



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 05:41 AM GMT

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 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/ValidationPDFNotes.html>

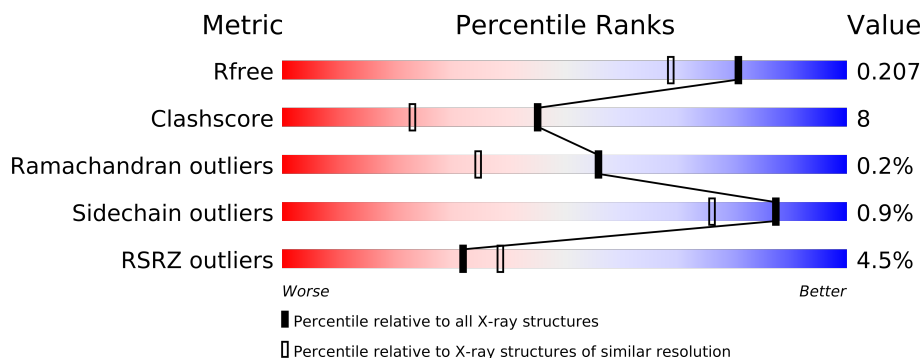
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance



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}	66092	1657 (1.76-1.72)
Clashscore	79885	1881 (1.76-1.72)
Ramachandran outliers	78287	1859 (1.76-1.72)
Sidechain outliers	78261	1859 (1.76-1.72)
RSRZ outliers	66119	1658 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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 hydrogen and 0 are deuterium.

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
1	A	620	Total	C	N	O	S	0	1	0
			4897	3098	858	932	9			
1	B	620	Total	C	N	O	S	0	1	0
			4897	3098	858	932	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	298	ALA	ASP	ENGINEERED	UNP P46881
A	382	TTS	TYR	MODIFIED RESIDUE	UNP P46881
B	298	ALA	ASP	ENGINEERED	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	B	1	Total	Cu	0	0
			1	1		
2	A	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		

4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 1.74Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.190 , 0.217 0.183 , 0.207	Depositor DCC
R_{free} test set	8601 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	22.7	Xtriage
Anisotropy	0.704	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 57.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	3 of 171652 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10930	wwPDB-VP
Average B, all atoms (Å ²)	31.0	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 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.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10930	0	9420	161	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (161) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:505:ARG:HD3	1:A:618:ASP:HB3	1.76	0.68
1:A:238:ILE:HG13	1:A:344:MET:HE1	1.75	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
1:A:261:ALA:HB1	1:A:268:LEU:HD22	1.85	0.58
1:A:260:ILE:N	1:A:260:ILE:HD12	2.17	0.58
1:A:599:TRP:CD2	1:A:600:PRO:HA	2.38	0.58
1:B:328:ILE:H	1:B:328:ILE:HD13	1.69	0.57
1:A:443:ILE:H	1:A:448:ASN:HD21	1.53	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:B:342:ILE:HD12	1:B:342:ILE:N	2.20	0.57
1:A:483:ALA:HB1	1:A:543:VAL:HB	1.86	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:B:222:ILE:N	1:B:222:ILE:HD12	2.22	0.54
1:A:144:TYR:CD2	1:A:188:ARG:NH1	2.76	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:HD12	1:A:321:ILE:N	2.25	0.51
1:A:220:ILE:HG22	1:A:222:ILE:HD11	1.92	0.51
1:B:379:ILE:O	1:B:382[A]:TTS:HD2	2.10	0.51
1:B:245:LEU:HB2	1:B:260:ILE:HD13	1.92	0.51
1:A:271:ILE:HG22	1:A:272:ILE:HG13	1.93	0.51
1:A:145:ALA:O	1:A:148:ARG:HD3	2.11	0.51
1:B:326:PRO:CD	1:B:342:ILE:HD13	2.40	0.51
1:A:246:ASP:HB2	1:A:258:HIS:HB2	1.93	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:C	1:B:530:ILE:HD13	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:379:ILE:O	1:B:382[B]:TTS:HD2	2.13	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:297:PHE:HB2	1:B:301:GLU:HG3	1.94	0.49
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:380:GLY:HA3	1:B:382[B]:TTS:C6'	2.44	0.48
1:B:317:CYS:HB3	1:B:321:ILE:HG12	1.95	0.48
1:A:550:GLU:HG2	1:A:570:TYR:CE1	2.49	0.48
1:A:373:ILE:N	1:A:373:ILE:HD12	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:B:245:LEU:CB	1:B:260:ILE:HD13	2.45	0.47
1:A:367:ARG:HD3	1:B:315:CYS:O	2.15	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:N	1:A:271:ILE:HD12	2.31	0.45
1:B:13:ARG:NH2	1:B:58:ARG:HG3	2.32	0.44
1:B:220:ILE:N	1:B:220:ILE:HD12	2.32	0.44
1:B:490:ARG:HH11	1:B:490:ARG:HG3	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:B:328:ILE:N	1:B:328:ILE:HD13	2.33	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:A:33:LEU:HD11	1:A:39:ILE:CD1	2.46	0.43
1:A:603:PRO:HG2	3:A:1174:HOH:O	2.17	0.43
1:A:319:GLY:C	1:A:321:ILE:HD12	2.38	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(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:HD23	1:A:42:LEU:C	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:B:219:PRO:C	1:B:220:ILE:HD12	2.40	0.42
1:A:260:ILE:H	1:A:260:ILE:HD12	1.83	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:HD12	1:B:582:ILE:C	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:260:ILE:N	1:A:260:ILE:CD1	2.83	0.41
1:A:72:PRO:HB2	1:A:98:LEU:HD11	2.02	0.41
1:B:342:ILE:CD1	1:B:342:ILE:N	2.83	0.41
1:B:280:MET:HG3	1:B:280:MET:O	2.21	0.41
1:A:460:MET:HE2	1:A:466:ARG:C	2.41	0.41
1:B:451:GLU:HG2	1:B:476:VAL:HG22	2.02	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:447:THR:HG21	1:A:501:GLU:OE2	2.20	0.41
1:B:282:VAL:HG21	1:B:296:TYR:CE2	2.55	0.41
1:A:280:MET:HG3	1:A:435:PHE:CD2	2.56	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:HD23	1:B:42:LEU:C	2.40	0.40
1:A:269:ARG:O	1:A:271:ILE:HD12	2.21	0.40
1:B:321:ILE:N	1:B:321:ILE:HD12	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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%)	56	35
1	B	617/638 (97%)	590 (96%)	26 (4%)	1 (0%)	56	35
All	All	1234/1276 (97%)	1184 (96%)	48 (4%)	2 (0%)	56	35

All (2) Ramachandran outliers are listed below:

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

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	512/528 (97%)	507 (99%)	5 (1%)	85	73
1	B	512/528 (97%)	508 (99%)	4 (1%)	89	80
All	All	1024/1056 (97%)	1015 (99%)	9 (1%)	87	76

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

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Mol	Chain	Res	Type
1	A	376	PHE
1	B	328	ILE
1	B	376	PHE
1	B	530	ILE
1	B	628	ASN

Some 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 ⓘ

There are no RNA chains in this entry.

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

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	24,24,25	4.54	12 (50%)	30,32,34	1.91	7 (23%)
1	TTS	A	382[B]	1	24,24,25	4.57	12 (50%)	30,32,34	1.97	7 (23%)
1	TTS	B	382[A]	1	24,24,25	4.54	12 (50%)	30,32,34	1.91	7 (23%)
1	TTS	B	382[B]	1	24,24,25	4.59	12 (50%)	30,32,34	1.97	7 (23%)

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	-	0/9/28/30	0/2/2/2
1	TTS	A	382[B]	1	-	0/9/28/30	0/2/2/2
1	TTS	B	382[A]	1	-	0/9/28/30	0/2/2/2
1	TTS	B	382[B]	1	-	0/9/28/30	0/2/2/2

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	382[B]	TTS	O-C	17.83	1.23	1.11
1	A	382[B]	TTS	O-C	17.76	1.23	1.11
1	B	382[A]	TTS	O-C	17.74	1.23	1.11
1	A	382[A]	TTS	O-C	17.73	1.23	1.11
1	B	382[A]	TTS	CE2-NE2	8.19	1.46	1.30
1	A	382[A]	TTS	CE2-NE2	8.19	1.46	1.30
1	B	382[B]	TTS	CE2-NE2	8.16	1.45	1.30
1	A	382[B]	TTS	CE2-NE2	8.14	1.45	1.30
1	B	382[B]	TTS	CE1-CZ	5.65	1.44	1.35
1	A	382[B]	TTS	CE1-CZ	5.63	1.44	1.35
1	A	382[A]	TTS	CE1-CZ	5.57	1.44	1.35
1	B	382[A]	TTS	CE1-CZ	5.55	1.44	1.35
1	B	382[B]	TTS	C5'-C4'	3.90	1.47	1.38
1	A	382[B]	TTS	C5'-C4'	3.85	1.47	1.38
1	A	382[A]	TTS	C5'-C4'	3.63	1.46	1.38
1	B	382[A]	TTS	C5'-C4'	3.61	1.46	1.38
1	B	382[A]	TTS	OD1-CD1	3.53	1.34	1.24
1	A	382[A]	TTS	OD1-CD1	3.52	1.34	1.24
1	B	382[B]	TTS	OD1-CD1	3.46	1.34	1.24
1	A	382[B]	TTS	OD1-CD1	3.44	1.34	1.24
1	B	382[B]	TTS	CD2-CG	3.42	1.44	1.34
1	A	382[B]	TTS	CD2-CG	3.41	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	382[A]	TTS	CD2-CG	3.38	1.44	1.34
1	A	382[A]	TTS	CD2-CG	3.37	1.44	1.34
1	B	382[B]	TTS	C5'-C6'	2.86	1.44	1.38
1	A	382[B]	TTS	C5'-C6'	2.83	1.44	1.38
1	B	382[B]	TTS	C2'-C3'	2.80	1.44	1.38
1	B	382[A]	TTS	C2'-C3'	2.77	1.44	1.38
1	A	382[A]	TTS	C2'-C3'	2.77	1.44	1.38
1	A	382[B]	TTS	C2'-C3'	2.72	1.44	1.38
1	B	382[B]	TTS	CG-CD1	-2.72	1.44	1.48
1	A	382[B]	TTS	CG-CD1	-2.71	1.44	1.48
1	B	382[A]	TTS	C5'-C6'	2.58	1.43	1.38
1	B	382[A]	TTS	CG-CD1	-2.57	1.45	1.48
1	A	382[A]	TTS	C5'-C6'	2.57	1.43	1.38
1	A	382[A]	TTS	CG-CD1	-2.56	1.45	1.48
1	A	382[B]	TTS	C2'-C1'	2.48	1.44	1.38
1	B	382[B]	TTS	C2'-C1'	2.47	1.44	1.38
1	A	382[A]	TTS	C2'-C1'	2.33	1.44	1.38
1	B	382[A]	TTS	C2'-C1'	2.32	1.44	1.38
1	B	382[B]	TTS	CA-C	2.23	1.52	1.48
1	B	382[A]	TTS	C6'-C1'	2.20	1.43	1.38
1	A	382[A]	TTS	C6'-C1'	2.20	1.43	1.38
1	A	382[B]	TTS	CA-C	2.18	1.52	1.48
1	B	382[B]	TTS	C6'-C1'	2.18	1.43	1.38
1	A	382[B]	TTS	C6'-C1'	2.15	1.43	1.38
1	B	382[A]	TTS	CA-C	2.08	1.52	1.48
1	A	382[A]	TTS	CA-C	2.07	1.52	1.48

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	382[B]	TTS	CD2-CE2-NE2	-6.45	121.67	128.16
1	A	382[B]	TTS	CD2-CE2-NE2	-6.45	121.67	128.16
1	B	382[A]	TTS	CD2-CE2-NE2	-6.23	121.89	128.16
1	A	382[A]	TTS	CD2-CE2-NE2	-6.23	121.89	128.16
1	B	382[A]	TTS	CD2-CG-CD1	3.83	122.51	118.24
1	A	382[A]	TTS	CD2-CG-CD1	3.83	122.51	118.24
1	A	382[B]	TTS	CD2-CG-CD1	3.78	122.45	118.24
1	B	382[B]	TTS	CD2-CG-CD1	3.76	122.42	118.24
1	A	382[B]	TTS	CA-CB-CG	3.48	121.47	114.41
1	B	382[B]	TTS	CB-CG-CD2	-3.45	116.16	122.61
1	B	382[A]	TTS	CB-CG-CD2	-3.45	116.17	122.61
1	B	382[B]	TTS	CA-CB-CG	3.44	121.39	114.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	382[A]	TTS	CB-CG-CD2	-3.44	116.17	122.61
1	A	382[B]	TTS	CB-CG-CD2	-3.43	116.20	122.61
1	B	382[A]	TTS	C1-NE2-CE2	3.20	127.64	120.64
1	A	382[A]	TTS	C1-NE2-CE2	3.21	127.64	120.64
1	A	382[B]	TTS	C1-NE2-CE2	3.12	127.47	120.64
1	B	382[B]	TTS	C1-NE2-CE2	3.11	127.44	120.64
1	B	382[B]	TTS	CD2-CE2-CZ	3.02	121.04	118.00
1	A	382[B]	TTS	CD2-CE2-CZ	2.98	121.01	118.00
1	A	382[A]	TTS	CA-CB-CG	2.94	120.36	114.41
1	B	382[A]	TTS	CA-CB-CG	2.92	120.33	114.41
1	B	382[A]	TTS	CD2-CE2-CZ	2.92	120.94	118.00
1	A	382[A]	TTS	CD2-CE2-CZ	2.92	120.94	118.00
1	B	382[B]	TTS	CE2-CD2-CG	-2.09	117.01	121.18
1	A	382[B]	TTS	CE2-CD2-CG	-2.07	117.04	121.18
1	B	382[A]	TTS	CE2-CD2-CG	-2.06	117.06	121.18
1	A	382[A]	TTS	CE2-CD2-CG	-2.06	117.06	121.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	620/638 (97%)	0.15	27 (4%)	33 39	20, 29, 45, 80	0
1	B	620/638 (97%)	0.07	29 (4%)	30 36	18, 26, 41, 79	0
All	All	1240/1276 (97%)	0.11	56 (4%)	32 38	18, 28, 43, 80	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	51	ALA	12.2
1	B	52	GLY	12.2
1	A	52	GLY	11.3
1	B	53	SER	10.1
1	A	51	ALA	9.7
1	B	54	GLU	9.3
1	B	55	ALA	8.6
1	B	50	GLY	7.7
1	A	54	GLU	7.2
1	A	53	SER	6.9
1	A	56	GLU	6.6
1	A	55	ALA	6.4
1	A	9	ALA	5.9
1	A	628	ASN	5.8
1	A	266	ASP	5.7
1	A	50	GLY	4.9
1	B	56	GLU	4.5
1	B	628	ASN	4.3
1	B	266	ASP	4.3
1	A	148	ARG	4.0
1	B	48	ALA	3.9
1	B	296	TYR	3.8
1	A	507	ASN	3.7
1	A	225	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	68	SER	3.5
1	B	225	PRO	3.4
1	A	265	GLY	3.2
1	B	194	VAL	3.2
1	A	296	TYR	3.2
1	A	462	PRO	3.1
1	B	414	GLY	3.1
1	A	48	ALA	3.0
1	A	339	ARG	3.0
1	B	413	GLU	2.9
1	B	462	PRO	2.9
1	B	265	GLY	2.9
1	B	215	THR	2.8
1	A	332	PHE	2.8
1	A	414	GLY	2.7
1	A	145	ALA	2.6
1	A	267	ARG	2.6
1	B	463	GLY	2.5
1	B	267	ARG	2.5
1	B	461	GLY	2.5
1	A	313	LEU	2.4
1	A	459	THR	2.4
1	B	9	ALA	2.4
1	B	507	ASN	2.3
1	B	459	THR	2.3
1	B	156	LEU	2.2
1	A	263	ARG	2.2
1	B	116	GLU	2.2
1	B	465	GLU	2.1
1	B	145	ALA	2.1
1	B	208	GLU	2.1
1	A	315	CYS	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	TTS	B	382[B]	23/24	0.22	2.96	26,43,55,56	23
1	TTS	B	382[A]	23/24	0.22	2.89	27,44,56,56	23
1	TTS	A	382[A]	23/24	0.17	1.85	25,44,57,58	23
1	TTS	A	382[B]	23/24	0.17	1.75	25,44,56,56	23

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CU	B	1002	1/1	0.05	-4.19	27,27,27,27	0
2	CU	A	1001	1/1	0.04	-5.13	27,27,27,27	0

6.5 Other polymers

There are no such residues in this entry.