	A	102	GLN
1	A	107	ASN
1	A	157	GLN
1	A	180	GLN
1	A	336	HIS
1	B	42	GLN
1	B	91	HIS
1	B	102	GLN
1	B	107	ASN
1	B	157	GLN

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Mol	Chain	Res	Type
1	B	180	GLN
1	B	336	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

2 ligands 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	TYA	A	1374	-	32,37,37	1.10	4 (12%)	32,54,54	1.77	3 (9%)
2	TYA	B	1374	-	32,37,37	1.13	5 (15%)	32,54,54	1.78	3 (9%)

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	TYA	A	1374	-	-	0/16/36/36	0/4/4/4
2	TYA	B	1374	-	-	0/16/36/36	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1374	TYA	OPP-C	-3.43	1.30	1.44
2	B	1374	TYA	OPP-C	-3.11	1.32	1.44
2	A	1374	TYA	CB-CG	2.13	1.56	1.51
2	A	1374	TYA	C6-N6	2.20	1.41	1.34
2	B	1374	TYA	C2-N3	2.27	1.36	1.32
2	B	1374	TYA	C6-N6	2.32	1.42	1.34
2	B	1374	TYA	CB-CG	2.50	1.57	1.51
2	B	1374	TYA	P-O1P	2.63	1.60	1.51
2	A	1374	TYA	P-O1P	2.87	1.61	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1374	TYA	N3-C2-N1	-8.57	122.33	128.89
2	B	1374	TYA	N3-C2-N1	-8.39	122.47	128.89
2	A	1374	TYA	C1'-N9-C4	-3.46	121.72	126.94
2	B	1374	TYA	C4-C5-N7	-2.74	106.95	109.48
2	A	1374	TYA	C4-C5-N7	-2.28	107.38	109.48
2	B	1374	TYA	CG-CB-CA	3.54	119.64	113.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1374	TYA	1	0
2	B	1374	TYA	2	0

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, 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	306/356 (85%)	0.80	36 (11%)	6	4	57, 91, 147, 185	1 (0%)
1	B	306/356 (85%)	1.05	62 (20%)	1	1	50, 91, 149, 184	1 (0%)
All	All	612/712 (85%)	0.93	98 (16%)	3	2	50, 91, 150, 185	2 (0%)

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	206	LEU	10.7
1	B	126	THR	7.5
1	B	339	GLU	7.3
1	B	338	LYS	7.2
1	A	337	VAL	7.1
1	B	372	ALA	6.6
1	A	368	ARG	6.4
1	A	341	GLU	5.3
1	B	78	CYS	5.2
1	B	373	LEU	5.1
1	A	342	ARG	4.9
1	B	374	TYR	4.9
1	B	331	HIS	4.7
1	B	334	GLN	4.7
1	B	204	VAL	4.7
1	B	289	ALA	4.6
1	B	212	GLU	4.6
1	A	369	CYS	4.5
1	B	211	PRO	4.4
1	B	127	LYS	4.4
1	B	37	GLY	4.4
1	A	261	LEU	4.4
1	B	263	GLY	4.3
1	B	208	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	166	GLY	4.3
1	B	202	GLN	4.1
1	A	105	GLY	4.0
1	A	265	ASP	3.9
1	A	310	PRO	3.9
1	B	371	GLN	3.8
1	A	156	GLN	3.8
1	B	335	LEU	3.8
1	A	340	PRO	3.7
1	B	162	GLY	3.6
1	A	338	LYS	3.6
1	B	297	THR	3.4
1	B	79	GLY	3.3
1	A	343	ARG	3.3
1	A	264	GLU	3.3
1	B	135	GLU	3.3
1	B	165	TRP	3.2
1	B	304	GLN	3.2
1	A	130	GLU	3.1
1	B	40	ALA	3.0
1	B	242	LEU	3.0
1	A	370	THR	3.0
1	A	372	ALA	3.0
1	B	305	PHE	3.0
1	B	300	PHE	3.0
1	A	164	SER	2.9
1	B	294	ARG	2.9
1	A	129	ARG	2.9
1	A	257	PHE	2.9
1	A	311	ASP	2.8
1	B	164	SER	2.8
1	B	133	GLU	2.8
1	A	263	GLY	2.8
1	A	220	PHE	2.7
1	B	80	PHE	2.7
1	B	337	VAL	2.7
1	B	369	CYS	2.7
1	B	96	LEU	2.7
1	B	111	LEU	2.7
1	B	342	ARG	2.6
1	B	92	LEU	2.6
1	A	79	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	162	GLY	2.6
1	B	322	THR	2.5
1	B	299	PRO	2.5
1	A	374	TYR	2.5
1	B	132	LEU	2.5
1	A	128	GLU	2.5
1	B	156	GLN	2.5
1	A	94	ALA	2.5
1	B	134	THR	2.5
1	A	373	LEU	2.4
1	B	291	TRP	2.4
1	B	298	SER	2.3
1	B	207	ARG	2.3
1	A	313	SER	2.3
1	A	371	GLN	2.3
1	B	225	GLN	2.3
1	A	78	CYS	2.2
1	A	127	LYS	2.2
1	B	224	LEU	2.2
1	B	366	ALA	2.2
1	A	132	LEU	2.2
1	B	321	PHE	2.2
1	B	222	GLN	2.2
1	B	77	TYR	2.2
1	B	131	ALA	2.1
1	B	311	ASP	2.1
1	B	368	ARG	2.1
1	B	290	VAL	2.1
1	B	221	TYR	2.1
1	B	199	LEU	2.0
1	A	242	LEU	2.0
1	B	94	ALA	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

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, 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	LLDF	B-factors(Å^2)	Q<0.9
2	TYA	A	1374	34/34	0.96	0.26	0.39	42,69,94,99	0
2	TYA	B	1374	34/34	0.94	0.26	-0.03	45,76,90,91	0

6.5 Other polymers (i)

There are no such residues in this entry.