



# Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2020 – 05:12 pm BST

PDB ID : 3PDX  
Title : Crystal structural of mouse tyrosine aminotransferase  
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Deposited on : 2010-10-25  
Resolution : 2.91 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

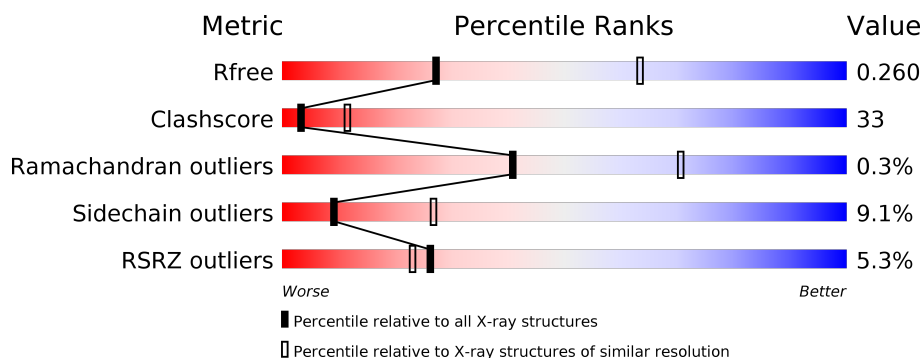
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.91 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))
$R_{free}$	130704	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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 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	402	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3014 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 Tyrosine aminotransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	P	S	0	0	0
			2976	1901	491	560	1	23			

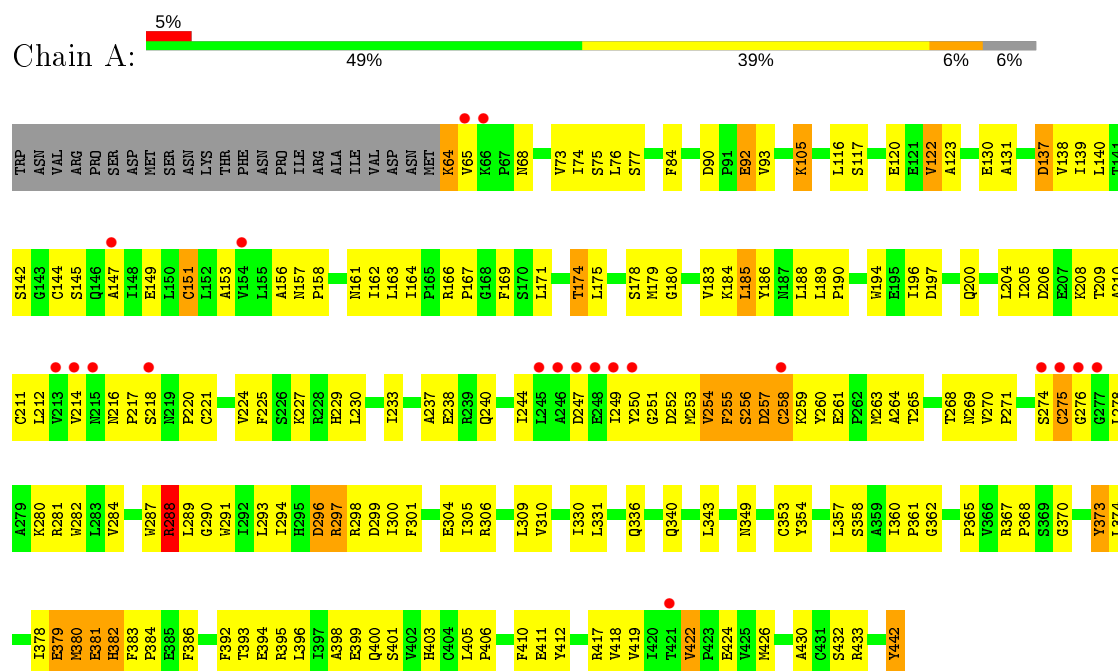
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	38	Total	O	0	0
			38	38		

### 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 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: Tyrosine aminotransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.28 Å   84.84 Å   157.99 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	28.94 – 2.91 28.94 – 2.91	Depositor EDS
% Data completeness (in resolution range)	87.3 (28.94-2.91) 87.3 (28.94-2.91)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.18 (at 2.90 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.263   ,   0.295 0.259   ,   0.260	Depositor DCC
$R_{free}$ test set	452 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	91.5	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 58.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3014	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: 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	0.85	1/3019 (0.0%)	0.83	5/4104 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	304	GLU	CG-CD	5.20	1.59	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	ALA	CB-CA-C	5.89	118.93	110.10
1	A	288	ARG	NE-CZ-NH1	5.89	123.24	120.30
1	A	254	VAL	CB-CA-C	-5.39	101.15	111.40
1	A	268	THR	N-CA-CB	-5.02	100.77	110.30
1	A	296	ASP	CB-CA-C	5.00	120.41	110.40

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	2976	0	2962	194	0
2	A	38	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3014	0	2962	194	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 33.

All (194) 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:251:GLY:HA2	1:A:260:TYR:OH	1.49	1.12
1:A:382:HIS:ND1	1:A:442:TYR:HE1	1.50	1.08
1:A:382:HIS:ND1	1:A:442:TYR:CE1	2.23	1.06
1:A:64:LYS:HD2	1:A:64:LYS:N	1.74	0.99
1:A:190:PRO:HG3	1:A:194:TRP:CZ3	2.01	0.95
1:A:158:PRO:HA	1:A:180:GLY:O	1.69	0.92
1:A:251:GLY:HA2	1:A:260:TYR:CZ	2.04	0.91
1:A:255:PHE:CE2	1:A:370:GLY:HA2	2.06	0.89
1:A:251:GLY:CA	1:A:260:TYR:OH	2.21	0.87
1:A:362:GLY:O	1:A:379:GLU:HG3	1.75	0.86
1:A:382:HIS:HD1	1:A:442:TYR:HE1	0.93	0.85
1:A:288:ARG:HH11	1:A:288:ARG:HG2	1.41	0.85
1:A:250:TYR:O	1:A:253:MET:HB2	1.77	0.84
1:A:256:SER:OG	1:A:258:CYS:SG	2.36	0.84
1:A:442:TYR:O	1:A:442:TYR:CG	2.30	0.84
1:A:183:VAL:HA	2:A:4:HOH:O	1.76	0.83
1:A:220:PRO:HG3	1:A:410:PHE:CG	2.18	0.79
1:A:65:VAL:HG23	2:A:26:HOH:O	1.81	0.79
1:A:380:MET:O	1:A:381:GLU:OE1	2.00	0.78
1:A:381:GLU:HB2	1:A:382:HIS:CD2	2.20	0.77
1:A:382:HIS:CB	1:A:442:TYR:CD1	2.68	0.76
1:A:373:TYR:HD2	1:A:419:VAL:HG12	1.50	0.75
1:A:288:ARG:CG	1:A:288:ARG:HH11	2.00	0.74
1:A:301:PHE:CD1	1:A:305:ILE:HG21	2.22	0.74
1:A:175:LEU:O	1:A:179:MET:HG2	1.86	0.74
1:A:205:ILE:HG21	1:A:240:GLN:HG2	1.70	0.74
1:A:296:ASP:CG	1:A:301:PHE:HB2	2.08	0.73
1:A:382:HIS:O	1:A:442:TYR:C	2.27	0.73
1:A:442:TYR:CD2	1:A:442:TYR:O	2.41	0.72
1:A:380:MET:HE1	1:A:386:PHE:O	1.88	0.72
1:A:382:HIS:HB2	1:A:442:TYR:CD1	2.24	0.72
1:A:220:PRO:HG3	1:A:410:PHE:CD1	2.25	0.72
1:A:373:TYR:CD2	1:A:419:VAL:HG12	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:PHE:HE2	1:A:370:GLY:HA2	1.54	0.70
1:A:75:SER:HA	1:A:403:HIS:HB2	1.74	0.70
1:A:161:ASN:HD21	1:A:208:LYS:HB2	1.57	0.69
1:A:381:GLU:CD	1:A:381:GLU:N	2.46	0.69
1:A:382:HIS:HB2	1:A:442:TYR:HD1	1.57	0.68
1:A:251:GLY:HA2	1:A:260:TYR:HH	1.56	0.68
1:A:166:ARG:CD	1:A:411:GLU:O	2.42	0.67
1:A:162:ILE:HG22	1:A:211:CYS:HB3	1.77	0.67
1:A:255:PHE:CD2	1:A:255:PHE:N	2.63	0.67
1:A:381:GLU:HB2	1:A:382:HIS:HD2	1.57	0.67
1:A:93:VAL:HG22	1:A:330:ILE:HG23	1.76	0.67
1:A:380:MET:C	1:A:381:GLU:CD	2.53	0.66
1:A:380:MET:C	1:A:381:GLU:OE1	2.33	0.66
1:A:255:PHE:HB2	2:A:9:HOH:O	1.95	0.66
1:A:380:MET:N	1:A:381:GLU:OE2	2.30	0.65
1:A:382:HIS:CD2	1:A:382:HIS:N	2.63	0.64
1:A:271:PRO:HB2	1:A:301:PHE:CE2	2.34	0.63
1:A:297:ARG:O	1:A:298:ARG:HB2	1.99	0.62
1:A:122:VAL:HG23	1:A:331:LEU:HD11	1.81	0.62
1:A:382:HIS:C	1:A:384:PRO:HD3	2.19	0.62
1:A:379:GLU:O	1:A:381:GLU:N	2.31	0.61
1:A:163:LEU:CD2	1:A:184:LYS:HB2	2.29	0.61
1:A:166:ARG:HG3	1:A:411:GLU:HB2	1.81	0.61
1:A:382:HIS:CG	1:A:442:TYR:CD1	2.88	0.61
1:A:123:ALA:HB2	1:A:138:VAL:HG21	1.82	0.61
1:A:161:ASN:ND2	1:A:208:LYS:HB2	2.15	0.60
1:A:166:ARG:HD2	1:A:411:GLU:O	2.02	0.60
1:A:382:HIS:CB	1:A:442:TYR:HD1	2.13	0.60
1:A:131:ALA:HB2	1:A:265:THR:HA	1.83	0.60
1:A:353:CYS:SG	1:A:374:LEU:HD21	2.43	0.59
1:A:214:VAL:HG11	1:A:263:MET:SD	2.42	0.59
1:A:382:HIS:ND1	1:A:442:TYR:CD1	2.70	0.59
1:A:254:VAL:O	1:A:343:LEU:HD13	2.02	0.59
1:A:227:LYS:HG3	1:A:261:GLU:HG2	1.84	0.58
1:A:300:ILE:H	1:A:300:ILE:HD12	1.68	0.58
1:A:162:ILE:HD12	1:A:164:ILE:HD11	1.85	0.57
1:A:167:PRO:HB3	1:A:412:TYR:HB2	1.86	0.57
1:A:383:PHE:CZ	1:A:442:TYR:HB2	2.38	0.57
1:A:289:LEU:HG	1:A:290:GLY:N	2.20	0.57
1:A:156:ALA:HB2	1:A:210:ALA:CB	2.35	0.57
1:A:396:LEU:HD12	1:A:400:GLN:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:PHE:CE2	1:A:370:GLY:CA	2.86	0.56
1:A:188:LEU:HD22	1:A:221:CYS:SG	2.46	0.56
1:A:400:GLN:O	1:A:401:SER:HB2	2.06	0.56
1:A:144:CYS:HA	1:A:147:ALA:HB3	1.87	0.56
1:A:73:VAL:HA	1:A:401:SER:HB3	1.88	0.56
1:A:254:VAL:HG11	1:A:260:TYR:HB2	1.88	0.55
1:A:188:LEU:HB3	1:A:194:TRP:HB3	1.89	0.55
1:A:142:SER:HA	1:A:288:ARG:O	2.06	0.55
1:A:378:ILE:HD13	1:A:392:PHE:CD2	2.42	0.55
1:A:288:ARG:NH1	1:A:288:ARG:HG2	2.07	0.55
1:A:217:PRO:HG3	1:A:224:VAL:HG22	1.90	0.54
1:A:211:CYS:SG	1:A:212:LEU:N	2.81	0.54
1:A:254:VAL:HG22	1:A:255:PHE:N	2.23	0.54
1:A:360:ILE:HG23	1:A:361:PRO:HD2	1.90	0.54
1:A:383:PHE:CE1	1:A:442:TYR:HB2	2.43	0.54
1:A:264:ALA:O	1:A:297:ARG:NH2	2.41	0.53
1:A:185:LEU:HD23	1:A:185:LEU:N	2.24	0.53
1:A:382:HIS:O	1:A:442:TYR:HA	2.09	0.52
1:A:147:ALA:O	1:A:151:CYS:HB2	2.09	0.52
1:A:188:LEU:O	1:A:190:PRO:HD3	2.09	0.52
1:A:251:GLY:CA	1:A:260:TYR:CZ	2.84	0.52
1:A:161:ASN:O	1:A:209:THR:HA	2.09	0.51
1:A:298:ARG:C	1:A:300:ILE:HD12	2.30	0.51
1:A:163:LEU:HD23	1:A:184:LYS:HB2	1.93	0.51
1:A:306:ARG:O	1:A:310:VAL:HG23	2.11	0.51
1:A:380:MET:CE	1:A:386:PHE:O	2.57	0.51
1:A:383:PHE:CE1	1:A:442:TYR:CB	2.93	0.51
1:A:255:PHE:HB3	1:A:343:LEU:HB3	1.93	0.51
1:A:164:ILE:O	1:A:186:TYR:CD2	2.63	0.50
1:A:383:PHE:N	1:A:384:PRO:HD3	2.24	0.50
1:A:393:THR:OG1	1:A:406:PRO:HG3	2.12	0.50
1:A:382:HIS:CG	1:A:442:TYR:HD1	2.29	0.50
1:A:298:ARG:CB	1:A:300:ILE:HD11	2.41	0.50
1:A:252:ASP:N	1:A:260:TYR:CZ	2.76	0.49
1:A:105:LYS:HD2	1:A:105:LYS:O	2.12	0.49
1:A:131:ALA:HA	1:A:297:ARG:NH2	2.28	0.49
1:A:196:ILE:HD12	1:A:233:ILE:HG12	1.93	0.49
1:A:362:GLY:C	1:A:379:GLU:HG3	2.33	0.49
1:A:382:HIS:N	1:A:382:HIS:HD2	2.10	0.49
1:A:166:ARG:NE	1:A:411:GLU:O	2.46	0.49
1:A:300:ILE:N	1:A:300:ILE:HD12	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:LEU:HD23	1:A:194:TRP:O	2.13	0.49
1:A:382:HIS:O	1:A:442:TYR:CA	2.61	0.49
1:A:395:ARG:O	1:A:399:GLU:HG3	2.13	0.49
1:A:130:GLU:HB3	1:A:265:THR:O	2.13	0.48
1:A:288:ARG:HH11	1:A:288:ARG:CB	2.25	0.48
1:A:189:LEU:C	1:A:194:TRP:HA	2.34	0.48
1:A:252:ASP:N	1:A:260:TYR:CE2	2.80	0.48
1:A:298:ARG:HB2	1:A:300:ILE:CD1	2.43	0.48
1:A:383:PHE:CD1	1:A:442:TYR:HA	2.49	0.48
1:A:238:GLU:OE1	1:A:269:ASN:HB2	2.14	0.48
1:A:247:ASP:OD1	1:A:249:ILE:HG22	2.13	0.48
1:A:76:LEU:HD13	1:A:418:VAL:HG23	1.95	0.47
1:A:197:ASP:O	1:A:200:GLN:HB2	2.14	0.47
1:A:254:VAL:CG2	1:A:255:PHE:N	2.78	0.47
1:A:298:ARG:CB	1:A:300:ILE:CD1	2.93	0.47
1:A:76:LEU:HB3	1:A:418:VAL:HG23	1.96	0.47
1:A:77:SER:O	1:A:417:ARG:NH2	2.46	0.46
1:A:175:LEU:O	1:A:179:MET:N	2.49	0.46
1:A:220:PRO:HB3	1:A:417:ARG:HD3	1.96	0.46
1:A:139:ILE:CD1	1:A:309:LEU:HB3	2.46	0.46
1:A:281:ARG:HB3	1:A:282:TRP:CE3	2.51	0.46
1:A:274:SER:HB2	1:A:293:LEU:HB2	1.97	0.46
1:A:379:GLU:C	1:A:381:GLU:OE2	2.54	0.45
1:A:174:THR:O	1:A:178:SER:OG	2.27	0.45
1:A:189:LEU:O	1:A:194:TRP:HA	2.16	0.45
1:A:405:LEU:HD23	1:A:410:PHE:CE2	2.51	0.45
1:A:116:LEU:O	1:A:120:GLU:HG3	2.15	0.45
1:A:166:ARG:CG	1:A:411:GLU:HB2	2.45	0.45
1:A:298:ARG:HB3	1:A:300:ILE:HD11	1.99	0.45
1:A:144:CYS:HB3	1:A:280:LLP:H6	1.98	0.45
1:A:288:ARG:HH11	1:A:288:ARG:CA	2.30	0.45
1:A:189:LEU:O	1:A:194:TRP:N	2.50	0.45
1:A:284:VAL:HB	1:A:287:TRP:CD2	2.52	0.45
1:A:336:GLN:O	1:A:340:GLN:HG2	2.17	0.45
1:A:137:ASP:HB3	1:A:294:ILE:HB	1.99	0.44
1:A:252:ASP:OD1	1:A:260:TYR:CD2	2.70	0.44
1:A:74:ILE:HG21	1:A:430:ALA:HB2	1.99	0.44
1:A:145:SER:O	1:A:149:GLU:HB2	2.18	0.44
1:A:90:ASP:OD2	1:A:92:GLU:HB2	2.18	0.44
1:A:196:ILE:HG13	1:A:229:HIS:NE2	2.32	0.43
1:A:212:LEU:O	1:A:244:ILE:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:VAL:CG1	1:A:260:TYR:HB2	2.49	0.43
1:A:278:LEU:HA	1:A:282:TRP:CE3	2.53	0.43
1:A:424:GLU:C	1:A:426:MET:N	2.72	0.43
1:A:225:PHE:HB2	1:A:230:LEU:HD21	2.00	0.43
1:A:353:CYS:O	1:A:357:LEU:HB2	2.19	0.43
1:A:68:ASN:N	1:A:398:ALA:O	2.52	0.43
1:A:275:CYS:SG	1:A:276:GLY:N	2.92	0.43
1:A:357:LEU:HB3	1:A:365:PRO:HG3	1.99	0.43
1:A:256:SER:O	1:A:257:ASP:C	2.56	0.43
1:A:271:PRO:HB2	1:A:301:PHE:CZ	2.54	0.43
1:A:354:TYR:C	1:A:354:TYR:CD2	2.92	0.43
1:A:140:LEU:HD23	1:A:291:TRP:HB3	2.00	0.42
1:A:166:ARG:HA	1:A:167:PRO:HA	1.75	0.42
1:A:216:ASN:HA	1:A:217:PRO:C	2.39	0.42
1:A:354:TYR:CE1	1:A:367:ARG:HB2	2.54	0.42
1:A:382:HIS:CE1	1:A:442:TYR:HE1	2.29	0.42
1:A:230:LEU:HA	1:A:233:ILE:HD12	2.01	0.42
1:A:218:SER:HB3	1:A:221:CYS:HB2	2.01	0.42
1:A:270:VAL:HG13	1:A:271:PRO:HD2	2.01	0.42
1:A:117:SER:O	1:A:120:GLU:HB2	2.20	0.42
1:A:237:ALA:HB2	1:A:244:ILE:HD11	2.01	0.42
1:A:169:PHE:CD2	1:A:171:LEU:HB3	2.54	0.42
1:A:76:LEU:HD13	1:A:418:VAL:CG2	2.50	0.42
1:A:189:LEU:HA	1:A:189:LEU:HD23	1.94	0.41
1:A:368:PRO:HG3	1:A:374:LEU:HB3	2.02	0.41
1:A:432:SER:O	1:A:433:ARG:C	2.58	0.41
1:A:405:LEU:HD23	1:A:410:PHE:HE2	1.86	0.41
1:A:251:GLY:HA3	1:A:260:TYR:OH	2.15	0.41
1:A:362:GLY:O	1:A:383:PHE:HE2	2.03	0.41
1:A:166:ARG:HD3	1:A:185:LEU:HD12	2.03	0.41
1:A:255:PHE:HE2	1:A:370:GLY:CA	2.27	0.41
1:A:64:LYS:N	1:A:64:LYS:CD	2.62	0.41
1:A:298:ARG:HB2	1:A:300:ILE:HD11	2.01	0.41
1:A:205:ILE:CG2	1:A:240:GLN:HG2	2.46	0.41
1:A:396:LEU:O	1:A:400:GLN:HB2	2.21	0.41
1:A:249:ILE:HA	1:A:276:GLY:HA2	2.03	0.40
1:A:76:LEU:CD2	1:A:422:VAL:HG11	2.52	0.40
1:A:424:GLU:C	1:A:426:MET:H	2.24	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	376/402 (94%)	344 (92%)	31 (8%)	1 (0%)	41 70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	380	MET

### 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	331/353 (94%)	301 (91%)	30 (9%)	9 27

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	LYS
1	A	84	PHE
1	A	92	GLU
1	A	105	LYS
1	A	122	VAL
1	A	137	ASP
1	A	151	CYS
1	A	157	ASN
1	A	174	THR
1	A	185	LEU

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Mol	Chain	Res	Type
1	A	204	LEU
1	A	206	ASP
1	A	255	PHE
1	A	256	SER
1	A	257	ASP
1	A	258	CYS
1	A	259	LYS
1	A	275	CYS
1	A	288	ARG
1	A	297	ARG
1	A	299	ASP
1	A	349	ASN
1	A	358	SER
1	A	373	TYR
1	A	379	GLU
1	A	381	GLU
1	A	382	HIS
1	A	394	GLU
1	A	422	VAL
1	A	442	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	160	GLN
1	A	215	ASN
1	A	231	GLN
1	A	295	HIS
1	A	332	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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
1	LLP	A	280	1	23,24,25	1.92	7 (30%)	25,32,34	1.54	2 (8%)

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	280	1	-	7/16/17/19	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	LLP	O3-C3	-4.63	1.26	1.37
1	A	280	LLP	C4-C4'	4.04	1.54	1.46
1	A	280	LLP	C2-N1	3.00	1.39	1.33
1	A	280	LLP	C4'-NZ	2.58	1.35	1.27
1	A	280	LLP	C6-N1	2.46	1.39	1.34
1	A	280	LLP	CE-NZ	2.40	1.52	1.46
1	A	280	LLP	C4-C3	2.24	1.44	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	LLP	OP4-C5'-C5	5.82	120.44	109.35
1	A	280	LLP	C4-C4'-NZ	-2.13	114.55	124.31

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	280	LLP	C5'-OP4-P-OP1
1	A	280	LLP	C5'-OP4-P-OP2
1	A	280	LLP	C5'-OP4-P-OP3
1	A	280	LLP	C4-C4'-NZ-CE

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Mol	Chain	Res	Type	Atoms
1	A	280	LLP	C3-C4-C4'-NZ
1	A	280	LLP	CD-CE-NZ-C4'
1	A	280	LLP	C5-C4-C4'-NZ

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	280	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	378/402 (94%)	0.29	20 (5%) 26 23	61, 105, 134, 140	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	275	CYS	4.7
1	A	215	ASN	4.6
1	A	214	VAL	3.6
1	A	246	ALA	3.6
1	A	249	ILE	3.2
1	A	247	ASP	3.2
1	A	276	GLY	3.1
1	A	245	LEU	3.0
1	A	147	ALA	2.7
1	A	258	CYS	2.5
1	A	274	SER	2.5
1	A	213	VAL	2.4
1	A	248	GLU	2.4
1	A	277	GLY	2.4
1	A	66	LYS	2.3
1	A	421	THR	2.2
1	A	250	TYR	2.2
1	A	154	VAL	2.1
1	A	65	VAL	2.1
1	A	218	SER	2.0

### 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, 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	B-factors( $\text{\AA}^2$ )	Q<0.9
1	LLP	A	280	24/25	0.94	0.29	76,102,106,107	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.