



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2021 – 09:02 PM EDT

PDB ID : 2D1W  
Title : Substrate Schiff-Base intermediate with tyramine in copper amine oxidase from *Arthrobacter globiformis*  
Authors : Murakawa, T.; Okajima, T.; Kuroda, S.; Nakamoto, T.; Taki, M.; Yamamoto, Y.; Hayashi, H.; Tanizawa, K.  
Deposited on : 2005-09-01  
Resolution : 1.74 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 : 2.23.2  
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) : 2.23.2

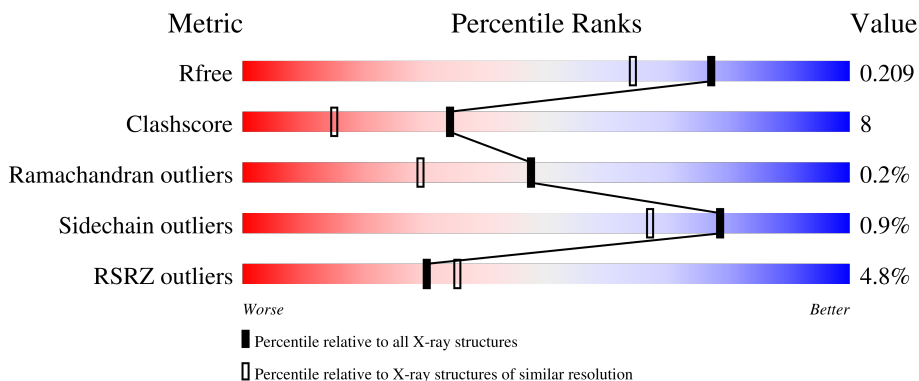
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.74 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	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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 of 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	638	
1	B	638	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10930 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 Phenylethylamine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	620	4897	3098	858	932	9	0	1	0
1	B	620	4897	3098	858	932	9	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	298	ALA	ASP	engineered mutation	UNP P46881
A	382	TTS	TYR	modified residue	UNP P46881
B	298	ALA	ASP	engineered mutation	UNP P46881
B	382	TTS	TYR	modified residue	UNP P46881

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cu	0	0
			1	1		
2	B	1	Total	Cu	0	0
			1	1		

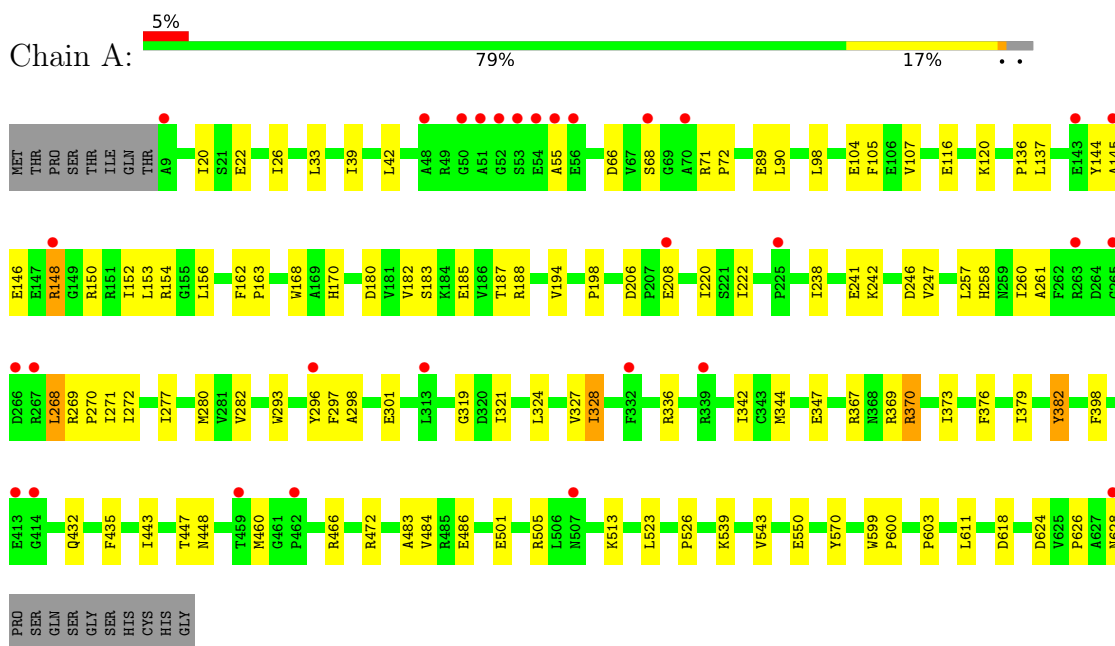
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	547	Total	O	0	0
			547	547		
3	B	587	Total	O	0	0
			587	587		

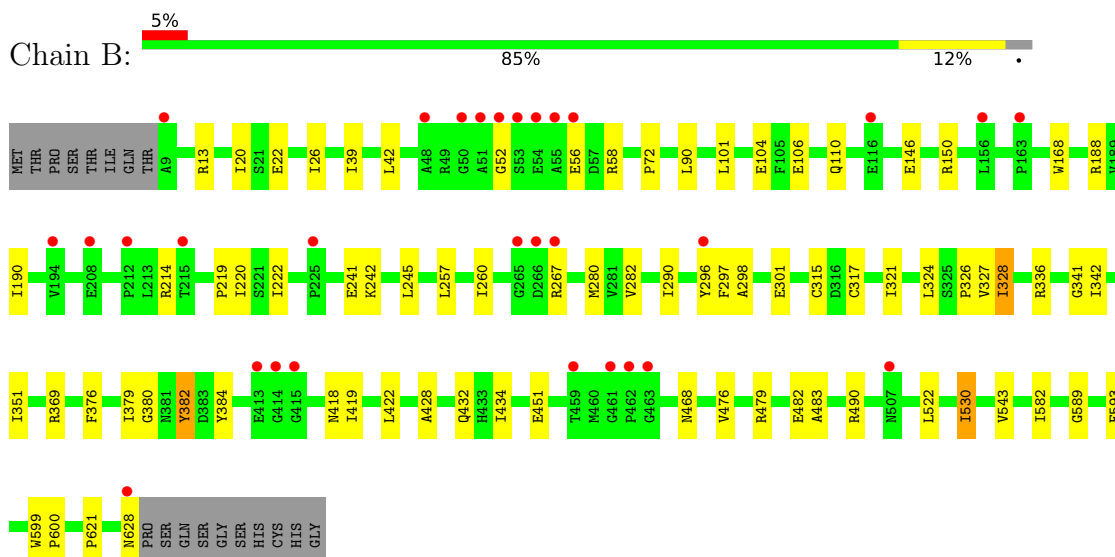
### 3 Residue-property plots i

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: Phenylethylamine oxidase



- Molecule 1: Phenylethylamine oxidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	157.57Å 63.35Å 183.65Å 90.00° 112.29° 90.00°	Depositor
Resolution (Å)	26.44 – 1.74 26.49 – 1.74	Depositor EDS
% Data completeness (in resolution range)	(Not available) (26.44-1.74) 99.8 (26.49-1.74)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.40 (at 1.74Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.190 , 0.217 0.183 , 0.209	Depositor DCC
$R_{free}$ test set	8601 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.7	Xtrriage
Anisotropy	0.704	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 63.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	10930	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.60 % 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 4.8718e-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, 0.333 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: TTS, CU

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	0.30	0/4972	0.64	0/6770
1	B	0.32	0/4972	0.64	1/6770 (0.0%)
All	All	0.31	0/9944	0.64	1/13540 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	593	PHE	N-CA-C	-5.04	97.40	111.00

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	4897	0	4711	90	0
1	B	4897	0	4709	76	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	547	0	0	6	0
3	B	587	0	0	4	0
All	All	10930	0	9420	161	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 8.

All (161) 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:168:TRP:HH2	1:B:382[A]:TTS:H5'	1.08	1.13
1:B:168:TRP:CH2	1:B:382[A]:TTS:H5'	2.00	0.95
1:B:382[A]:TTS:O1	3:B:1411:HOH:O	1.97	0.81
1:B:341:GLY:C	1:B:342:ILE:HD12	2.08	0.73
1:B:422:LEU:HD11	1:B:428:ALA:HB2	1.71	0.72
1:A:104:GLU:O	1:A:107:VAL:HG22	1.90	0.71
1:B:328:ILE:HD13	1:B:336:ARG:O	1.91	0.70
1:B:326:PRO:HD3	1:B:342:ILE:HD13	1.74	0.69
1:A:238:ILE:HG13	1:A:344:MET:HE1	1.75	0.68
1:A:505:ARG:HD3	1:A:618:ASP:HB3	1.76	0.68
1:A:22:GLU:O	1:A:26:ILE:HG12	1.94	0.68
1:A:624:ASP:CG	1:B:214:ARG:HD2	2.13	0.68
1:B:220:ILE:HG22	1:B:222:ILE:HD11	1.74	0.68
1:A:328:ILE:HD13	1:A:336:ARG:O	1.94	0.67
1:A:66:ASP:OD1	1:A:68:SER:HB3	1.95	0.67
1:A:168:TRP:HH2	1:A:382[A]:TTS:H5'	1.60	0.66
1:A:180:ASP:OD1	1:A:182:VAL:HG22	1.97	0.65
1:A:33:LEU:HD11	1:A:39:ILE:HD11	1.79	0.64
1:A:170:HIS:HD2	1:A:198:PRO:O	1.81	0.64
1:A:187:THR:O	1:A:188:ARG:HG3	1.98	0.64
1:A:206:ASP:CG	1:A:208:GLU:HG2	2.18	0.64
1:B:257:LEU:HB3	1:B:260:ILE:HD11	1.80	0.64
1:A:347:GLU:OE1	1:A:370:ARG:HD3	1.97	0.63
1:A:247:VAL:HG21	1:A:344:MET:HE1	1.80	0.62
1:A:247:VAL:HG21	1:A:344:MET:CE	2.30	0.62
1:A:146:GLU:O	1:A:150:ARG:HD3	1.99	0.62
3:A:1174:HOH:O	1:B:621:PRO:HD2	1.99	0.62
1:B:599:TRP:CD2	1:B:600:PRO:HA	2.35	0.62
1:A:206:ASP:OD1	1:A:208:GLU:HG2	2.00	0.62
1:A:137:LEU:HD12	1:A:293:TRP:HH2	1.64	0.61
1:B:146:GLU:O	1:B:150:ARG:HD3	2.00	0.61
1:B:530:ILE:HD13	1:B:530:ILE:O	2.00	0.61
1:A:328:ILE:HD13	1:A:328:ILE:H	1.65	0.61
1:A:162:PHE:HB2	1:A:163:PRO:HD2	1.84	0.60
1:B:220:ILE:HG22	1:B:222:ILE:CD1	2.31	0.60
1:A:472:ARG:HD3	3:A:1490:HOH:O	2.01	0.59
1:B:290:ILE:HD12	1:B:290:ILE:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:ALA:HB1	1:A:268:LEU:HD22	1.85	0.58
1:A:260:ILE:HD12	1:A:260:ILE:N	2.17	0.58
1:A:599:TRP:CD2	1:A:600:PRO:HA	2.38	0.58
1:A:443:ILE:H	1:A:448:ASN:HD21	1.53	0.57
1:B:328:ILE:HD13	1:B:328:ILE:H	1.69	0.57
1:A:526:PRO:HG3	3:B:1208:HOH:O	2.04	0.57
1:A:282:VAL:HB	1:A:296:TYR:CE2	2.40	0.57
1:A:483:ALA:HB1	1:A:543:VAL:HB	1.86	0.57
1:B:342:ILE:HD12	1:B:342:ILE:N	2.20	0.57
1:A:72:PRO:HG2	1:A:90:LEU:HB2	1.85	0.56
1:B:106:GLU:O	1:B:110:GLN:HG3	2.05	0.56
1:A:432:GLN:HE22	1:A:523:LEU:H	1.53	0.56
1:B:39:ILE:HD12	1:B:39:ILE:N	2.22	0.55
1:A:222:ILE:HD12	1:A:222:ILE:N	2.22	0.55
1:A:144:TYR:CD2	1:A:188:ARG:NH1	2.76	0.54
1:B:222:ILE:HD12	1:B:222:ILE:N	2.22	0.54
1:A:277:ILE:HD12	1:A:277:ILE:N	2.22	0.54
1:A:324:LEU:HB2	1:A:342:ILE:HB	1.90	0.53
1:A:137:LEU:HD12	1:A:293:TRP:CH2	2.43	0.53
1:B:280:MET:CG	1:B:298:ALA:HB3	2.39	0.52
1:B:296:TYR:HH	1:B:384:TYR:HE2	1.56	0.51
1:A:321:ILE:N	1:A:321:ILE:HD12	2.25	0.51
1:A:220:ILE:HG22	1:A:222:ILE:HD11	1.92	0.51
1:B:245:LEU:HB2	1:B:260:ILE:HD13	1.92	0.51
1:B:379:ILE:O	1:B:382[A]:TTS:HD2	2.10	0.51
1:A:145:ALA:O	1:A:148:ARG:HD3	2.11	0.51
1:A:271:ILE:HG22	1:A:272:ILE:HG13	1.93	0.51
1:A:246:ASP:HB2	1:A:258:HIS:HB2	1.93	0.51
1:B:326:PRO:CD	1:B:342:ILE:HD13	2.40	0.51
1:B:72:PRO:HG2	1:B:90:LEU:HB2	1.94	0.50
1:A:39:ILE:HD12	1:A:39:ILE:N	2.26	0.50
1:B:324:LEU:HB2	1:B:342:ILE:HB	1.94	0.49
1:B:530:ILE:HD13	1:B:530:ILE:C	2.33	0.49
1:A:182:VAL:HG23	1:A:183:SER:N	2.27	0.49
1:B:241:GLU:O	1:B:242:LYS:HB2	2.12	0.49
1:A:194:VAL:HG13	3:A:1041:HOH:O	2.13	0.49
1:A:624:ASP:OD2	1:B:214:ARG:HD2	2.12	0.49
1:A:626:PRO:HG2	1:A:628:ASN:ND2	2.28	0.49
1:B:280:MET:HG3	1:B:298:ALA:HB3	1.95	0.49
1:B:297:PHE:HB2	1:B:301:GLU:HG3	1.94	0.49
1:B:379:ILE:O	1:B:382[B]:TTS:HD2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ILE:HD12	1:A:327:VAL:HG12	1.95	0.49
1:B:351:ILE:HD12	1:B:351:ILE:N	2.27	0.49
1:A:369:ARG:CZ	1:B:220:ILE:HD13	2.43	0.48
1:A:261:ALA:CB	1:A:268:LEU:HD22	2.42	0.48
1:A:379:ILE:O	1:A:382[B]:TTS:HD2	2.12	0.48
1:A:370:ARG:O	1:A:370:ARG:HG2	2.13	0.48
1:A:238:ILE:HG13	1:A:344:MET:CE	2.42	0.48
1:A:297:PHE:HB2	1:A:301:GLU:HG3	1.96	0.48
1:A:183:SER:OG	1:A:185:GLU:HG2	2.13	0.48
1:B:522:LEU:HD11	1:B:530:ILE:HD12	1.96	0.48
1:B:317:CYS:HB3	1:B:321:ILE:HG12	1.95	0.48
1:B:380:GLY:HA3	1:B:382[B]:TTS:C6'	2.44	0.48
1:A:550:GLU:HG2	1:A:570:TYR:CE1	2.49	0.48
1:A:373:ILE:HD12	1:A:373:ILE:N	2.28	0.47
1:B:483:ALA:HB1	1:B:543:VAL:HB	1.96	0.47
1:B:267:ARG:HG2	1:B:267:ARG:HH11	1.80	0.47
1:B:369:ARG:HG3	3:B:1414:HOH:O	2.15	0.47
1:A:367:ARG:HD3	1:B:315:CYS:O	2.15	0.47
1:B:245:LEU:CB	1:B:260:ILE:HD13	2.45	0.47
1:A:136:PRO:HD2	1:A:382[B]:TTS:C4'	2.46	0.46
1:A:163:PRO:HG2	3:A:1362:HOH:O	2.14	0.46
1:B:282:VAL:HB	1:B:296:TYR:CD2	2.51	0.46
1:A:369:ARG:NH2	1:B:220:ILE:HD13	2.31	0.46
1:A:484:VAL:HG12	1:A:539:LYS:HG3	1.97	0.46
1:A:105:PHE:HB3	1:A:136:PRO:HG2	1.97	0.46
3:A:1134:HOH:O	1:B:351:ILE:HD13	2.16	0.46
1:A:145:ALA:O	1:A:148:ARG:CD	2.64	0.45
1:A:241:GLU:O	1:A:242:LYS:HB2	2.16	0.45
1:A:271:ILE:HD12	1:A:271:ILE:N	2.31	0.45
1:B:13:ARG:NH2	1:B:58:ARG:HG3	2.32	0.44
1:B:220:ILE:HD12	1:B:220:ILE:N	2.32	0.44
1:B:490:ARG:HG3	1:B:490:ARG:HH11	1.82	0.44
1:B:220:ILE:CG2	1:B:222:ILE:HD11	2.45	0.44
1:A:152:ILE:CG2	1:A:153:LEU:N	2.80	0.44
1:A:71:ARG:HD3	1:A:89:GLU:HG2	1.98	0.44
1:A:282:VAL:HB	1:A:296:TYR:CD2	2.53	0.44
1:B:188:ARG:HD3	3:B:1306:HOH:O	2.18	0.44
1:B:328:ILE:HD13	1:B:328:ILE:N	2.33	0.44
1:A:33:LEU:HD11	1:A:39:ILE:CD1	2.46	0.43
1:A:319:GLY:C	1:A:321:ILE:HD12	2.38	0.43
1:A:603:PRO:HG2	3:A:1174:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:VAL:HB	1:B:296:TYR:CE2	2.54	0.43
1:A:513:LYS:O	1:A:611:LEU:HA	2.18	0.43
1:B:56:GLU:OE2	1:B:58:ARG:HG2	2.18	0.43
1:B:190:ILE:HD12	1:B:190:ILE:N	2.34	0.43
1:A:42:LEU:C	1:A:42:LEU:HD23	2.39	0.43
1:B:296:TYR:OH	1:B:384:TYR:HE2	2.02	0.43
1:B:22:GLU:O	1:B:26:ILE:HG12	2.19	0.42
1:B:298:ALA:HB1	1:B:379:ILE:CD1	2.49	0.42
1:A:296:TYR:CE1	1:A:298:ALA:HB2	2.54	0.42
1:B:418:ASN:C	1:B:419:ILE:HD12	2.39	0.42
1:A:260:ILE:HD12	1:A:260:ILE:H	1.83	0.42
1:B:219:PRO:C	1:B:220:ILE:HD12	2.40	0.42
1:A:137:LEU:HD11	1:A:156:LEU:HD12	2.02	0.42
1:A:116:GLU:O	1:A:120:LYS:HG3	2.20	0.42
1:B:20:ILE:HD12	1:B:327:VAL:HG12	2.02	0.42
1:B:479:ARG:O	1:B:482:GLU:HG2	2.19	0.42
1:A:277:ILE:HD11	1:A:398:PHE:CE1	2.55	0.42
1:B:290:ILE:HD12	1:B:290:ILE:H	1.85	0.41
1:B:434:ILE:HD13	1:B:589:GLY:HA3	2.02	0.41
1:B:582:ILE:C	1:B:582:ILE:HD12	2.40	0.41
1:B:282:VAL:HA	1:B:432:GLN:O	2.20	0.41
1:B:290:ILE:N	1:B:290:ILE:CD1	2.82	0.41
1:B:468:ASN:HD22	1:B:468:ASN:H	1.68	0.41
1:A:154:ARG:HD2	1:A:293:TRP:CE3	2.55	0.41
1:A:270:PRO:C	1:A:271:ILE:HD12	2.40	0.41
1:A:72:PRO:HB2	1:A:98:LEU:HD11	2.02	0.41
1:A:260:ILE:N	1:A:260:ILE:CD1	2.83	0.41
1:B:342:ILE:N	1:B:342:ILE:CD1	2.83	0.41
1:A:460:MET:HE2	1:A:466:ARG:C	2.41	0.41
1:B:280:MET:HG3	1:B:280:MET:O	2.21	0.41
1:B:451:GLU:HG2	1:B:476:VAL:HG22	2.02	0.41
1:A:447:THR:HG21	1:A:501:GLU:OE2	2.20	0.41
1:A:486:GLU:OE1	1:A:539:LYS:NZ	2.51	0.41
1:B:101:LEU:HB2	1:B:104:GLU:HG3	2.01	0.41
1:A:280:MET:HG3	1:A:435:PHE:CD2	2.56	0.41
1:B:282:VAL:HG21	1:B:296:TYR:CE2	2.55	0.41
1:A:146:GLU:OE1	1:A:188:ARG:NH1	2.54	0.41
1:A:257:LEU:HB3	1:A:260:ILE:HD11	2.03	0.41
1:A:319:GLY:O	1:A:321:ILE:HD12	2.21	0.40
1:B:42:LEU:C	1:B:42:LEU:HD23	2.40	0.40
1:A:269:ARG:O	1:A:271:ILE:HD12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:ILE:HD12	1:B:321:ILE:N	2.37	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	617/638 (97%)	594 (96%)	22 (4%)	1 (0%)	47 29
1	B	617/638 (97%)	590 (96%)	26 (4%)	1 (0%)	47 29
All	All	1234/1276 (97%)	1184 (96%)	48 (4%)	2 (0%)	47 29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	ALA
1	B	52	GLY

### 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	512/528 (97%)	507 (99%)	5 (1%)	76 63
1	B	512/528 (97%)	508 (99%)	4 (1%)	81 72
All	All	1024/1056 (97%)	1015 (99%)	9 (1%)	78 67

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	ARG
1	A	268	LEU
1	A	328	ILE
1	A	370	ARG
1	A	376	PHE
1	B	328	ILE
1	B	376	PHE
1	B	530	ILE
1	B	628	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	HIS
1	A	309	ASN
1	A	345	HIS
1	A	432	GLN
1	A	448	ASN
1	A	507	ASN
1	A	515	HIS
1	A	519	GLN
1	A	628	ASN
1	B	224	GLN
1	B	306	GLN
1	B	421	GLN
1	B	468	ASN
1	B	507	ASN
1	B	519	GLN
1	B	628	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 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	TTS	A	382[A]	1	21,24,25	2.44	10 (47%)	23,32,34	1.86	5 (21%)
1	TTS	A	382[B]	1	21,24,25	2.49	10 (47%)	23,32,34	1.94	5 (21%)
1	TTS	B	382[A]	1	21,24,25	2.44	10 (47%)	23,32,34	1.86	5 (21%)
1	TTS	B	382[B]	1	21,24,25	2.51	10 (47%)	23,32,34	1.94	5 (21%)

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	TTS	A	382[A]	1	-	3/11/28/30	0/2/2/2
1	TTS	A	382[B]	1	-	2/11/28/30	0/2/2/2
1	TTS	B	382[A]	1	-	3/11/28/30	0/2/2/2
1	TTS	B	382[B]	1	-	2/11/28/30	0/2/2/2

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	382[B]	TTS	CE1-CZ	6.06	1.44	1.35
1	A	382[B]	TTS	CE1-CZ	6.04	1.44	1.35
1	A	382[A]	TTS	CE1-CZ	5.98	1.44	1.35
1	B	382[A]	TTS	CE1-CZ	5.95	1.44	1.35
1	B	382[B]	TTS	C5'-C4'	4.29	1.47	1.38
1	A	382[B]	TTS	C5'-C4'	4.24	1.47	1.38
1	A	382[A]	TTS	C5'-C4'	3.99	1.46	1.38
1	B	382[A]	TTS	C5'-C4'	3.97	1.46	1.38
1	B	382[A]	TTS	OD1-CD1	3.86	1.34	1.24
1	A	382[A]	TTS	OD1-CD1	3.84	1.34	1.24
1	B	382[B]	TTS	OD1-CD1	3.78	1.34	1.24
1	A	382[B]	TTS	OD1-CD1	3.76	1.34	1.24
1	B	382[B]	TTS	CD2-CG	3.73	1.44	1.34
1	A	382[B]	TTS	CD2-CG	3.73	1.44	1.34
1	B	382[A]	TTS	CD2-CG	3.70	1.44	1.34
1	A	382[A]	TTS	CD2-CG	3.68	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	382[B]	TTS	C5'-C6'	3.02	1.44	1.38
1	A	382[B]	TTS	C5'-C6'	2.99	1.44	1.38
1	B	382[B]	TTS	C2'-C3'	2.95	1.44	1.38
1	A	382[A]	TTS	C2'-C3'	2.92	1.44	1.38
1	B	382[A]	TTS	C2'-C3'	2.92	1.44	1.38
1	A	382[B]	TTS	C2'-C3'	2.87	1.44	1.38
1	B	382[B]	TTS	CG-CD1	-2.85	1.44	1.49
1	A	382[B]	TTS	CG-CD1	-2.85	1.44	1.49
1	B	382[A]	TTS	C5'-C6'	2.72	1.43	1.38
1	A	382[A]	TTS	C5'-C6'	2.72	1.43	1.38
1	B	382[A]	TTS	CG-CD1	-2.70	1.45	1.49
1	A	382[A]	TTS	CG-CD1	-2.69	1.45	1.49
1	A	382[B]	TTS	C2'-C1'	2.62	1.44	1.38
1	B	382[B]	TTS	C2'-C1'	2.62	1.44	1.38
1	A	382[A]	TTS	C2'-C1'	2.47	1.44	1.38
1	B	382[A]	TTS	C2'-C1'	2.46	1.44	1.38
1	B	382[A]	TTS	C6'-C1'	2.33	1.43	1.38
1	A	382[A]	TTS	C6'-C1'	2.32	1.43	1.38
1	B	382[B]	TTS	C6'-C1'	2.30	1.43	1.38
1	A	382[B]	TTS	C6'-C1'	2.28	1.43	1.38
1	B	382[A]	TTS	C3'-C4'	2.14	1.43	1.38
1	A	382[A]	TTS	C3'-C4'	2.13	1.43	1.38
1	B	382[B]	TTS	C3'-C4'	2.09	1.42	1.38
1	A	382[B]	TTS	C3'-C4'	2.07	1.42	1.38

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	382[A]	TTS	CD2-CG-CD1	5.04	122.51	118.64
1	B	382[A]	TTS	CD2-CG-CD1	5.04	122.51	118.64
1	A	382[B]	TTS	CD2-CG-CD1	4.96	122.45	118.64
1	B	382[B]	TTS	CD2-CG-CD1	4.93	122.42	118.64
1	A	382[B]	TTS	CB-CA-C	-4.24	103.53	111.47
1	B	382[B]	TTS	CB-CA-C	-4.23	103.54	111.47
1	A	382[B]	TTS	CA-CB-CG	4.16	121.47	113.51
1	B	382[B]	TTS	CA-CB-CG	4.13	121.39	113.51
1	A	382[A]	TTS	CB-CA-C	-3.84	104.26	111.47
1	B	382[A]	TTS	CB-CA-C	-3.84	104.27	111.47
1	A	382[A]	TTS	CA-CB-CG	3.59	120.36	113.51
1	B	382[A]	TTS	CA-CB-CG	3.57	120.33	113.51
1	B	382[B]	TTS	CD2-CE2-CZ	2.97	121.04	117.91
1	A	382[B]	TTS	CD2-CE2-CZ	2.94	121.01	117.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	382[A]	TTS	CD2-CE2-CZ	2.87	120.94	117.91
1	B	382[A]	TTS	CD2-CE2-CZ	2.87	120.94	117.91
1	A	382[A]	TTS	C1-NE2-CE2	2.82	127.64	121.36
1	B	382[A]	TTS	C1-NE2-CE2	2.82	127.64	121.36
1	A	382[B]	TTS	C1-NE2-CE2	2.74	127.47	121.36
1	B	382[B]	TTS	C1-NE2-CE2	2.73	127.44	121.36

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	382[A]	TTS	O-C-CA-CB
1	A	382[A]	TTS	NE2-C1-C2-C1'
1	A	382[B]	TTS	O-C-CA-CB
1	B	382[A]	TTS	O-C-CA-CB
1	B	382[A]	TTS	NE2-C1-C2-C1'
1	B	382[B]	TTS	O-C-CA-CB
1	A	382[A]	TTS	N-CA-CB-CG
1	B	382[A]	TTS	N-CA-CB-CG
1	A	382[B]	TTS	N-CA-CB-CG
1	B	382[B]	TTS	N-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	382[A]	TTS	1	0
1	A	382[B]	TTS	2	0
1	B	382[A]	TTS	4	0
1	B	382[B]	TTS	2	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	382[A]:TTS	C	383:ASP	N	1.17
1	B	382[B]:TTS	C	383:ASP	N	1.14



## 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	619/638 (97%)	0.12	30 (4%) 30 35	20, 29, 45, 80	0
1	B	619/638 (97%)	0.04	30 (4%) 30 35	18, 26, 40, 79	0
All	All	1238/1276 (97%)	0.08	60 (4%) 30 35	18, 28, 43, 80	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	51	ALA	12.5
1	A	52	GLY	11.7
1	B	52	GLY	11.7
1	A	51	ALA	11.3
1	B	53	SER	11.2
1	B	55	ALA	10.1
1	B	54	GLU	9.8
1	B	50	GLY	8.0
1	A	54	GLU	7.8
1	A	55	ALA	7.5
1	A	56	GLU	7.2
1	A	628	ASN	6.7
1	A	53	SER	6.4
1	A	9	ALA	5.9
1	A	50	GLY	5.8
1	A	266	ASP	5.4
1	B	56	GLU	5.0
1	B	266	ASP	4.4
1	B	628	ASN	4.2
1	B	296	TYR	4.1
1	B	414	GLY	3.8
1	A	148	ARG	3.7
1	A	265	GLY	3.7
1	B	48	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	414	GLY	3.7
1	A	507	ASN	3.6
1	A	296	TYR	3.4
1	B	265	GLY	3.4
1	B	225	PRO	3.4
1	A	68	SER	3.3
1	B	194	VAL	3.3
1	A	48	ALA	3.3
1	A	225	PRO	3.2
1	A	462	PRO	3.2
1	B	462	PRO	3.1
1	A	313	LEU	2.9
1	B	413	GLU	2.8
1	A	145	ALA	2.8
1	A	332	PHE	2.7
1	A	339	ARG	2.6
1	B	9	ALA	2.6
1	B	461	GLY	2.5
1	B	215	THR	2.5
1	B	463	GLY	2.5
1	A	267	ARG	2.4
1	B	267	ARG	2.4
1	A	459	THR	2.4
1	B	208	GLU	2.4
1	A	143	GLU	2.3
1	A	263	ARG	2.3
1	B	116	GLU	2.3
1	B	459	THR	2.2
1	A	70	ALA	2.2
1	B	507	ASN	2.2
1	B	163	PRO	2.2
1	B	415	GLY	2.1
1	B	156	LEU	2.1
1	A	413	GLU	2.1
1	B	212	PRO	2.1
1	A	208	GLU	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. 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	TTS	B	382[A]	23/24	0.82	0.22	27,44,56,56	23
1	TTS	B	382[B]	23/24	0.82	0.22	26,43,55,56	23
1	TTS	A	382[A]	23/24	0.91	0.16	25,44,57,58	23
1	TTS	A	382[B]	23/24	0.91	0.16	25,44,56,56	23

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 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
2	CU	A	1001	1/1	1.00	0.05	27,27,27,27	0
2	CU	B	1002	1/1	1.00	0.05	27,27,27,27	0

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

There are no such residues in this entry.